Verification of RADTRAN*

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Introduction

The RADTRAN computer code calculates risk estimates for radioactive materials transportation by highway, rail, air, and waterborne modes. RADTRAN was first developed by Sandia National Laboratories (SNL) in 1977 in conjunction with NUREG-0170, "Final Environmental Statement on the Transportation of Radioactive Material by Air and Other Modes" (NRC 1977; Taylor and Daniel 1982). Subsequent releases of RADTRAN to date are RADTRAN II (Taylor and Daniel 1982), RADTRAN III (Madsen et al. 1986), and RADTRAN 4 (Neuhauser and Kanipe 1992). RADTRAN 5 is currently in development. This paper discusses verification of the RADTRAN computer code. Verification is the process of determining that a code correctly performs the calculations embodied in it by the code developers; this is distinct from the separate process of validation in which the correctness of the algorithms and equations is determined. With all releases, the NUREG-0170 data file is used for verification of the code output. The capabilities of RADTRAN have been enhanced over the years, and the NUREG-0170 input format has been altered to accommodate these changes. In order to test other new capabilities, additional test files have been added to the verification regimen. The test files for RADTRAN 5 are not the same files as those used with RADTRAN 4; however, they were originally created from the latter and have evolved as RADTRAN 5 has evolved.

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Types of Code Modifications

Four types of changes that may be made to RADTRAN affect the output files. One is modification of input formats, which will affect the input echo. The second is changes in algorithms within RADTRAN as new models are introduced. The third type of change involves adding intermediate results to the output. The fourth type of change is error correction.

Should an error be found in RADTRAN, corrections are made immediately. These changes result in changes to RADTRAN output files to one degree or another. Actual risk values will change only for two types of changes: model changes and error correction. An example of each is described later in this paper.

Verification Process - Documentation

Each time a change or series of changes is made, a verification process is performed. The verification process requires making changes and documenting them on change sheets. Test input files are run and the outputs from these tests are compared to archived output values produced with the previous release of RADTRAN. Differences, if any, in the test files are noted and are filed in the programmer's log along with the change sheets and any other pertinent information, such as plots or spreadsheets identifying reasons for differences in outputs. Often, derivations of equations are included in the log. The change sheets are incorporated into an askSam™ data base (askSam Systems) and are also kept in ASCII format.

The askSam™ data base is a useful tool for retrieving information on RADTRAN changes. Searches in askSam™ are not limited to certain search keys, so that any word can be used as a search key. For example, the programmer need only query for a subroutine name to have all changes that affected the subroutine pulled up for viewing. The programmer may refer to the log for more information if necessary.

For RADTRAN 4 intermediate releases, descriptions of the changes and expected outcomes are also described in the revision history available on-line to RADTRAN users via the TRANSNET computer system. TRANSNET currently hosts RADTRAN 4 as well as other transportation risk-assessment tools.

Verification Process - Hand Calculations

Hand calculations are performed for all major releases of RADTRAN. Figure 1 shows a sequence for a hand calculation check of the storage dose in RADTRAN 4.

Figure 1 Hand Calculation of Storage Dose

Storage Dose equation from RADTRAN 4 Technical Manual:

$$Dose = Q_2 \cdot k_0 \cdot DR_p \cdot PPS \cdot SPY \cdot T_{stor} \cdot P_{stor} / r_{stor}^2$$

A RADTRAN input file:

```
TITLE  TEST
PARM  1 1 2 4 0
NORMAL NMODE=1 1 0 0 8.6E+01 4.03E+01 2.41E+01
                    0 0 0 0 0 0 0
                    1 1 8.0 100.0 100.0 0
                    0 0 0 0 0 0
EOF
ISOTOPES 1 2 3 4.0 0.5 0.5 TEST
DISTKM NMODE=1 1000
PKGSIZ TEST 5.0
EOF
EOI
```

Using the equation with constant Q_2 *= 1.0E-03 rem/mrem and values:*

DR_p = 4.0 mrem/hr/package
PPS = 3.0 packages/shipment
SPY = 2.0 shipments
T_{stor} = 8.0 hr
P_{stor} = 100.0 persons
r_{stor} = 100.0 m

and intermediate value produced by RADTRAN 4 Technical Manual equations and input value d_p *= 5.0 m:*

$d_e = 2(1+d_p/2)^{3/4} - .55 = 4.57$ m
$k_0 = (1 + d_e/2)^2 = 10.79$ m^2

Hand calculation value for the storage dose in person-rem:

$$Dose = 1E\text{-}3(10.79)(4.0)(3.0)(2.0)(8.0)(100.0)/100.0^2 = 2.07E\text{-}02$$

Storage dose in RADTRAN 4 output file produced by the above file:

Storage Dose = 2.07E-02 person-rem

Verification for Model Changes - Sample Case

In RADTRAN 5 there has been a model change to the handler dose calculations. For the handler dose in RADTRAN 4, the use of a point-source equation or a line-source equation is determined by the sizes of the packages; a threshold value distinguishes between medium and large package sizes. Previously, with a very large package, the handlers were modeled as being exposed to a line-source and for the medium-sized packages the handlers were modeled as being exposed to a point-source. Because of the source-to-receptor distances involved in handling these sizes of packages, the new model (RADTRAN 5) determines point-source and line-source equation usage by the distance of the handler from the package and by the size of the package. If the handler is at a distance of less than two times the package size, then the line-source equation is used. If the handler is farther away, then the point-source equation is used. The equation for small packages (generally less than .5 meters) has remained the same. The results should differ for medium and large packages depending on the previous threshold values and the package sizes.

Table 1 shows results from the handler-dose model change. Three samples were taken from the NUREG-0170 test file. The sample of material AM241-A shows no change between the previous value and the new value. The package was considered small (less than .5 meters). The other two, however, produced changes in the values that are in accord with the changes predicted during model development. The previous values for materials AM241-B and CO60-LSA were produced with the code's point-source equation, and the new values were produced using the code's line-source equation. The original values were altered to produce results as if a line-source equation were used. These altered results are shown in Table 1. The result is that differences greater than 10 percent can be accounted for by the model changes. With the model change taken into consideration, the difference is not greater than 10 percent.

Table 1 Handler-Dose Model Change (values in Person-rem)

NUREG-0170 Test File	AM241-A	AM241-B	CO60-LSA
Previous values	7.90E+01	8.18E-01	1.49E+02
New values	7.90E+01	6.27E-01	1.15E+02
Difference greater than 10%	none	-1.90E-01	-3.40E+01
New values that use line-source	N/A	6.27E-01	1.15E+02
Previous values modified to line-source	N/A	6.27E-01	1.14E+02
Difference greater than 10%	N/A	none	none

Error Correction - Sample Case

Discussed below is the treatment of a calculational error that was discovered in August 1990 by a member of the International Atomic Energy Agency Coordinated Research Program on the Development of Probabilistic Safety Assessment Techniques Relating to the Safe Transport of Radioactive Material (Florentin Lange 1990). The problem concerned the plotting of the characteristic package dimension (CPD) versus the package coefficient (K_0). K_0, in square meters, is calculated within RADTRAN to allow the dose-rate value to be extrapolated back to the center of the package to achieve a true point-source configuration. The CPD is used for determining dose to persons potentially exposed during the incident-free transportation of nuclear materials. At a distance of 4 meters, the slope of the K_0 vs CPD plot becomes too steep and the package dimension is converted to an effective package dimension that produces a more level curve. The plot of K_0 versus CPD, though level, produced a discontinuity at 4 meters.

The first step in this revision was to produce pairs of package dimension and K_0 values and plot them. The plot showed the discontinuity at a package dimension of 4 meters. Second, the CPD equation was reexamined, and it was determined that the constant in the equation was incorrect. A series of plots was created, showing the effect of a range of constant values. The values for this constant were narrowed down until a value was found that produced no discernible discontinuity. Upon examination of the corrected value, the error is believed to have arisen when a measurement in feet was not properly converted to a measurement in meters.

With the problem now identified and understood, RADTRAN was updated to include the correct constant. As is done with all major releases, the RADTRAN 4 release number and date were also updated. A change sheet was prepared describing the problem and the correction that was made. Test files were run and comparisons were made (see Table 2). The NUREG-0170 test file contains only packages with CPDs less

Table 2 Output Comparisons (Values in Person-rem)

	Previous Values	New Values	Actual Difference	Expected Difference	Differences > 10%
TEST FILE 1 (AM241-A)					
Passengers	1.87E+01	1.87E+01	0	0	none
Crew	1.49E+02	1.49E+02	0	0	none
Handlers	7.90E+01	7.90E+01	0	0	none
Off-link	1.36E+01	1.36E+01	0	0	none
On-link	4.35E+01	4.35E+01	0	0	none
Stops	1.77E+02	1.77E+02	0	0	none
Storage	7.97E+00	7.97E+00	0	0	none
TEST FILE 2					
Passengers	0.00E+00	0.00E+00	0	0	none
Crew	9.21E+01	1.39E+02	4.69E+01	4.74E+01	none
Handlers	0.00E+00	0.00E+00	0	0	none
Off-link	1.49E+01	2.14E+01	6.50E+00	6.54E+00	none
On-link	6.53E+01	9.39E+01	2.86E+01	2.87E+01	none
Stops	4.51E+02	6.49E+02	1.98E+02	1.98E+02	none
Storage	0.00E+00	0.00E+00	0	0	none

than 4 meters; therefore there were no differences except in the release number and date. The other seven test files, which include data for large packages, did produce differences in the incident-free risks consistent with predictions. Each difference was examined and determined to be appropriate by both the scientific programmer and the RADTRAN principal engineer. The change sheet was filed along with the plots and test file differences.

In addition, development had been started on RADTRAN 5, so the correction was incorporated into RADTRAN 5 also. A new release number was not necessary, however, since the code was in development. A change sheet was also created for RADTRAN 5, and the same procedure of testing and archiving was followed.

Summary

The RADTRAN verification process has been illustrated using two examples showing that the methodology is reliable. This process has been applied to all calculational sequences in RADTRAN 4 and RADTRAN 5. In the later case, the process was repeated at each stage of code development and the final prototype yields acceptable results for all calculational sequences. The process will be performed if any changes are made to RADTRAN 5 in the future. The archival procedures allow all changes to be easily retrieved and reviewed.

References

Lange, Florentin, personal communication (1990).

Madsen, M.M., J.M. Taylor, R.O. Ostmeyer, and P.C. Reardon, "RADTRAN III," SAND84-0036, Sandia National Laboratories, Albuquerque, NM (1986).

Neuhauser, K.S. and F.L. Kanipe, "RADTRAN 4: Volume 3, User Guide," SAND89-2370, TTC-0943, Sandia National Laboratories, Albuquerque, NM (1992).

NRC, "Final Environmental Statement on the Transportation of Radioactive Material by Air and Other Modes," NUREG-0170, U.S. Nuclear Regulatory Commission, Washington D.C. (1977).

Taylor, J.M. and S.L. Daniel, "RADTRAN II: A Revised Computer Code to Analyze Transportation of Radioactive Material," SAND80-1943, Sandia National Laboratories, Albuquerque, NM (1982).