NUMERICAL
APPLICATIONS, INC.
SOLUTIONS IN ENGINEERING AND SOFTWARE

September 12, 2000

Mr. WM Blumberg
USNRC
MS-O-10H4
Washington, DC

Dear Mr. Blumberg,

NAI has completed their review of the RADTRAD Version 3.01/3.02 computer program and documentation. The enclosed report summarizes the scope of the review and code and documentation deficiencies discovered during the review. Some of the noted deficiencies will result in lower dose estimates than obtained from a corrected version of the code.

This report is presented to the USNRC to satisfy our obligations under the RADTRAD distribution agreement. The agreement stipulates that errors be communicated to the contractor assigned to code development. Based on our telephone conversation, a contractor is not currently assigned to the software development, so the errors are presented directly to the NRC per your request.

Please contact me if you have any questions regarding this report.

Sincerely,

Thomas L. George
President

cc F. Eltawila
cc J. Flack

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RADTRAD-NAI

Introduction

Over the past year, Numerical Applications, Inc. (NAI) has completed a formal, comprehensive verification and validation of the RADTRAD computer code (versions 3.01 and 3.02) under NAI's 10CFR50 Appendix B program. The V&V effort resulted in the identification and correction of several deficiencies in the code and the addition of several enhancements. A detailed Design Review report documents the entire process. The scope of the V&V effort and the nature of the resulting code modifications are summarized here.

As required by the NRC, NAI's Revised Version of RADTRAD is named **RADTRAD-NAI** to distinguish it from the original code. **RADTRAD-NAI** is currently being maintained under NAI's 10CFR50 Appendix B program, which has been NUPIC-audited and approved by numerous utilities and fuel vendors. This is the same Quality Assurance program under which the **GOTHIC** computer code is being maintained by NAI for the nuclear industry.

RADTRAD-NAI

RADTRAD-NAI began with versions 3.01 and 3.02 of the NRC's RADTRAD computer code, originally developed by Sandia National Laboratory (SNL). The code, acceptance case input and output and documentation were received on a distribution Compact Disk (CD) from Scientech, Inc. (currently Information Systems Laboratories, Inc.). The code was initially modified to compile on a UNIX system. Once compiled, an extensive design review/verification and validation process began on the code and documentation. The subject of the review also included the source code for the solver, which was made available in a separate distribution from the NRC. The review is described in Attachment A.

In the course of the review, several deficiencies were identified in the code and documentation. Some of the deficiencies would result in a reduced estimate of the dose. The identified deficiencies are listed in Attachment B.

In addition to reviewing the code, several improvements/additions were made. These include:

- A model to track the pH of a pool, accounting for contributions from the source term, user specified acid and base sources and the temperature dependence of the ionization constant of water
- Modifications to the output to ensure all input is echoed

- Removal of a significant amount of unused coding; in particular, related to revolatilization models
- Restructure of the solver input to eliminate inactive input placeholders and other unused parameters, allow free format of input data and allow unrestricted commenting of the input file
- Elimination of redundant input, including various flags and, for example, compartment and pathway flow rates associated with the different transport groups for various removal mechanisms
- A change that shifts the code transient time scale so that transient time is relative to the start of an event rather than the start of a release.

All changes to the solver were tracked through the RADTRAD-NAI Action Reporting System as part of NAI's 10CFR50 Appendix B program. All major changes to the documentation were tracked through the design review process/report. The new code package includes the solver and documentation. The documentation includes User Instructions, Technical Basis/Theory Manual, and Programmer Information.

ATTACHMENT A
DESCRIPTION OF DESIGN REVIEW

Code and Documentation Review

The review covered the following elements.

User Instructions

- Does the code install according to the description given in the User Manual?
- Are the contents of the installation directory and subdirectories clearly defined in the User Manual?
- Are the contents and purpose of the files associated with the source term clearly documented?
- Can the acceptance cases provided with the code be duplicated by the installed code?
- Does the code operate according to the description given in the User Manual?
- Does the User Manual describe in detail how to prepare input for the solver?
- Does the User Manual provide an adequate description of the output?
- Does the User Manual provide guidelines for use of the code?

Technical Basis/Theory

- Are the governing equations that apply to the source, transport, removal and decay of radionuclides adequately described?
- Are source terms adequately described?
- Are the spray models adequately described?
- Are the natural deposition models adequately described?
- Are the overlying pool removal models adequately described?
- Are the leakage models adequately described?
- Are the suppression pool models adequately described?
- Are the piping deposition models adequately described?
- Are the consequence analyses adequately described?
- Is the solution method adequately described?

Programmer Information

- Is the structure of the code adequately described?
- Is the function of each code module adequately described?
- Is the input consistent with the description given in the User Manual?
- Is the solver code logic and solution scheme adequately described?
- Assess the extent to which code comments contribute to the function of the Programmer Manual.

Verification

- Is the code input structure consistent with the documentation?
- Are the coded spray models consistent with the documentation?
- Do the coded spray models accurately represent the references for those models?
- Are the coded natural deposition models consistent with the documentation?
- Do the coded natural deposition models accurately represent the references for those models?
- Are the coded overlying pool removal models consistent with the documentation?
- Do the coded overlying pool removal models accurately represent the references for those models?
- Are the coded leakage models consistent with the documentation?
- Do the coded leakage models accurately represent the references for those models?
- Are the coded suppression pool models consistent with the documentation?
- Do the coded suppression models accurately represent the references for those models?
- Are the coded piping deposition models consistent with the documentation?
- Do the coded piping deposition models accurately represent the references for those models?
- Is the code output a complete and accurate representation of the calculations performed by the code?

Validation

- Run acceptance cases provided with the original code distribution and determine that the results, which were also provided with the distribution, can be duplicated.
- Do the source terms perform as described?
- Do the natural deposition models perform as described?
- Do the overlying pool models perform as described?
- Do the leakage models perform as described?
- Do the suppression pool models perform as described?
- Do the piping deposition models perform as described?
- Do the spray models perform as described?
- Do the radioactive decay models perform as described?

Summary of Validation Tests

Validation was performed with three different types of tests:

- Comparison of selected Acceptance Test Case results with Excel spreadsheet solutions.
- Separate effects tests, and
- Recent industry examples.

Each of these test types is described below.

Acceptance Test Cases

Input and output files for Acceptance Test Cases 1 through 24A come with versions 3.01 and/or 3.02 of RADTRAD. The basis for each case is presented in section 3.3 of NUREG/CR-6604. The results of selected cases, listed in Table 1 below, were checked with a combination of analytical solutions and Excel spreadsheets. These solutions were not provided with the RADTRAD distribution. The analytical portion is usually the solution of a set of differential equations, including evaluation of multiple:

- locations (EAB vs. LPZ),
- time periods with different values for dispersion and breathing rates, and
- isotopes.

Table 1 Acceptance Cases Used for Verification

Acceptance Test Case number	Description
1	I-131 only, with no radioactive decay. EAB and LPZ doses are a result of Containment leakage. Tested fission yield, transport, integration of release over time and combination of dose conversion factors, breathing rates and X/Q dispersion.
2	Same as Case 1, except with the addition of other isotopes. Additionally tested addition of 13 TID isotopes (fission yield and dose conversion factor).
2A	Same as Case 2, except with the addition of radioactive decay. Additionally tested half-life implementation for decay.
2B	Same as Case 2A, except with the addition of Daughter In-growth. Additionally tested decay of iodine to produce xenon.
3	Same as Case 2, except with the additional calculation of Control Room dose. Additionally tested transport to and within the Control Room, including recirculating filter.
4	Similar to Case 2 and Case 3 (with no radioactive decay), except the release fraction is doubled and iodine is removed from the air inside Containment by means of natural deposition. Additionally tested user-specified constant rate of natural deposition.
6	Similar to Case 1, except the release is based on NUREG-1465 instead of TID-14844: I-131 only, no radioactive decay. Tested release fraction and timing tables, dose conversion factors and TEDE with a single isotope.
7	Same as Case 6, except for the addition of other isotopes and elements. Tested addition of NUREG isotopes, including fission yield and dose conversion factors.
7A	Same as Case 7, except with the addition of radioactive decay for each isotope. Additionally tested half-life implementation for decay.
9	Same as Case 7, except with the addition of a constant rate of removal of iodine from the atmosphere inside Containment. Additionally tested natural deposition.
11	As the first BWR example, the most important difference is the release path. The Containment building leaks to the Condenser (via Main Steamline) and it is the Condenser that leaks to the outside environment. I-131 only with no radioactive decay. Similar to case 1, but also tested transport through an intermediate compartment.
12	Same as Case 11, except with the addition of Control Room dose. Additionally tested transport to the Control Room and the geometric factor for cloudshine contribution to TEDE.

15	comparable to Case 11, except - a NUREG-1465 source term instead of TID-14844, and - ECCS leakage to the Auxiliary Building instead of Condenser leakage to the Turbine Building. Additionally tested complex transport through multiple compartments.

Separate Effects Test Cases

The separate effects test cases were specifically designed to check a single option or code model. Examples are shown in Table 2 below:

Table 2 Separate Effects Test Cases

Test Case number	Description
NAI-1	Daughter in-growth The amount of Xenon produced by Iodine decay at 100 hours is compared with the solution of differential equations.
NAI-2	Powers model for removal/retention of aerosol in an Overlying Pool Pool retention is compared with corresponding value for Decontamination Factor derived from correlation.
NAI-3	Suppression pool pathway Rate of transport of activity checked with simple "hand" calculation
NAI-4	Powers model for Natural Deposition of Aerosol (1) Input data chosen to match example calculation in source reference and (2) slope of mass fraction plotted on log scale compared with corresponding λ derived from table
NAI-5	Powers model for Aerosol removal by Spray semi-log plot of amount of aerosol as a function of time
NAI-6 (set or series)	Brockman and Bixler models for Deposition in Piping (1) check of applicable variables (while these are not normally included in the output, a temporary change was made to the source code to invoke or activate print statements included in the original BROCK subroutine) (2) comparison of relative amounts on "pipe wall" versus downstream
NAI-7	Suppression Pool pH tracking (1) comparison to results of Grand Gulf calculation (2) observation of expected (qualitative) trend for temperature dependence
NAI-8	Nuclide conservation: In a single-compartment model without decay, verify that the nuclide and transport group quantities are preserved throughout the transient.
NAI-9	Nuclide conservation: In a two-compartment model with balanced recirculation between compartments, verify that the nuclide and transport group quantities are preserved throughout the transient and agree with the nuclide and transport group quantities from NAI-8.

NAI-10	Nuclide conservation: In a single-compartment model with an overlying pool, verify that the nuclide and transport group quantities are preserved.
NAI-11	Nuclide conservation: In a single-compartment model with a recirculating filter, verify that the nuclide and transport group quantities are preserved.
NAI-12	Nuclide conservation: In a single-compartment model with natural deposition, verify that the nuclide and transport group quantities are preserved.
NAI-13	Nuclide conservation: In a single-compartment model with compartment sprays, verify that the nuclide and transport group quantities are preserved.
NAI-14	Nuclide conservation: In a two-compartment model connected by a piping pathway, verify that the nuclide and transport group quantities are preserved.
NAI-15	Nuclide conservation: In a two-compartment model connected by a filter pathway, verify that the nuclide and transport group quantities are preserved.
NAI-16	Nuclide conservation: In a two-compartment model connected by a suppression pool pathway, verify that the nuclide and transport group quantities are preserved.
NAI-17	Nuclide conservation: In a two-compartment model connected by a convection pathway, verify that the nuclide and transport group quantities are preserved.
NAI-18	Nuclide conservation: In a multi-compartment, multi-pathway model in which all removal mechanisms are active, verify that the nuclide and transport group quantities are preserved.
NAI-19	Nuclide conservation: In a multi-compartment model with flows to and from an environment compartment, verify that the nuclide and transport group quantities are preserved.

Recent Industry Examples

Several cases were run to compare with previous plant analyses to provide additional independent checks. They are:

- Wolf Creek Fuel Handling Accident
- Perry (BWR) Main Steamline Break
- Grand Gulf (BWR) LOCA
- Surry (PWR) LOCA.

ATTACHMENT B

IDENTIFIED DEFICIENCIES IN RADTRAD VERSION 3.02

In the process of completing the Design Review of RADTRAD version 3.01, several deficiencies were noted in the solver source code and in the documentation. All items noted below are also applicable to RADTRAD version 3.02. These deficiencies were corrected in **RADTRAD-NAI.**

Identified Code Deficiencies

1. For any case in which radioactive decay is calculated, the Compartment Atmosphere Nuclide Inventory does not match the corresponding Compartment Atmosphere Transport Group Inventory in the output file. (Action Report 17)
   Consequence: The code cannot be validated for nuclide conservation by examination of the output. Consequences depend on application and interpretation of output.
2. For any case in which radioactive decay is calculated, the transport group quantities for the compartment and pathway retention locations do not reflect decay at those locations. (Action Report 17)
   Consequence: Nuclide conservation cannot be validated in models that include any of the various removal mechanisms and with decay active.
3. Noble gases given off by daughter in-growth at the retention locations are effectively discarded rather than being released to the atmosphere. (Action Report 17)
   Consequence: This would underestimate the dose.
4. The daughter in-growth algorithm fails to account for in-growth to another transport group. This includes the previously noted problem with noble gases, and would also include in-growth to an iodine for which the distribution to the elemental, organic and aerosol forms is not considered. (Action Report 17)
   Consequence: With daughter in-growth active, the distribution of nuclides to the various transport groups will, in general, be incorrect.
5. The output transport group quantities for Overlying Pools are always zero. (Action Report 16)
   Consequence: Nuclide conservation cannot be validated in models that include an overlying pool.
6. The distribution of iodine from a source beneath an overlying pool is not adjusted in consideration of the removal mechanisms in the pool. (Action Report 17)

Consequence: The distribution of iodine in the effective source to the compartment atmosphere above the pool will not, in general, be correct.

7. In a general model that includes an environment compartment and the various removal mechanisms, conservation of the nuclides is not maintained. (Action Report 17)
   Consequence: Consequence depends on application.
8. Distribution of the source to a multiple number of compartments results in accelerated decay. (Action Report 18 and 7)
   Consequence: The dose will be under estimated.
9. Use of Powers model for removal of aerosol by spray over-predicts removal. According to the referenced source, the decontamination coefficient should decrease as the aerosol concentration decreases. RADTRAD does not exhibit this behavior. (Action Report 19 and 2)
   Consequence: Aerosol removal would be over predicted and, therefore, dose would be under predicted.
10. RADTRAD does not properly account for the bend angle in aerosol deposition in piping. (Action Report 15)
    Consequence: Aerosol retention in piping with bends would be underpredicted.
11. Treatment of flow through a Suppression Pool pathway is inconsistent with the input. (Action Report 14)
    Consequence: Dependent upon the connected compartment volumes, this error could over predict or under predict doses.
12. Table 2.2.2.1-5 in NUREG/CR-6604 for the Advanced PWR lists incorrect deposition coefficient values for the 10th and 90th percentiles for the 13.8 to 24 hour period. (Action Report 20)
    Consequence: Deposition during this time period would be slightly under predicted.
13. The reference height for Henry's correlation for Natural Deposition is not consistent with the referenced source. (Action Report 21)
    Consequence: Natural deposition would be under predicted.
14. The last coefficient in Equation 23 in NUREG/CR-6604 is incorrect. The referenced source is in error. (Action Report 22)
    Consequence: Deposition on pipe walls would be underpredicted.

Identified Documentation (NUREG/CR-6604) Deficiencies: no change to coding

1. Values for spray flux presented in section 2.2.1.1 should be divided by 10,000.
2. There is a typographical error in Equation 15. In its current form, the term in brackets is zero.
3. Equation 18 is not consistent with the coding without inclusion of the slip correction.
4. The discussion of Gravitational Settling is not complete in that laminar flow conditions are not addressed. In the coding, Equation 18 is only applicable to turbulent flow conditions.
5. In order to be consistent with the definition of "η" as deposition efficiency, Equation 23 should be subtracted from "1.0".
6. "D_{iff}" in Equation 24 is described as the "particle diffusion coefficient", but not defined mathematically.
7. In Equations 30 and 32, the deposition velocities for elemental and organic iodine within piping should be expressed as exponential.
8. The discussion of deposition in piping bends is not complete in that laminar flow conditions are not appropriately addressed. In the coding, Equation 27 is only applicable to turbulent flow conditions and Equation 26 is "bypassed".
9. Equation 39 should not include the geometric factor, G_F.
10. Equation 37 should include the Occupancy Factor.