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RADTRAN 5.5 Validation and Verification Plan

D.M. Osborn, R.F. Weiner, S.C. Hamp

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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D.M. Osborn, R.F. Weiner, S.C. Hamp
Transportation Risk & Packaging Department
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-0718

ABSTRACT

This document contains a description of the verification and validation (V&V) plan used for the RADTRAN 5.5 code. The V&V plan will ensure the proper calculational models and mathematical and numerical methods are used in the RADTRAN 5.5 code for the determination of risk and consequence assessments in accordance with approved standards.

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1. INTRODUCTION

RADTRAN[®] (Copyright: Sandia National Laboratories 2003; current version RADTRAN 5) is the national standard for transportation risk assessment computer codes. The international version, INTERTRAN, is based on RADTRAN. RADTRAN combines user-determined meteorological, packaging, demographic, transportation, and material data with health physics data to calculate the expected radiological consequences and accident risk of transporting radioactive material.

RADTRAN was initially developed for the “Environmental Impact Statement (EIS) for the Transportation of Radioactive Materials by Air and Other Means” (NUREG-0170) in 1977. RADTRAN 5, the current version, allows complete user input and contains several improved utilities. RADCAT[®] (Copyright: Sandia National Laboratories 2004; current version RADCAT 1.0) is a graphical user interface (GUI). It is coupled with a downloadable PC version of RADTRAN 5 and acts as the input file generator.

RADTRAN 5.5, which is to be launched in the first quarter of 2005, will have the same capabilities as RADTRAN 5 plus a fully functional user-defined atmospheric dispersion model. The radionuclide library will be expanded from 60 nuclides presently available to 148 nuclides. There are additional tables that have been added to the output file, and the ingestion dose model, COMIDA, has also been updated to reflect the addition of the extra nuclides.

The RADTRAN code is in the operation and maintenance phase of its life-cycle according to the ANSI/ANS software standard (ANS, 1987). Since additional capabilities and improved performance characteristics will be incorporated into the RADTRAN 5.5 code, a validation and verification plan is needed to meet the minimum requirements for establishing the correctness of the RADTRAN risk assessment tool.

The primary objectives of this validation and verification (V&V) plan are twofold:

1. Validate the performance of the program revisions and new capabilities incorporated into RADTRAN 5.5.
2. Benchmark RADTRAN 5.5 against earlier validated versions of RADTRAN and other industry recognized computer programs appropriate for this type of analysis.

Sandia National Laboratories Organization 06143 is responsible for the maintenance and operation of the RADTRAN 5.5 code. The manager of 06143 designates a Member of the Technical Staff as the Principle Investigator responsible for RADTRAN. In addition, there is generally a scientific programmer assisting the Principle Investigator.

2. DESCRIPTION OF REVISIONS AND NEW CAPABILITIES

The major revisions in RADTRAN 5.5 are the addition of new tables, expansion of the radionuclide library, and an update of the COMIDA file. Other differences between the

current RADTRAN 5 version and the new RADTRAN 5.5 are in the location or content of the following output tables:

1. Dilution Factors – Chi Values after Depletion ($\text{Ci-sec/m}^3/\text{Ci-released}$)
2. Release Fractions
3. Deposition Velocities
4. Deposition Factors – Chi Deposited ($\text{Ci/m}^2/\text{Ci-released}$)
5. Dilution Factors for Pasquill Category **X** – Chi Values after Depletion ($\text{Ci-sec/m}^3/\text{Ci-released}$). This table is only listed when the average Pasquill dispersion option is selected, and where “**X**” is the Pasquill wind stability category A, B, C, D, E, or F.
6. Expected Values of Population Risk in Person-REM. This table lists results for each radionuclide in each package for each link in the output file rather than a separate file.

In the “Dilution Factors – Chi Values after Depletion ($\text{Ci-sec/m}^3/\text{Ci-released}$)” table, the RADTRAN 5 output has the isopleth areas listed for each isopleth while the RADTRAN 5.5 output has the downwind distance listed for each isopleth. The “Release Fraction” table echos the release fractions listed for each severity category in each physical chemical group listed in the input. The “Deposition Velocities” table echos the deposition velocities for each physical chemical group listed in the input. The “Deposition Factors – Chi Deposited ($\text{Ci/m}^2/\text{Ci-released}$)” is calculated by taking the “Dilution Factors – Chi Values after Depletion ($\text{Ci-sec/m}^3/\text{Ci-released}$)” and multiplying it by the deposition velocity (m/sec). The “Expected Values of Population Risk in Person-REM” tables are calculated using the equations listed in Section 5.3 of the RADTRAN 5 Technical Manual (Neuhauser, 2000) for each isotope. When the average Pasquill dispersion option is chosen then the tables “Dilution Factors for Pasquill Category **X** – Chi Values after Depletion ($\text{Ci-sec/m}^3/\text{Ci-released}$),” (where “**X**” is the Pasquill wind stability category A, B, C, D, E, or F) are produced. RADTRAN 5 uses the isopleth areas while RADTRAN 5.5 uses the downwind centerline distances. Also when the average Pasquill dispersion option is chosen the tables for the “Release Fractions” and the “Deposition Velocities” are listed for each of the Pasquill dispersion categories.

The expanded radionuclide library expands the original 60 isotopes and expands it to 148. The library has also updated the following for each isotope according to the source listed:

1. Half Life (days) source: ICRP 38 (as reported in Federal Guidance Report (FGR) 12)
2. Photon Energy (Mev) source: ICRP 38
3. Cloud/Immersion Dose Factor ($\text{REM-m}^3/\text{Ci-sec}$) source: FGR 12
4. Groundshine Dose Factor ($\text{REM-m}^2/\mu\text{Ci-day}$) source: FGR 12
5. Inhalation Value – 50 year Effective Dose (REM/Ci) source: ICRP 72
6. Inhalation Value – 50 year Dose to Gonads (REM/Ci) source: ICRP 72

7. Inhalation Value – 1 year Dose to Lungs (REM/Ci) source: ICRP 72
8. Inhalation Value – 1 year Dose to Bone Marrow (REM/Ci) source: ICRP72
9. Nuclide Name for Ingestion Date (RT5INGEST.BIN) source: COMIDA2
10. A1 Activity Limit Value (Ci) source: 10CFR71 Appendix A as of 01/01/2004
11. A2 Activity Limit Value (Ci) source: 10CFR71 Appendix A as of 01/01/2004

In determining the 50 year dose, ICRP 72 assigns the dose commitments to adult members of the public (age 20) assumed to live another 50 yrs. The inhalation values are based on 1.0-micron AMAD particles with the exception of the following radioisotopes:

1. Kr-85, Xe-133m, and Xe-133 are gases
2. H-3(water) is tritiated water
3. H-3(gas) is elemental hydrogen vapor
4. C-14(organic) is organic gases and vapors
5. C-14(gas) is carbon dioxide.

All the radioisotopes are assumed to have no progeny contribution with the exception of the following radionuclides:

1. Mo-99 includes the weighted contribution from its Tc-99m daughter
2. Ru-103 includes the weighted contribution from its short half-life Rh-103 daughter
3. Ru-106 includes the weighted contribution from its short half-life Rh-106 daughter. The inhalation dose conversion factors were determined for Ru-106 only since there is no information on Rh-106.
4. Cs-137 includes the weighted contribution from its short half-life Ba-137m daughter. Inhalation dose conversion factors were determined for Cs-137 only since there is no information on Ba-137m.
5. Ce-144 includes the weighted contribution from its two short half-life daughters Pr-144 and Pr-144m. Inhalation dose conversion factors were determined with Ce-144 and Pr-144 since there is no information on Pr-144m.

The updated COMIA file, COMIDA2, has an expanded library that incorporates all of the additional radionuclides. The current version of COMIDA was updated in July 2003. A slight correction in the output of the Backyard Farmer Dose will be made. This is to reflect the 0.00 REM for the ingestion dose when an area has been interdicted just like the Societal Ingestion Dose.

The new capability that has been added to RADTRAN 5.5 offers the option to the user to better define the atmospheric conditions for an accident release. The atmospheric model computes dispersion from a “Puff” release at a certain release height. This User-Define option incorporates the following meteorological conditions:

1. Release Height (in meters)
2. Heat Flux (in calories per second)
3. Source Width (in meters)
4. Source Height (in meters)
5. Wind Speed (in meters per second)
6. Dispersion Type (Pasquill or Briggs)
7. Wind Stability Class (A through F)
8. Rainfall Rate (in millimeters per hour)
9. Deposition Velocity (in meters per second)
10. Anemometer Height (in meters)
11. Ambient Temperature (in Kelvin)
12. Atmospheric Mixing Height (in meters)
13. Population Zone (suburban/urban or rural)

3. VALIDATON AND VERIFICATION APPROACH

The V&V of RADTRAN 5.5 will address the following areas:

1. Program requirements
2. Program design
3. Source code, program integration and documentation
4. Program testing
5. Test results-validation
6. V&V review report

Many of these areas have been previously addressed and are documented in the validation of earlier versions of the RADTRAN code (Neuhauser 1994; Neuhauser 2000). Therefore, the required extent of review for each of these areas will vary accordingly. The specific aspects that are to be reviewed are discussed in detail in the following sections.

3.1 PROGRAM REQUIREMENTS

As previously discussed, the earlier versions of RADTRAN have been documented and these documents are the basis for the program requirements. This V&V will primarily review the mathematical models and solution algorithms used by the program for the purpose of determining any known limitations to the code and the classes of problems that they best represent. The primary focus of this V&V is on the ability of the RADTRAN 5.5 code to model the incident-free, accident, and ingestion exposures and consequences to the public, workers, and a maximally exposed individual.

3.2 PROGRAM DESIGN

This V&V will not include a review of the program design. Since RADTRAN is an existing program that has undergone previous validation and verification and has been used for 27 years, it was determined that a detailed review of the program is not required.

3.3 SOURCE CODE, PROGRAM INTEGRATION, AND DOCUMENTATION

The review of the source code, program integration, and documentation will be limited to the following areas:

1. Configuration control of source code changes
2. Program installation
3. User documentation

These reviews and/or tests will be documented in the V&V report.

3.4 PROGRAM TESTING

This aspect of the V&V plan is crucial to ensuring that the two primary objectives of this plan will be accomplished. The tests in each of the series are designed to fulfill one or both of the primary objectives. The test series are the following:

- Series 1: Tests will utilize an old RADTRAN 5 truck input file that was used to validate and verify RADTRAN 5 with RADTRAN 4. The primary objective of this series is Objective 1.
- Series 2: Tests will utilize a RADTRAN 5 truck input file with the average Pasquill atmospheric dispersion model. The primary objective of this series is Objective 1.

- Series 3: Tests will provide a baseline for the average Pasquill atmospheric dispersion model with the new User-Defined atmospheric dispersion model. The primary objective of this series is Objective 2.
- Series 4: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Pasquill dispersion model for an elevated release in a suburban/urban population zone. The primary objective of this series is Objective 2.
- Series 5: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Pasquill dispersion model for an elevated release in a rural population zone. The primary objective of this series is Objective 2.
- Series 6: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Briggs dispersion model for an elevated release in a suburban/urban population zone. The primary objective of this series is Objective 2.
- Series 7: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Briggs dispersion model for an elevated release in a rural population zone. The primary objective of this series is Objective 2.
- Series 8: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Pasquill dispersion model for an ground level release in a suburban/urban population zone. The primary objective of this series is Objective 2.
- Series 9: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Pasquill dispersion model for an ground level release in a rural population zone. The primary objective of this series is Objective 2.
- Series 10: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Briggs dispersion model for an ground level release in a suburban/urban population zone. The primary objective of this series is Objective 2.
- Series 11: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a Briggs dispersion model for an ground level release in a rural population zone. The primary objective of this series is Objective 2.
- Series 12: Tests will utilize a RATRAN 5 rail input file. The primary objective of this series is Objective 1.

- Series 13: Tests will utilize a RADTRAN 5 barge input file. The primary objective of this series is Objective 1.
- Series 14: Tests will utilize a RADTRAN 5 truck input file defining a radionuclide that is not in the library. The primary objective of this series is Objective 1.
- Series 15: Tests will utilize a RADTRAN 5 truck input file with 21 different severity categories. The primary objective of this series is Objective 1.
- Series 16: Tests will utilize a RADTRAN 5 truck input file with a neutron exposure. The primary objective of this series is Objective 1.
- Series 17: A test will utilize a RADTRAN 5.5 input file with various deposition velocities for different physical chemical groups for the new User-Defined atmospheric dispersion model. The primary objective of this series is Objective 1.
- Series 18: A test will utilize a RADTRAN 5.5 input file with all the radionuclides listed in the expanded library. The primary objective of this series is Objective 1.
- Series 19: A test will utilize a RADTRAN 5.5 input file that will determine whether the Backyard Farmer Dose will provide the zero-values when an area is to be interdicted. The primary objective of this series is Objective 1.
- Series 20: Tests will provide a baseline for the new User-Defined atmospheric dispersion model using a rainfall scenario. The primary objective of this series is Objective 2.
- Series 21: A test will utilize a RADTRAN 5.5 input file that will determine whether the Societal Ingestion Dose will provide a correct output for the new User-Defined atmospheric dispersion model using a rainfall scenario. The primary objective of this series is Objective 1.

These test series will evaluate most of the changes and additions and will also demonstrate that the changes do not inadvertently affect other functions within the program. Table 1 provides the test matrix for these series.

Table 1: Test Matrix

Test Series/Case No.	Description
1a	Verify that a standardized truck route run with RADTRAN 5 on TRANSNET with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator
1b	Verify that a standardized truck route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator and the average weather dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET.
1c	Verify that a standardized truck route run with RADTRAN 5.5 PC-Version with the average weather dispersion model produces the same results as those run with RADTRAN 5 with the RADCAT 1.0 input file generator with the exception of those results affected by the new expanded radioisotope library and the updated COMIDA file
1d	Verify that a standardized truck route run with RADTRAN 5.5 with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the exception of those results affected the updated COMIDA file
1e	Verify that a standardized truck route run with RADTRAN 5.5 with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the exception of those results affected by the new expanded radioisotope library
2a	Verify that a standardized truck route run with RADTRAN 5 on TRANSNET with the Pasquill dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator
2b	Verify that a standardized truck route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the Pasquill dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET.
2c	Verify that a standardized truck route run with RADTRAN 5.5 with the Pasquill dispersion model using the old radionuclide library and COMIDA files from RADTRAN 5 produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator

Table 1: Test Matrix

Test Series/Case No.	Description
3a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator using the Pasquill dispersion model with test case 3b
3b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 with the old radionuclide library and COMIDA files from RADTRAN 5 using the new User-Defined Pasquill dispersion model with test case 3a
4a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Pasquill dispersion model for an elevated release in a suburban/urban population zone with test case 4b
4b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Pasquill dispersion model for an elevated release in a suburban/urban population zone with test case 4a
5a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Pasquill dispersion model for an elevated release in a rural population zone with test case 5b
5b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Pasquill dispersion model for an elevated release in a rural population zone with test case 5a
6a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Briggs dispersion model for an elevated release in a suburban/urban population zone with test case 6b
6b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Briggs dispersion model for an elevated release in a suburban/urban population zone with test case 6a

Table 1: Test Matrix

Test Series/Case No.	Description
7a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Briggs dispersion model for an elevated release in a rural population zone with test case 7b
7b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Briggs dispersion model for an elevated release in a rural population zone with test case 7a
8a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Pasquill dispersion model for a ground level release in a suburban/urban population zone with test case 4b
8b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Pasquill dispersion model for a ground level release in a suburban/urban population zone with test case 4a
9a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Pasquill dispersion model for a ground level release in a rural population zone with test case 5b
9b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Pasquill dispersion model for a ground level release in a rural population zone with test case 5a
10a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Briggs dispersion model for a ground level release in a suburban/urban population zone with test case 6b
10b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Briggs dispersion model for a ground level release in a suburban/urban population zone with test case 6a

Table 1: Test Matrix

Test Series/Case No.	Description
11a	Compare the dilution factors (Chi/Q) for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Briggs dispersion model for a ground level release in a rural population zone with test case 7b
11b	Compare the dilution factors (Chi/Q) for a simplified truck route run with RISKIND 2.0 using the Briggs dispersion model for a ground level release in a rural population zone with test case 7a
12a	Verify that a standardized rail route run with RADTRAN 5 on TRANSNET with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator
12b	Verify that a standardized rail route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the average weather dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET.
12c	Verify that a standardized rail route run with RADTRAN 5.5 with the average weather dispersion model using the old radionuclide library and COMIDA files from RADTRAN 5 produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator
13a	Verify that a standardized barge route run with RADTRAN 5 on TRANSNET with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator
13b	Verify that a standardized barge route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the average weather dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET.
13c	Verify that a standardized barge route run with RADTRAN 5.5 with the average weather dispersion model using the old radionuclide library and COMIDA files from RADTRAN 5 produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator

Table 1: Test Matrix

Test Series/Case No.	Description
14a	Verify that a standardized truck route run with RADTRAN 5 on TRANSNET with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator when the DEFINE statement is used
14b	Verify that a standardized truck route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the average weather dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET when the DEFINE statement is used.
14c	Verify that a standardized truck route run with RADTRAN 5.5 with the average weather dispersion model using the old radionuclide library and COMIDA files from RADTRAN 5 produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator when the DEFINE statement is used
15a	Verify that a standardized rail route run with RADTRAN 5 on TRANSNET with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator when 21 different severity categories are used
15b	Verify that a standardized rail route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the average weather dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET when 21 different severity categories are issued.
15c	Verify that a standardized rail route run with RADTRAN 5.5 with the average weather dispersion model using the old radionuclide library and COMIDA files from RADTRAN 5 produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator when 21 different severity categories are used
16a	Verify that a standardized truck route run with RADTRAN 5 on TRANSNET with the average weather dispersion model produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator when neutron dose is calculated

Table 1: Test Matrix

Test Series/Case No.	Description
16b	Verify that a standardized truck route run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator with the average weather dispersion model produces the same results as those run with RADTRAN 5 on TRANSNET when neutron dose is calculated
16c	Verify that a standardized truck route run with RADTRAN 5.5 with the average weather dispersion model using the old radionuclide library and COMIDA files from RADTRAN 5 produces the same results as those run with RADTRAN 5 PC-Version with the RADCAT 1.0 input file generator when neutron dose is calculated
17	Verify that the RADTRAN 5.5 User-Defined atmospheric dispersion model can calculate a series of different deposition velocities from various physical chemical groups
18	Verify that all 148 radionuclides in the RADTRAN 5.5 isotope library provide the correct output
19	Verify that the Backyard Farmer Dose provides zero-values in areas that have been interdicted.
20a	Compare the dilution factors (Chi/Q) and the ground deposition for each isopleth for a simplified truck route run with RADTRAN 5.5 using the new User-Defined Briggs dispersion model for an elevated release in a rural population zone which has rainfall with test cases 20b and 20c.
20b	Compare the dilution factors (Chi/Q) and the ground deposition for each isopleth for a simplified truck route run with RISKIND 2.0 using the new User-Defined Briggs dispersion model for an elevated release in a rural population zone which has rainfall with test cases 20a and 20c.
20c	Compare the dilution factors (Chi/Q) and the ground deposition for each isopleth for a simplified truck route run with HOTSPOT 2.05 using the new User-Defined Briggs dispersion model for an elevated release in a rural population zone which has rainfall with test cases 20a and 20b.
21	Verify that the Societal Ingestion Dose will provide a correct output for the new User-Defined atmospheric dispersion model using a rainfall scenario.

3.5 REVIEW OF TEST RESULTS

Test results will be reviewed to assure that program requirements have been fully tested and that the tests have met the requirements of this V&V project. Some tests will also be verified by hand calculations and will be made available upon request. Discrepancies will be noted in the V&V report. If additional tests are required, they too will be documented. Test results will be evaluated relative to acceptance criteria as stated within the test matrix. Exceptions will be noted and causes will be determined. The determination of potential in program limitations will also be examined and reported.

3.6 V&V REPORT

The results of the RADTRAN 5.5 code evaluation will be fully documented in a V&V report. This report will provide a clear indication of how the requirements and the objectives of this V&V plan were met. Specific detailed discussion will be provided for each test together with documentation of the results. Results of the program testing will also be summarized for convenient review. Traceability will be provided for all the test case input, output results, and hand calculations.

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