

## A Posteriori Verification and Validation of a Tritium Dispersion & Consequence Model<sup>1</sup>

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### Abstract

An American National Standards Institute (ANSI) posteriori (backfit) process, available to provide software quality assurance (SQA) for software developed outside of required qualification protocol, has been applied to the special-purpose, versatile tritium dispersion and consequence model, UFOTRI, a computer model developed at the German Karlsruhe laboratory. UFOTRI was chosen because of its strengths in initial tritium-related consequence analyses and its potential for application in a Department of Energy accident analysis context. The six-task process met key ANSI requirements and was performed during a several-month level of effort. Included project deliverables were Assessment, Test Plan, Configuration Procedure, Error Notification Procedure, Comprehensive Technical Report, and SQA Qualification Report documentation. Comparison to acute release conditions is still in progress, but results to date indicate satisfactory, bounding predictions can be achieved with UFOTRI relative to measurements. Results of this compact effort have identified UFOTRI as a suitable candidate for a software “toolkit,” i.e., minimum verification and validation (V & V) requirements are satisfied, and a configuration controlled version is deemed appropriate for use in a DOE accident analysis context.

### Introduction

The accident analysis sections of Safety Analysis Reports (SARs) and Basis for Interim Operation (BIO) reports for Department of Energy (DOE) nuclear facilities usually contain the methods and quantification of radiological exposures due to postulated accident conditions. In principle, SAR-related doses are calculated applying a qualified spreadsheet or other software package using conservative inputs and user assumptions. In practice, many of the computer-based options available to DOE accident analysts are not supported with adequate SQA, and little validation evidence that the model is fit for the specific applications exists. This issue has been identified by the staff of the Defense Nuclear Facilities Safety Board and highlighted in their recent Technical Report (DNFSB, 2000).

The analyses supporting SARs and BIOs for DOE tritium storage and processing facility operation face the same SQA issues. Unless sufficient justification can be provided demonstrating the pedigree of the software, including quality assurance and fitness for application to accident conditions, it is difficult for independent review of the analyses to draw any conclusion on the associated consequences calculated with the model. This may be especially problematic with software developed without a formal Software Development Plan (SDP) that is tailored to meet certain customer’s requirements, and then made available for users. However, an ANSI standard exists that details a posteriori (backfit) process, applicable to many accident analysis software models used for DOE nuclear facilities. The standard, ANSI/ANS-10.4-1987, provides assurance that software developed outside a defined SDP qualification protocol is applied within the proper context and meets minimum V & V standards [ANSI/ANS, 1987].

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<sup>1</sup> **Acknowledgment.** This abstract was prepared in connection with work done under Contract No. DE-AC09-96SR18500 for the U. S. Department of Energy. By acceptance of this abstract, the publisher and/or recipient acknowledges the U. S. Government’s right to retain a nonexclusive, royalty-free license in and to any copyright covering this abstract, along with the right to reproduce and to authorize others to reproduce all or part of the copyrighted abstract.

The ANSI backfit process has been applied to UFOTRI, a special-purpose, tritium dispersion and consequence model. The process demonstrating UFOTRI as “fit” for tritium consequence analysis for Savannah River Site (SRS) and other DOE facilities is described in this paper. It may be of particular interest since the ANSI standard is applied to a computer model that is foreign-developed.

## UFOTRI Dispersion and Consequence Model

The Defense Nuclear Facilities Safety Board staff recently reviewed the application of safety analysis software and its associated quality assurance in the DOE Complex [DNFSB 2000]. Technical Report 25 recommended improvements in the SQA practices, processes, and procedures used for accident analysis and process control of DOE nuclear facilities. Of particular significance in the report was the class of computer models for dispersion and consequence analysis, and the suggestion to establish a “toolkit” of verified and validated models with identified regimes of applicability. In principle, the accident analysis toolkit would be a repository of verified and validated computer models that are configuration-controlled and made available for specific applications. Because of UFOTRI's strengths in tritium-related consequence analysis, the SQA program for UFOTRI Version 93/4.20P for Personal Computers was chosen to be upgraded with the ANSI standard process. Equivalent goals were to benchmark the resource commitment to conduct the a posteriori V & V (or Design) Review and to ultimately establish UFOTRI as a primary software model for the toolkit.

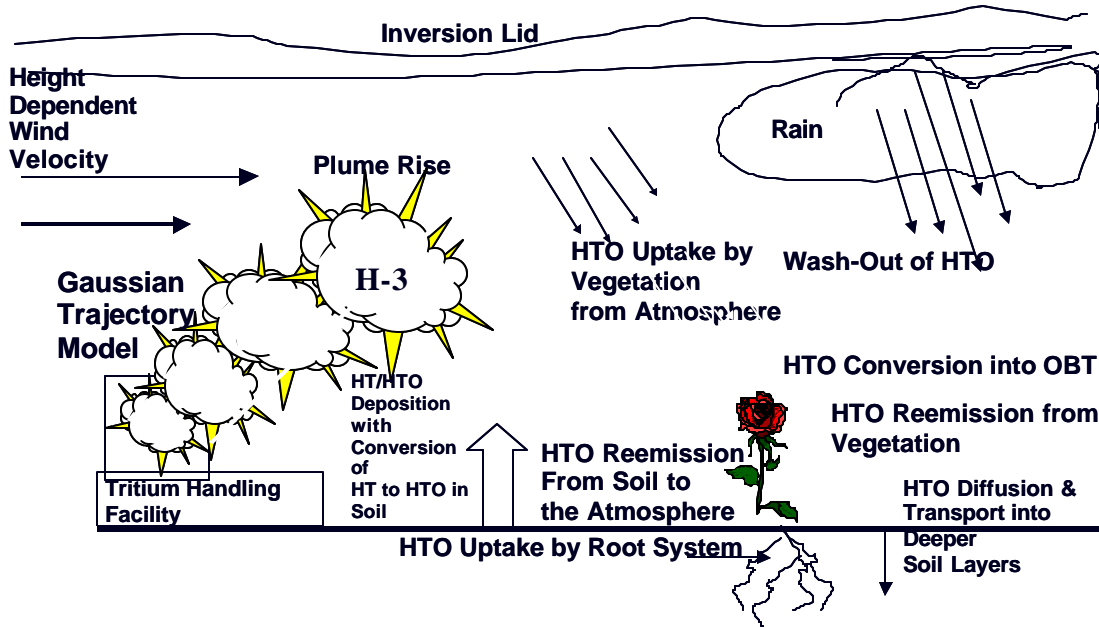
The UFOTRI (Unfallfolgenmodell für Tritiumfreisetzungen) computer model was developed by the German national laboratory Karlsruhe (Kernforschungszentrum Karlsruhe GmbH, or KfK) to assess the radiological consequences due to postulated accidental atmospheric releases from nuclear facilities [Raskob 1990, 1992, 1993]. The first version of UFOTRI was released in mid-1991 [Raskob, 1990]. An update was released in late 1993 incorporating several significant improvements to plant/soil exchange, soil/atmosphere exchange, plant, and photosynthesis (OBT formation) models [Raskob, 1992 and 1993].

UFOTRI describes the behavior of tritium in the biosphere and calculates the radiological impact on individual receptors and populations due to inhalation, skin absorption and uptake of contaminated foodstuffs. Although individual and population doses can be calculated, UFOTRI does not calculate health effects. Time-dependent processes modeled include dispersion, deposition, reemission, conversion of tritium gas (HT) into tritiated water vapor (HTO) by the soil, and conversion of HTO into organically bound tritium (OBT) (Figure 1). The source term model accounts for release duration, release height, tritium species being released, and thermal energy released. A Gaussian module is applied for the initial release of HT/HTO and reemission up to seven days after the release event. The reemission model addresses evaporation from soil and transpiration from vegetation. UFOTRI considers all relevant transfer processes in the environment (atmosphere, soil, plant, and animal), and is unique in that the initial plume passage model is integrated with the reemission (area source) model.

UFOTRI features an acute atmospheric model of transfer processes from the postulated event (~ first one hundred hours), coupled to a first-order compartment module for the longer-term behavior of two different chemical forms of tritium species in the food chain. The long-term model accounts for food ingestion doses from contaminated foodstuffs, but does not include ingestion doses from potable water consumption. Typically, for individual dose calculations for SARs, the food ingestion doses are not calculated. The Radiological Dispersion/Consequence Working Group of the Accident Progression and Consequence (APAC) Evaluation Project recommended UFOTRI over other software packages for deterministic safety analyses (SARs and BIOs), Environmental Impacts Statements, and probabilistic safety assessments of tritium nuclear facilities [O’Kula et al., 1996].

The code can execute with meteorological data treated either in a deterministic manner, using prescribed meteorological conditions, or in a probabilistic manner, using a stratified random sampling algorithm.

## ***UFOTRI Models Key Biophysical Processes of Tritium in the Environment***



**Figure 1. UFOTRI Model of Environmental Processes for Acute Tritium Releases**

When meteorological data is treated in a probabilistic manner, a set of “start times” is selected from consequence bins (sampled from meteorological data representative of the site). The consequences for the respective source terms are weighed by the probability of the consequence category, such that the output is in the form of a complementary cumulative distribution function (CCDF) table, providing median, 95<sup>th</sup> percentile, and other consequence levels.

UFOTRI has been applied primarily for fusion safety and design projects. The major applications have been for fusion studies such as the Next European Tokamak (NET) and the International Thermonuclear Experimental Reactor (ITER). Experimental studies in Canada indicate good agreement for use of UFOTRI for tritiated water vapor release [BIOMOVs, 1996]. Testing with HT species in Canada has shown good agreement with field measurements, despite data collection and modeling uncertainties [Raskob, 1990].

The model used for most consequence analyses of postulated accident conditions for SRS safety documentation is MACCS version 1.5.11.1 [Chanin et al., 1990, 1993; Jow et al., 1990; Rollstin et al., 1990]. Despite completion of the UFOTRI V & V process, MACCS will continue to be applied for most SRS tritium consequence analyses. UFOTRI will be applied in a supplemental and confirmatory context. Table 1 compares the two models, UFOTRI and MACCS.

### **ANSI-10.4 Compliant Process**

In order for UFOTRI to be used with confidence for the calculation of doses associated with authorization basis (AB) documentation, the code must have a graded V & V effort that defines the qualification of the

software. The ANSI and IEEE software quality assurance standards [ANSI/ANS, 1987 and IEEE, 1984] both contain sections that deal with software that is developed outside the respective standards.

**Table 1. Comparison of MACCS with Tritium-Specific UFOTRI Computer Model**

Phenomenon or Model Feature	MACCS	UFOTRI
1. Gaussian release model	Yes	Yes
2. Sensible heat/release duration	Yes	Yes
3. Deposition (wet/dry)	Yes (simple model only)	Yes - the option used by MACCS and a detailed biophysics option
4. Stratified Random Sampling of Site Meteorology option	Yes (10 samples x 36 categories = 360 sequences)	Yes (1 sample from 144 categories = 144 sequences)
5. Dispersion parameterization	Yes (Pasquill-Gifford; User-Specified Diffusion Parameters)	Yes (MOL, Belgium Briggs, Pasquill-Gifford sets)
6. HTO – HT differentiation	No	Yes
7. Tritium model after plume passage	Resuspension model	Detailed reemission physics model accounting for soil/vegetation interaction with HTO/HT in atmosphere
8. Tritium conversion from HT to HTO	No	Yes
9. Uptake of HTO by Vegetation	No	Yes
10. Conversion of HTO into OBT	No	Yes
11. 1 <sup>st</sup> Order Compartment Model for Long-term behavior in Food Chain	No	Yes

A “backfit” process may make sense for a computer model that is the end product of a research program [ANSI/ANS, 1987]. In this context, a parallel V & V program may be impracticable until after the development process is completed. The ANSI standard details a backfit or *a posteriori* process that recovers some measure of V & V previously missing by taking advantage of available computer model products and collective user experience. Its purpose is to determine whether the computer model produces valid responses within a specific domain, and to document that an appropriate level of V & V has been conducted.

Six tasks defining the *a posteriori* V & V program were performed for UFOTRI. The tasks meet the ANSI requirements and define the minimum steps completed before the UFOTRI code was deemed suitable for Authorization Basis applications. Included are:

1. An *Assessment Document* containing listing of, or reference to, technical data pertaining to existing software requirements and documentation, code source listing, test data, validation experiments, and technical literature search.
2. A *Test Plan* defining tests performed and expected results, evaluation criteria, and technical bases for test data.
3. A *Configuration Procedure* defining code installation, a maintenance procedure for software/operating system modifications, test set contents, and a routine testing procedure.
4. An *Error Notification Procedure* that defines user qualifications and approvals, maintenance of user and software error lists, and indicates the process for user notification.

5. *A Comprehensive Technical Report* containing results of testing program, identifying areas of code applicability and potential limitations.
6. *SQA Qualification Report* containing completed SQA checklist, supplemental material and explanation, including software management and inventory program interfaces.

A modest effort was undertaken to complete these tasks. A flowchart of phases is discussed in the next section.

### **UFOTRI Software Evaluation Process**

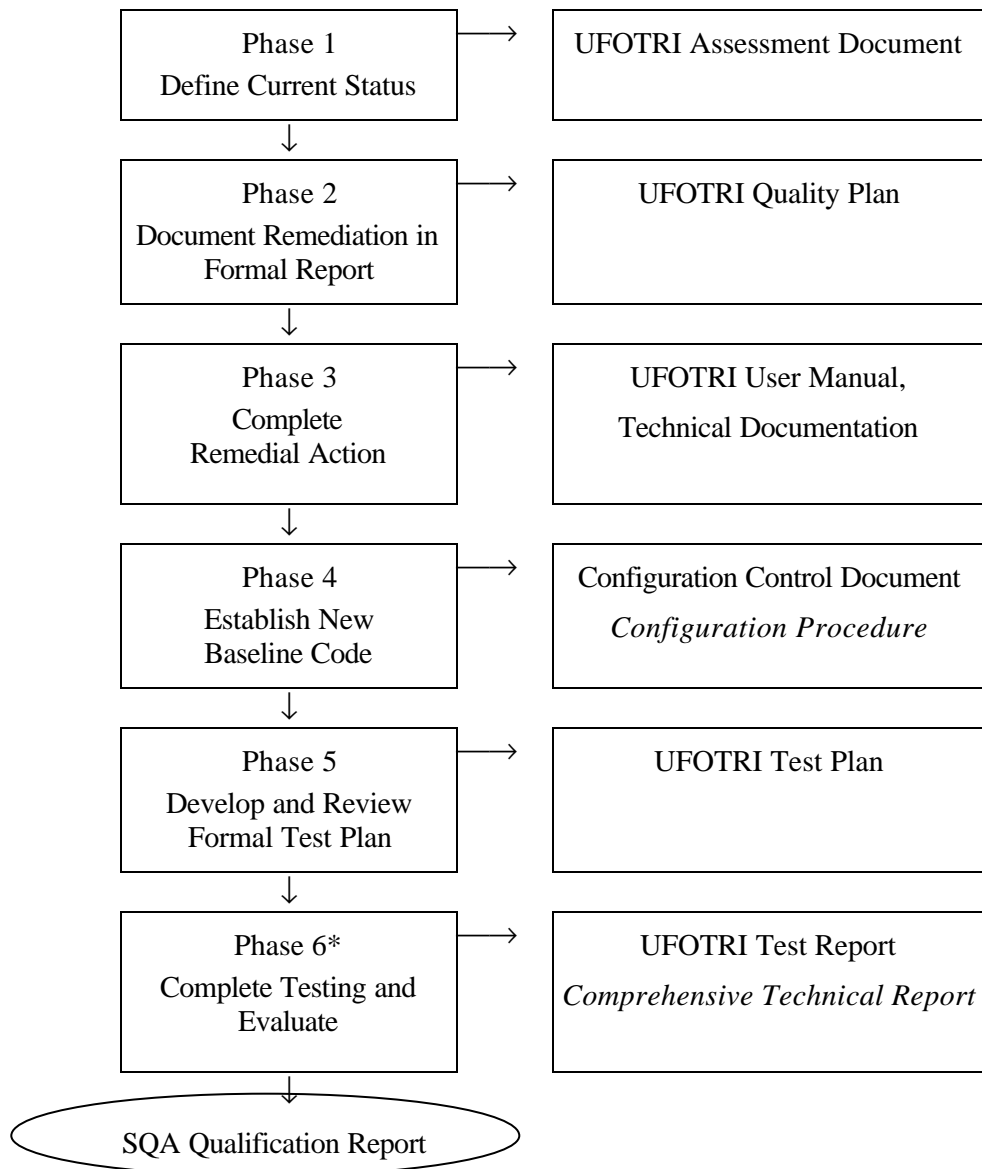
A compact process was executed to ensure that key V & V tasks were completed to bring the UFOTRI software into compliance with major requirements of the ANSI and IEEE standards. Phases and activities included:

- Phase 1 - **Defining Current UFOTRI Status:** The initial phase documents the current computer model status, origin and development of the executable, operating system requirements, and intended applications, and existing configuration control.
- Phase 2 - **Planning Remedial Action:** This step evaluates inadequacies in the software and specifies upgrade plans, including source code, documentation, test plans, test results, and documented reviews of these items. Phase 2 forms the basis for further action and outlines requirements for final acceptance of the software and the extent of remediation planning to correct deficiencies in the source code and documentation.
- Phase 3 - **Complete Remedial Action:** This phase executes all tasks defined in Phase 2, and defers or redefines activities as priorities change.
- Phase 4 - **Establish New Baseline:** A new baseline is defined for UFOTRI in terms of execution, configuration, documentation, and user access. All elements are reviewed to ensure compliance with Remediation Plan.
- Phase 5 - **Develop and Review Formal Test Plan:** Establish a testing plan of the new baseline code based on the objectives listed in the Remediation Plan
- Phase 6 - **Complete Testing and Evaluation:** Demonstrate the compliance of the software against the objectives listed in the Remediation and Test Plans. A test report describes the outcome of testing of the UFOTRI software.

Independent review of Phases 2 through 6 was periodically performed to ascertain if any aspect of work needed to be revised or redone. Based on our experience with the UFOTRI program, by far the most resource-intensive phase was the Phase 3 (approximately 70% of the overall effort).

The effort to perform the six tasks was conducted over two periods. The overall level of effort, including technical report generation, technical and management, and quality assurance review was approximately 3 person-months.

Figure 2 is a representative process flowsheet that was followed for configuration control of the UFOTRI software. It indicates the deliverable for each of the component phases.



**Figure 2. Diagram of Qualification Process for Non-Compliant Software.**

Phases 2 through 6 were repeated as needed.

### Software Quality Assurance Documentation

As an independent check of the SQA performed under the ANSI posteriori process, the V & V qualification process sheet was assessed for compliance against the relevant IEEE standard [IEEE, 1984]. The UFOTRI project was performed at a level where many requirements were consolidated, but in a manner that still complied with most of the applicable IEEE Standard requirements.

Table 2 is a list and description of the necessary documents needed for a complete SQA package as taken from these standards. The phase in which the IEEE standard was met is listed next before each document or activity. While it is designed to be implemented in a software development activity, a project assessment demonstrated that the UFOTRI qualification process met the intent of these items.

**Table 2. UFOTRI V & V Process Compliance Against IEEE Standard**

UFOTRI Process	IEEE Standard
Phase 2	<p><b>Project Plan:</b> The project plan is a brief overview of the project. It defines the project, describes the organization, proposes schedules and milestones, and defines procedures to ensure the quality of the final product.</p>
Phase 3	<p><b>Software Requirements Specification (SRSp):</b> The SRSp is a description of the external interfaces and essential requirements of the software in terms of functions, performance, constraints, and attributes. Requirements are objective and measurable. The SRSp is concerned with what is required, not how to achieve it. This document is reviewed by project members, users, and management. It is verify that the intent of the SRSp is clear, the software proposed by the SRSp is what is desired, and that the project can proceed to the next development stage.</p> <p><b>Design Description:</b> A Design Description documents the design work accomplished during the design phase. Documenting the design prior to coding avoids (or reduces) any design misunderstandings and subsequent recoding.</p> <p><b>Design Review Results:</b> The results of the Design Review are documented in a report, which identifies all deficiencies discovered during the review along with a plan and schedule for corrective actions. The updated design description document, when placed under configuration control, will establish the baseline for subsequent phases of the software life cycle.</p> <p><b>Maintenance Documentation:</b> Well-documented code and the software design document provide the backbone of maintenance documentation and the starting point for determining training needs.</p> <p><b>Training Plan:</b> The preparation of a well thought out training plan is an essential part of bringing a system into smooth operation. If the people, documents, and training techniques are not considered in the early planning for a new system, resources may not be available and training will be haphazard.</p> <p><b>User's Manual:</b> A user's manual is organized to contain practical information for the individuals required to put the software into action. Depending on the size and type of system, operating procedures may be required as a separate document to cover management of the logical and physical components. Without a properly prepared User's or Operator's Manual, either the time of the user will be wasted determining what to do, or the system will be inappropriately used, or both.</p>
Phase 4	<p><b>Structured Source Code:</b> Implementation is the translation of the detailed design into a computer language; a process commonly called coding.</p> <p><b>Configuration Management Plan:</b> The Configuration Management Plan lists all modules used by the project, module locations, personnel responsible for controlling changes, and change procedures.</p> <p><b>Baseline Table:</b> The Baseline Table lists modules and versions in the project's baselined system.</p> <p><b>Change Table:</b> The Change Table lists all changes and enhancements made to the modules. Additional update supporting documents reflect changes and enhancements made to the system.</p>
Phase 5	<p><b>Test Set:</b> The Test Set includes "rich" test data and relevant test procedures and tools to adequately test the application's response to valid as well as invalid data.</p> <p><b>Test Set Documentation:</b> The Test Set Documentation (or Software Test Plan) describes the test data, procedures, tools, and overall plan.</p>
Phase 6	<p><b>Test Results:</b> The results of the tests are documented to identify outcome of all testing and whether any deficiencies were identified.</p>

## Comparison to Acute Release Measurements

Several prediction-to-measurement comparisons of UFOTRI to field data are contained in the User's Manual. A comparison to a predominantly tritium gas release was performed based on an event occurring at SRS on May 2, 1974.

The release was caused by a valve failure and resulted in a stack release of approximately 49 g from the central area of SRS [Murphy and Wortham, 1997]. The release occurred over a 4-minute period beginning at 0755 hours Eastern Standard Time (EST). The tritium form was estimated to be primarily tritiated hydrogen gas with less than 1% tritiated water. At the time of the release, light winds carried the tritium in a northeasterly direction at 6.4 to 9.7 km/h. Cloud cover recorded nearby in Augusta, GA was 90% - 100%. The atmospheric stability was predominantly neutral. The trajectory of the release carried the tritium north of Columbia, SC, beyond which point it was difficult to predict because of complex weather patterns.

Table 3 compares several environmental measurements of tritium concentrations with quantities calculated by the UFOTRI model. In this case, meteorology at the time of the release is used along with a 80-km grid specific to SRS and surrounding areas. The computer estimates are considerably above ground measurements for most quantities compared, including air, vegetable tritiated water (HTO), surface water, and milk concentrations. From the standpoint of safety analysis, this is preferred to under-predicting measurements. This trend is consistent with measured-to-observed data reported from an intended field release of HT conducted in Canada [Raskob, 1990].

The major factors leading to the over-prediction of tritium concentrations by the UFOTRI model are primarily

- One-hour averaging of meteorology applied to a short-duration release (<five minutes) - UFOTRI interprets changes in weather, including windspeed and wind direction, on an hourly frequency basis. The HT release modeled here occurred over less than five minutes, thus Briggs dispersion puff parameterization can be subject to appreciable error in defining peak maxima when one-hour meteorology periods are averaged.
- Sampling location error – The release was accidental as opposed to a planned experiment. Thus, positioning of instrumentation was not planned beforehand. In effect, the plume was being “chased” and assayed, based on the weather forecasting performed at SRS. It is highly improbable that computer model peaks coincided with recorded data from environmental sampling.
- Spatial uniformity assumed by UFOTRI – While UFOTRI provides concentrations using 5-degree arc resolution, all aspects of the compartment model considering air, soil, vegetation, grass, and consumption by humans and animals, assumes uptake at the peak sectors. In reality, grass, pine tree, crop, and dairy locations are spatially dependent. It is very unlikely that particular sampling locations were in the path of the plume centerline.

While this comparison resulted in satisfactory performance relative to “puff” release conditions, other types of releases will need to be evaluated with UFOTRI. Included are HTO and longer duration “plume” type releases.

Based on the outcome of this modest V and V program, and the demonstrated conservative results relative to comparison to field data, this version of UFOTRI will be placed in configuration control for use in SRS safety analysis. While tritium facilities will continue to be assessed using the general purpose code, MACCS, it is clear that UFOTRI can be applied as a supplemental tool. Additionally, it is a preferred option in cases where simple single-species, inhalation dose only analysis is insufficient, and longer-term food chain assessment models are required.

**Table 3. Comparison of UFOTRI Predictions to 1974 Release from Savannah River Site**

<b>Quantity</b>	<b>Measurement</b>	<b>Calculated Peak (Plume Centerline), Unless otherwise noted</b>	<b>Calculated/ Measured</b>
<b>Average air concentration five hours after release, [pCi/m<sup>3</sup>]</b>	<b>3.9E+05</b>	<b>6.7E+7; 3-sector average</b>	<b>170</b>
<b>Maximum Vegetation HTO, [pCi/ml]</b>	<b>Perimeter: 4630 40 km: 310</b>	<b>Perimeter: 4644 40 km: 1430</b>	<b>Perimeter: 1.0 40 km: 4.6</b>
<b>Peak Surface Water Concentration, [pCi/ml]</b>	<b>10,000</b>	<b>Not computed.</b>	<b>-</b>
<b>Maximum Soil Water Concentration, [pCi/ml]</b>	<b>138</b>	<b>1.647E+04</b>	<b>120</b>
<b>Maximum Milk Concentration, [pCi/ml]</b>	<b>375</b>	<b>1.290E+03</b>	<b>3.4</b>

### Summary and Conclusions

Version 93/4.20P of the UFOTRI code has been verified and validated applying ANSI standard 10.4-1987 in an a posteriori (backfit) manner. The effort was maintained at a low resource commitment level (~ three person-months). The V & V process provides sufficient assurance that UFOTRI can be one of a group of software models that is available for tritium accident analysis for DOE facilities, as part of a toolkit of configuration-controlled models for specific applications.

The major observations and lessons learned through the V & V process for UFOTRI are as follows:

- Overall duration of the six-phase process, including: (1) UFOTRI Status Definition; (2) Remedial Action Plan; (3) Completion of all Remedial Actions; (4) Establishing New Baseline; (5) Development and Review of Formal Test Plan; and (6) Complete Testing and Evaluation phases required 3 person-months.
- These tasks met applicable ANSI software quality assurance documentation requirements, and resulted in an Assessment Document, a Test Plan, a Configuration Procedure, an Error Notification Procedure, a Comprehensive Technical Report, and a SQA Qualification Report.
- Although not as rigorous as a V and V process integrated into software development, the a posteriori process still could be shown to comply favorably with the most critical items from the IEEE software standard.
- Comparison to field data from actual accidental release events show that the UFOTRI model can be exercised in a bounding, conservative manner appropriate for accident analysis applications.

The project described here serves as a useful pilot application in the sense of qualifying “toolkit” computer models. In principle, the compact, targeted activity can be a useful template for other source term and dispersion identifying models in DOE Complex applications, and adding remedial V & V to reach adequate software quality assurance levels. It can be easily extended to other DOE sites.

### Acknowledgment

The UFOTRI V & V process discussed in this paper required extensive input and recommendations from many sources. While the SQA Process team is appreciative of all contributions and suggestions, it is especially indebted to Dr. Wolfgang Raskob of KfK (UFOTRI developer and maintainer) and Mr. Eric Hope of Westinghouse Safety Management Solutions (Software Quality Assurance issues).

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