Selection of a Tritium Dose Model: Defensibility and Reasonableness for DOE Authorization Basis Calculations

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Selection of a Tritium Dose Model: Defensibility and Reasonability for DOE Authorization Basis Calculations (U)

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Introduction

The Savannah River Site (SRS) is a major center in the Department of Energy (DOE) Complex featuring a number of nuclear facilities containing appreciable inventories of tritium. In the facility authorization basis, the safety “case” is developed by examining a number of design and evaluation basis accidents. Accident sequences include postulated upset conditions in tritium processing, storage, transport, and other associated operations. Analysis of these conditions with conservative inputs and assumptions helps ensure that radiological exposures can be precluded or minimized through design, passive and active design features, and administrative controls. Thus, for the final phase of the sequence analysis, the quantification of radiological doses from atmospheric releases under hypothetical accident conditions is a critical part of the overall accident and consequence task.

At SRS, several methodology options exist for the tritium dispersion and consequence calculations for ultimately determining doses in safety analysis. The analysis options span simple spreadsheet-based, Gaussian models to full assessment (acute plume passage and chronic phase) models. The basis for the particular calculation option is developed from an integrated review of the hazard category of the facility, the life-cycle phase of safety documentation, and the receptor range of interest. This paper highlights the logic used to select a dispersion/consequence methodology, describes the collection of tritium models contained in the suite of analysis options (the “tool kit”), and provides application examples.

Methodology Selection

Selection of a consequence methodology for Savannah River tritium facilities is based on analyst understanding and preference. However, two end-point objectives are integrated into the selection process, in that the identified approach must be both defensible for the particular analysis need, and reasonable depending on the constraints of the phase of analysis. Specifically, the analyst must be able to technically defend the method(s) applied for quantification of consequences due to postulated acute release of tritium, implement phenomenological models within the regimes of applicability, and incorporate site/facility data required using conservative values. The method should be reasonable, or commensurate to the facility hazard category, the phase of safety analysis, and the particular receptor group being evaluated, in the manner of graded approach practices.¹
In an application context, the method selection for tritium consequence analysis is illustrated by considering a three-dimensional matrix (Figure 1). The dimensions are a series of factors that although can be addressed in any order, the process for safety application at SRS to address the complete set in entirety as follows:

- The first dimension is **facility hazard categorization**. In application of a dispersion/consequence model for tritium accident analysis, a model should be selected commensurate to the hazard category of the subject facility. In this study, the Category 3 to 2 boundary is used to delineate simple to more complex models. For example, most Category 3 facilities do not warrant complex, detailed source term and dispersion analysis. In most cases, an engineering spreadsheet determination of radiological exposure conditions is sufficient. Conversely, a tritium Category 2 facility should be treated in a manner consistent with a higher hazard category, and the associated consequence analysis may need to implement increased-capability methods.

- A second dimension is **facility life-cycle stage of safety documentation**. For facilities preparing for startup or restart with greater than five years operational lifetime remaining, more effort and enhanced methods are warranted. Similarly, scoping and preliminary hazard analyses should be performed with bounding, conservative assumptions. As events are identified and are propagated into the accident analysis phase leading to the basis for functional classification, there may be a need to examine the safety margins. In some situations, implementation of a more detailed model is justified.

- A final dimension is **source-to-receptor complexity**. The graded approach philosophy that is applied to many phases of DOE facility analysis can be extended to cover environmental and topographic complexity once the atmospheric dispersion and uptake of hazardous material become the focus. In many applications, the source-to-receptor conditions are amenable to simple Gaussian models. In other examples, where collocated buildings or terrain features lead

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\(^a\) A five-year breakpoint can be adjusted depending on the site and facility.
to complex flow patterns, the applications of these same models could result in misleading results.

Suite of Analysis Options

The Savannah River Site safety organization currently applies three computer models in hazard and accident analyses.b The set of models, or includes AXAIRQ, MACCS, and UFOTRI. A short review of each of the three models follows before the selection framework is described.

1. AXAIRQ (Westinghouse Savannah River Company), is a Gaussian model that provides conservative assessment of airborne tritium vapor releases.
   - Savannah River Site-developed AXAIR8Q code for predicting downwind doses following a postulated atmospheric release of short (less than two hours) duration. Page 3
   - Code is compliant with Regulatory Guide 1.145. AXAIR89Q was retired, and replaced by AXAIRQ. Page 3
   - Uses a Gaussian plume model and an Eulerian coordinate system.
   - The code is configured to take advantage of the one-hour time averaged five-year meteorological data bases collected at each of the major facility clusters at SRS.
   - Doses are determined for the inhalation and cloudshine pathways using a joint frequency distribution process.
   - AXAIRQ allows a fixed deposition velocity for non-noble gas radionuclides, and permits selection of dispersion coefficients.

2. MACCS2 (Sandia National Laboratories) is a Gaussian model that uses Latin Hypercube Sampling of site meteorology to provide an additional level of sophistication with user-specified input to deposition and resuspension models, and can assess both acute and long-term phase doses. Page 3
   - MACCS2 is PC-compatible, written in both FORTRAN 77 and 90.
   - Supported at Sandia National Laboratories (SNL) under the sponsorship of DOE as an update of the United States Nuclear Regulatory Commission's (USNRC's) MACCS. Page 3
   - For regulatory applications, MACCS2 calculates the fifty-year Effective Dose Equivalent (EDE) to specified stationary receptors from the plume passage phase of a hypothetical release.
   - Sensitivity studies may also be performed with MACCS2 to show the relative benefits of evacuation, sheltering, interdiction, and the effects of various shielding assumptions.
   - MACCS2 predicts dispersion of radionuclides by the use of multiple, straight-line Gaussian plumes. Although each plume treats the released material as a neutrally buoyant gas, the direction, duration, sensible heat, and initial radionuclide concentration may be varied from plume to plume.
   - Meteorological variability is treated in MACCS2 with a stratified random sampling algorithm. MACCS2 uses Latin Hypercube Sampling (LHS) to process site-specific meteorological data.
   - Complementary cumulative distribution functions (CCDFs) are calculated for various measures of consequence, including individual and population dose, conditional risk, and health effects.

3. UFOTRI (German Karlsruhe Laboratory) is also a Gaussian model similar to MACCS in terms of meteorology sampling, but able to model both vapor and gas species of tritium.
   - UFOTRI (Unfallfolgenmodell für Tritiumfreisetzungen) computer model was developed in Germany at Karlsruhe (Kernforschungszentrum Karlsruhe GmbH, or KfK) to assess tritium alone. Page 3

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b HOTSPOT (Homann, S. G., 1994: HOTSPOT Health Physics Codes for the PC. UCRL-MA-106315 Lawrence Livermore National Laboratory, Livermore, California 94551. 78 pp.) is also used at SRS, but primarily for emergency management action level determination.

c MACCS 1.5.11.1 is applied for purposes of this paper. The description given is applicable to MACCS for tritium modeling.
Describes 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.

Individual and population doses can be calculated with UFOTRI, but not 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).

Source term model accounts for release duration and height, tritium species, and thermal energy.

A segmented Gaussian module treats the initial release of HT/HTO. Reemission is treated up to seven days after the release event. UFOTRI factors in all relevant transfer processes in the environment (atmosphere, soil, plant, and animal). UFOTRI is unique in that the initial plume passage model is integrated with a reemission (area source) model. The reemission model addresses evaporation from soil and transpiration from vegetation.

Atmospheric model is coupled to a first-order compartment module, which describes dynamically the longer-term behavior of the two different chemical forms of tritium in the food chain.

Executes in a deterministic or probabilistic mode, applying either prescribed meteorological conditions or a stratified random sampling algorithm, respectively.

Table 1 compares features of UFOTRI to MACCS2 and other similar Gaussian models. The differences are based primarily on the tritium biophysics models in UFOTRI.

**Tritium Consequence Model Recommendations**

Table 2 is an outline of the preferred modeling options that have been developed for Savannah River tritium consequence analysis. The options are grouped by phase of the analysis and the hazard category for the receptor groups of concern, and take into account the capabilities of AXAIRQ, MACCS, and UFOTRI. Recommendations are made from the standpoint of achieving

<table>
<thead>
<tr>
<th>Phenomenon or Model Feature</th>
<th>UFOTRI</th>
<th>General Purpose Gaussian Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Gaussian release model</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>2. Sensible heat/release duration</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>3. Deposition (wet/dry)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>4. Stratified Random Sampling of Site Meteorology option</td>
<td>Yes (sample size smaller than MACCS)</td>
<td>Yes</td>
</tr>
<tr>
<td>5. Prescribed meteorology option</td>
<td>Yes (Default: European Study-Based Dispersion Parameters)</td>
<td>Yes</td>
</tr>
<tr>
<td>6. HTO – HT differentiation</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>7. Reemission from Soil/Vegetation</td>
<td>Detailed reemission physics model</td>
<td>Resuspension model</td>
</tr>
<tr>
<td>8. Tritium conversion from HT to HTO</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>9. Uptake of HTO by Vegetation</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>10. Conversion of HTO into OBT</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>11. 1st Order Compartment Model for Long-term Behavior in Food Chain</td>
<td>Yes, for HT and HTO</td>
<td>Yes in some codes, but usually applicable to Sr, Cs, etc., occasionally HTO</td>
</tr>
</tbody>
</table>
Table 2. Analysis Options for Tritium Modeling of Airborne Releases

<table>
<thead>
<tr>
<th>Analysis Phase</th>
<th>AXAIRQ</th>
<th>AXAIRQ</th>
<th>MACCS2</th>
<th>MACCS2</th>
<th>UFOTRI</th>
<th>UFOTRI</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Scoping/Preliminary</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hazard Analysis</td>
<td>Onsite</td>
<td>Offsite</td>
<td>Onsite</td>
<td>Offsite</td>
<td>Onsite</td>
<td>Offsite</td>
</tr>
<tr>
<td>2. Category 2 or greater</td>
<td>NR (Note)</td>
<td>NR</td>
<td>Yes</td>
<td>Yes</td>
<td>NR</td>
<td>NR</td>
</tr>
<tr>
<td>2. Category 3 or less</td>
<td>Yes</td>
<td>Yes</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
<td>NR</td>
</tr>
</tbody>
</table>

| Accident Analysis/               |        |        |        |        |        |        |
| Functional                      |        |        |        |        |        |        |
| Classification                   |        |        |        |        |        |        |
| 2. Category 2 or greater        | NR | NR | CR | Yes | Yes | Yes |
| 2. Category 3 or less           | Yes | Yes | Yes | Yes | NR | Yes |

Note: NR = Computer Model can be used but it is Not Recommended for this application.
CR = Conditionally Recommended; acceptable under some conditions.

Conservative results, while maintaining defensibility in terms of model selected and reasonableness for the particular intent of analysis. For scoping and preliminary hazard assessment purposes, the MACCS2 computer code provides sufficient analytical capability for Category 2 facilities, for both receptor types. For Category 3 facilities at the same stage of analysis, AXAIRQ is satisfactory. At the accident analysis and functional classification phase of Category 2 safety analysis, MACCS2 is adequate for most offsite calculations, but the preference is for UFOTRI for both onsite and offsite calculations. Although there is no strong guidance for Category 3 facility accident analysis for offsite receptor doses, AXAIRQ and MACCS2 are recommended for onsite dose determinations.

Application of Selection Methodology

Prescriptive Meteorology

An initial comparison of the three models can be made using a simple test scenario and prescribed, persistent meteorology. The scenario is a one-hour stack release of 1000 Ci of tritium oxide, under three sets of stability/windspeed conditions. No building wake effects are assumed and receptors are located at 100m, 640m, and 8 km (MOI).

Table 3 compares the code estimates for three receptor locations and the three persistent weather sets. The dose estimates show lower dose estimates from MACCS (Version 1.5.11.1) for all meteorological conditions for exposure to the close-in 100m receptor. UFOTRI (Version 4.02) doses are lower than MACCS estimates at both the 640m and MOI receptor distances, the latter by 27% - 68% for B/3.5, D/4.5, and F/1.0, respectively. An alternative representation of the differences is portrayed as the three-dimensional bar graph in Figure 2. For each receptor distance, the two model dose estimates are compared for each stability category and windspeed combination. Dose differences are due primarily to the dispersion parameters applied, and secondarily to differences in the surface roughness length. Since AXAIRQ is not configured to calculate prescribed meteorology doses, it was possible to report only the median and 95th doses obtained from the Joint Frequency Distribution sampling of SRS meteorology. For this elevated
release case, the AXAIRQ-obtained median and 95th percentile doses are approximately the same as the prescribed D/4.5 (at 640m) and F/1.0 (at MOI) doses using MACCS.

Table 3. Comparison of AXAIRQ, MACCS, and UFOTRI results for a 1000 Ci HTO release using persistent meteorology.

<table>
<thead>
<tr>
<th>Computer Model</th>
<th>Stability/Wind Speed; or Percentile Consequence</th>
<th>Dose to Receptor @ 100 m (rem)</th>
<th>Dose to Receptor @ 640 m (rem)</th>
<th>Dose to Receptor @ MOI (8 km) (rem)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AXAIRQ</td>
<td>50th</td>
<td>7.7E-17</td>
<td>2.0E-04</td>
<td>3.8E-05</td>
</tr>
<tr>
<td></td>
<td>95th</td>
<td>8.8E-04</td>
<td>4.8E-04</td>
<td>1.2E-04</td>
</tr>
<tr>
<td>MACCS2</td>
<td>B/3.5</td>
<td>5.1E-09</td>
<td>1.4E-04</td>
<td>2.2E-06</td>
</tr>
<tr>
<td></td>
<td>D/4.5</td>
<td>3.8E-09</td>
<td>2.1E-04</td>
<td>1.1E-05</td>
</tr>
<tr>
<td></td>
<td>F/1.0</td>
<td>3.6E-08</td>
<td>8.7E-05</td>
<td>1.8E-04</td>
</tr>
<tr>
<td>UFOTRI</td>
<td>B/3.5</td>
<td>3.5E-05</td>
<td>7.7E-05</td>
<td>1.6E-6</td>
</tr>
<tr>
<td></td>
<td>D/4.5</td>
<td>7.1E-08</td>
<td>1.3E-04</td>
<td>4.2E-6</td>
</tr>
<tr>
<td></td>
<td>F/1.0</td>
<td>0</td>
<td>3.9E-06</td>
<td>5.7E-5</td>
</tr>
</tbody>
</table>

Site-Specific Meteorology

An illustrative application of the selection methodology can provide additional insight into the relative capabilities of the tritium consequence models. This example considers a revision to the authorization basis documentation for Category 2 tritium facilities at the Savannah River Site. To support this analysis, the SRS meteorology is sampled rather than prescriptive meteorology, and SRS source to receptor distances are used relative to the facility location (Figure 3). Table 2 indicates that for Category 2 facilities and the offsite MOI, MACCS is the appropriate model for hazard analysis phase of work while both MACCS and UFOTRI could support accident analysis phase. In the accident analysis phase, the application of UFOTRI could be useful to verify and refine the MACCS-calculated dose values before finalizing functional classification decisions.

During PHA and initial accident analyses of SRS facilities, it is customary to calculate dose per activity released, and then scale the resultant doses by the calculated source term. Table 4 shows the calculated MOI dose per unit activity for an unfiltered, ground-level release, for periods of 3 to 60 minutes, inclusive. The AXAIRQ results (Column 4.a) are obtained from a two-hour release using one-hour meteorological sampling from the calculated JFD of SRS meteorology. The MACCS dose values (Column 4.b) also apply Pasquill-Gifford dispersion parameters and use the LHS mode of sampling, but the largest source of the factor of four reduction is from crediting dry deposition. Column 4.c results from UFOTRI indicate approximately 40% reduction relative to MACCS. UFOTRI has a wind-shift model allows changes in hourly wind
Figure 2. Comparison of MACCS and UFOTRI dose estimates at three receptor distances and prescriptive meteorology sets.

Figure 3. SRS map indicating reservation boundary and MOI distance.
Table 4. Comparison of Computer Model Calculations for Unit HTO Activity Release (1 Ci)

<table>
<thead>
<tr>
<th>Computer Model</th>
<th>a. AXAIRQ P-G$^1$</th>
<th>b. MACCS P-G</th>
<th>c. UFOTRI P-G</th>
<th>d. UFOTRI $&gt;$-1m K-J$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release Duration (min.)</td>
<td>95th Percentile Dose to MOI (rem/Ci)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>4.8E-08</td>
<td>2.8E-08</td>
<td>-</td>
</tr>
<tr>
<td>10</td>
<td>-</td>
<td>-</td>
<td>2.2E-08</td>
<td>-</td>
</tr>
<tr>
<td>20</td>
<td>-</td>
<td>3.1E-08</td>
<td>1.9E-08</td>
<td>-</td>
</tr>
<tr>
<td>40</td>
<td>-</td>
<td>2.8E-08</td>
<td>1.7E-08</td>
<td>-</td>
</tr>
<tr>
<td>60</td>
<td>1.0E-07</td>
<td>2.4E-08</td>
<td>1.5E-08</td>
<td>1.2E-08</td>
</tr>
</tbody>
</table>

1. Pasquill-Gifford
2. Karlsruhe-Julich parameters for surface roughness length $\rightarrow 1$ m

direction to be credited. The MACCS algorithm for maximum centerline dose transports the plume in the same direction throughout travel to the MOI distance. A fourth result (4.d) is from UFOTRI and a one-hour averaging time, using the wind-shift option and Karlsruhe-Julich dispersion parameters. Application of the longer time scale Karlsruhe-Julich dispersion parameters increases vertical dispersion, since the air concentration is proportional to $1/\sigma_z$. The larger roughness length is appropriate for SRS environmental characteristics based on evergreen coverage of greater than 50%. Both MACCS and UFOTRI consider a seven-day acute exposure period. In the case of UFOTRI, plume passage contributes 85% - 95% of the overall dose in probabilistic sampling of SRS meteorology. The fraction of dose from re-emit tritium is a function of the specific stability/windspeed condition and source-receptor distance, and in general, the dispersion parameter set applied.

Application to Accident Analysis

Once final accident sequences are defined by the accident analysis team including specification of release duration, height of release, sensible energy released, and tritium release quantities, the consequence estimates may be updated. Typically, material-at-risk inventories and release periods are adjusted, and other aspects of the accident sequence description are given one additional review. Additional systems, structures, and components may also be credited, so the functional classification process may also be reaching a decision-making stage.

To illustrate several insights gained at this point in the analysis, a fire release accident sequence is considered involving several rooms of one of the tritium facilities. It is assumed that all tritium released is the oxide species (100% oxidation) and that the release is at ground level. Applying MACCS and UFOTRI for single-release periods ranging from twenty minutes to one hour indicate the following:

- **Conservative/best-estimate doses** - The MACCS-based, 95th percentile, direction-independent dose to the MOI receptor is 0.90 rem (20 minutes). This dose is conservative relative to the environmental model applied. The 95th percentile dose, developed using more realistic modeling of the SRS release environment with UFOTRI, at the same consequence level is 0.55 rem (20 minutes).
- **Plume duration and meander influence** – Assuming the same amount of tritium oxide is released, but over a sixty-minute period, the new MACCS and UFOTRI doses are 0.70 rem
and 0.44 rem, respectively. The crosswind distribution of the tritium air concentration at the 11.85 km MOI distance is more likely to broaden as the release duration increases.

- **Sensible heat input** – At the MOI distance, any sensible heat partitioned into convective energy from the fire does not appreciably change the dose versus no sensible heat. As can be demonstrated with either MACCS or UFOTRI, this factor is important at closer distances (e.g. within several kilometers).

- **Reemission dose** – UFOTRI indicates that the fraction of dose from re-emitted tritium increases with distance from the source, and ranges from ~0% at ~100m to over 15% at the MOI distance for the SRS environment.

The input files for the models discussed here use SRS-specific input. Thus, it would be inappropriate to scale any of the dose estimates presented to other sites. Key sources of difference include source-receptor distances, terrain, and vegetation characteristics.

### CONCLUSIONS

A selection framework has been established for selection and application of tritium dispersion and consequence computer models for accident analysis at the Savannah River Site, that is translatable to other sites and facilities. The framework is based on objectives of defensibility and reasonability, and has dimensions of hazard category, lifecycle stage of safety documentation, and complexity of the source-receptor environment. The resulting selection criteria establish MACCS as the most broadly applicable model in hazard analysis applications for Category 2 facilities. Either UFOTRI or MACCS may be applied to the accident analysis phase. Several sets of analysis types are used to illustrate the applications of the selection framework to “generic” and site-specific conditions. In the case of a Category 2 tritium facility situated on a large DOE site with significant forested areas, the selection logic identifies MACCS as the most appropriate computer model for scoping and hazard analysis. Although UFOTRI provides a more realistic alternative for later-phase accident analysis, MACCS can be also be applied particularly for far-field offsite calculations (greater than several kilometers distance).

UFOTRI dose estimates for the SRS MOI receptor relative to hypothetical tritium releases are less than fifty percent of that predicted by MACCS. This is due principally to the more realistic UFOTRI model, which can accommodate wind-shift after the initial plume segment is released, while MACCS transports the plume in the initial direction throughout transport. Secondly, UFOTRI incorporates dispersion parameter sets that are more appropriate to the surface scale lengths representative of the heavily forested Savannah River Site. Predicted one-hour release doses to the MOI are 2.4E-08 rem/Ci for MACCS, 1.5E-08 rem/Ci (Pasquill-Gifford dispersion set) and 1.2E-08 rem/Ci (Karlsruhe-Julich dispersion set) for UFOTRI. Results are based on SRS characteristics omitting farmland, grassland and do not include food pathways. Results obtained here are not scaleable to other DOE Complex sites since distances, terrain, and land use characteristics vary widely.

### Acknowledgments

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