

SANDIA REPORT

SAND2023-10896

Printed October 2023

**Sandia
National
Laboratories**

Comparison of Tritium Dose Calculations from MACCS, UFOTRI, and ETMOD

Kyle A. Clavier
Mariah L. Smith

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

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology & Engineering Solutions of Sandia, LLC.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@osti.gov
Online ordering: <http://www.osti.gov/scitech>

Available to the public from

U.S. Department of Commerce
National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.gov
Online order: <https://classic.ntis.gov/help/order-methods/>



ABSTRACT

Tritium exhibits unique environmental behavior because of its potential interactions with water and organic substances. Modeling the environmental consequences of tritium releases can be relatively complex and thus an evaluation of MACCS is needed to understand what updates, if any, are needed in MACCS to account for the behavior of tritium. We examine documented tritium releases and previous benchmarking assessments to perform a model intercomparison between MACCS and state-of-practice tritium-specific codes UFOTRI and ETMOD to quantify the difference between MACCS and state of practice models for assessing tritium consequences. Additionally, information to assist an analyst in judging whether a postulated tritium release is likely to lead to significant doses is provided.

ACKNOWLEDGEMENTS

The authors would like to thank the members of the larger MACCS team for their contributions to this effort, these contributors include Dan Clayton and John Fulton. The authors are deeply appreciative of the support from Wolfgang Raskob (UFOTRI/KfK) particularly for time spent addressing questions with the code as well as Sohan Chouhan and Luke Lebel, both of Canadian Nuclear Laboratories, for administrative and technical assistance with ETMOD. The authors would also like to acknowledge the technical contributions and input from the US Nuclear Regulatory Commission, including Keith Compton and Salman Haq. This research was funded by the US Nuclear Regulatory Commission under agreement number 31310020F0032.

CONTENTS

Abstract.....	3
Acknowledgements	4
Acronyms and Terms	8
1. Motivation and Scope.....	9
2. Introduction	11
2.1. Tritium Overview	11
2.2. Documented Tritium Releases	13
2.3. Hypothetical Dose Assessments for Postulated Releases	15
2.3.1. Major Findings of the Model Defensibility and Reasonability Study [8].....	17
2.3.2. Major Findings of the APAC Radiological Dispersion/Consequence Working Group Report [16].....	17
2.3.3. Long-Term Environmental Tritium Processes Assessments.....	18
2.3.4. Summary.....	20
3. Tritium Model Overview	21
3.1. UFOTRI.....	21
3.2. ETMOD.....	21
4. Establishing a Baseline Scenario	23
5. Baseline Scenario Results	25
6. Sensitivity Analyses	27
6.1. Chemical Speciation	27
6.2. Release Height.....	30
6.3. Receptor Distance.....	30
6.4. Nighttime Release	32
6.5. Extreme Summer Release.....	33
7. Unit Dose-Distance Relationships	35
8. Conclusions and Recommendations	37
References	39
Distribution.....	41

LIST OF FIGURES

Figure 2-1. Key processes of tritium behavior in the environment. From UFOTRI Model Description [7].....	12
Figure 5-1. Baseline scenario modeling results at 500 m for a 1 hour, 5000 Ci release of HTO.....	25
Figure 6-1. Inhalation dose chemical speciation comparison at 500 m	28
Figure 6-2. Receptor distance sensitivity comparison.....	31
Figure 7-1. Normalized unit dose-distance plot for total inhalation in UFOTRI	35
Figure 7-2. Normalized unit dose-distance plot for total ingestion in UFOTRI.....	36

LIST OF TABLES

Table 2-1. Tritium process descriptions in MACCS	12
Table 2-2. Overview of documented tritium releases described in [10].....	14

Table 2-3. Overview of tritium model benchmarking assessments available in open literature	
[8][16]	16
Table 4-1. Baseline scenario assumptions	23
Table 4-2. Additional scenario input assumptions	23
Table 5-1. Tabular baseline scenario modeling results.....	25
Table 5-2. Baseline scenario ingestion modeling results at 500 m for a 1 hour, 5000 Ci release of	
HTO.....	26
Table 6-1. Tabular chemical speciation comparison results.....	28
Table 6-2. Ingestion dose chemical speciation comparison at 500 m	29
Table 6-3. Release height sensitivity inhalation dose comparison at 500 m.....	30
Table 6-4. Release height sensitivity ingestion dose comparison at 500 m	30
Table 6-5. Tabular receptor distance sensitivity total inhalation dose comparison for a 100%	
HTO release.....	31
Table 6-6. Tabular receptor distance sensitivity total inhalation dose comparison for a 100% HT	
release.....	31
Table 6-7. Nighttime release sensitivity inhalation dose comparison at 500 m	32
Table 6-8. Nighttime release sensitivity ingestion dose comparison at 500 m.....	33
Table 6-9. Extreme summer release sensitivity inhalation dose comparison at 500 m	33
Table 6-10. Extreme summer release sensitivity ingestion dose comparison at 500 m.....	34

This page left blank

ACRONYMS AND TERMS

Acronym/Term	Definition
CANDU	Canadian Deuterium Uranium
CEDE	Committed Effective Dose Equivalent
CTEM	Canadian Terrestrial Ecosystem Model
DOE	Department of Energy
ETMOD	Environmental Tritium Model
HT	Gaseous Tritium
HTO	Tritiated Water or Oxidized Tritium
IAEA	International Atomic Energy Agency
IH	Direct Inhalation
IHR	Inhalation Resuspension/Reemission
LOCA	Loss-of-Coolant Accident
MODARIA	Modelling and Data for Radiological Impact Assessments
Non-LWR	Non-Light Water Reactor
NRC	US Nuclear Regulatory Commission
OBT	Organically-Bound Tritium
SAR	Safety Analysis Report
SRS	Savannah River Site
STC	Special Tritium Compound

1. MOTIVATION AND SCOPE

The US Nuclear Regulatory Commission's (NRC) Non-Light Water Reactor (non-LWR) Vision and Strategy Volume 3 report [1] identifies a need to understand whether updates to the MACCS model are needed to account for the unique environmental behavior of tritium. In contrast to many radionuclides typically included in severe accident consequence analysis, tritium can be released in different chemical forms with significantly different dose coefficients. It is also highly mobile in the environment and can undergo transformations that change its chemical form. Preliminary efforts have identified that tritium may be important for certain non-LWR reactor types [2] and that MACCS is fundamentally capable of handling tritium consequence calculations but may benefit from updates to improve the fidelity of calculations involving tritium [3]. These largely qualitative efforts highlight a need to understand the quantitative differences in tritium consequence calculations across state of practice models so that specific areas where calculations using MACCS may differ from state of practice tritium consequence models can be addressed. Further, it is currently unclear whether risk-significant quantities of tritium could be released in a hypothetical severe accident for a non-LWR. Information to assist an analyst in judging whether a postulated tritium release is likely to be risk-significant can help in determining when higher-fidelity tritium models are needed.

Given that MACCS does not have dedicated tritium modeling capabilities, severe accident research applications can be informed by a model intercomparison exercise. Accordingly, this report examines MACCS as it relates to UFOTRI and ETMOD, two state of practice tritium models. A benchmarking study is conducted assuming a standard scenario, with several sensitivity analyses geared towards understanding the most impactful modeling parameters for estimating consequences of tritium releases.

This page left blank

2. INTRODUCTION

Section 2 provides a tritium overview, as well as discusses documented cases of tritium releases to the environment and previously conducted benchmarking assessments available in the open literature. Although routine tritium releases are well-documented in the literature, the focus of this study is on the short-term release characteristics of potential accident scenarios. A more detailed review of tritium environmental fate and transport processes may be found in CNSC (2009) [4], and a detailed review of tritium dosimetry and health effects may be found in CNSC (2010) [5].

2.1. Tritium Overview

Small amounts of the tritium isotope are produced naturally in the environment from sunlight interactions, as well as anthropogenically from nuclear weapons testing and the routine operation of nuclear facilities. An isotope of hydrogen, tritium has a half-life of approximately 12.3 years and behaves similarly to hydrogen in the environment as it is incorporated into water, soil, and biota. The similarity of tritium to the abundant and mobile non-radioactive isotope of hydrogen results in phenomena of tritium transport and transformation in the environment that make accurate quantification of acute tritium release consequences challenging. Accurately accounting for the chemical form of tritium in the environment is of special importance for tritium consequence calculations. Inhaling gaseous tritium (typically in the form of HT) is associated with fairly low radiological risk when compared to inhaling oxidized tritium (in the form of HTO), which has orders of magnitude higher dose coefficients for inhalation. For example, Federal Guidance Report 13 mortality and morbidity risk coefficients for inhalation are 10,000 times higher for HTO than for HT [6]. Tritium is otherwise a weak external exposure hazard (low-energy beta emitter).

Tritium's ability to interact with natural processes such as the water cycle, carbon cycle, and natural soil oxidation processes present unique challenges for dose quantification. As shown in Figure 2-1, the environmental transport and transformation processes impacting tritium dose estimations are numerous. These processes are summarized in Table 2-1, along with the existing capabilities in MACCS to address these processes. A comprehensive tritium model would therefore need to account for the processes documented in Table 2-1. A review of MACCS capabilities to represent each process is also provided in the table. This table was adapted from Table 1 in [8].

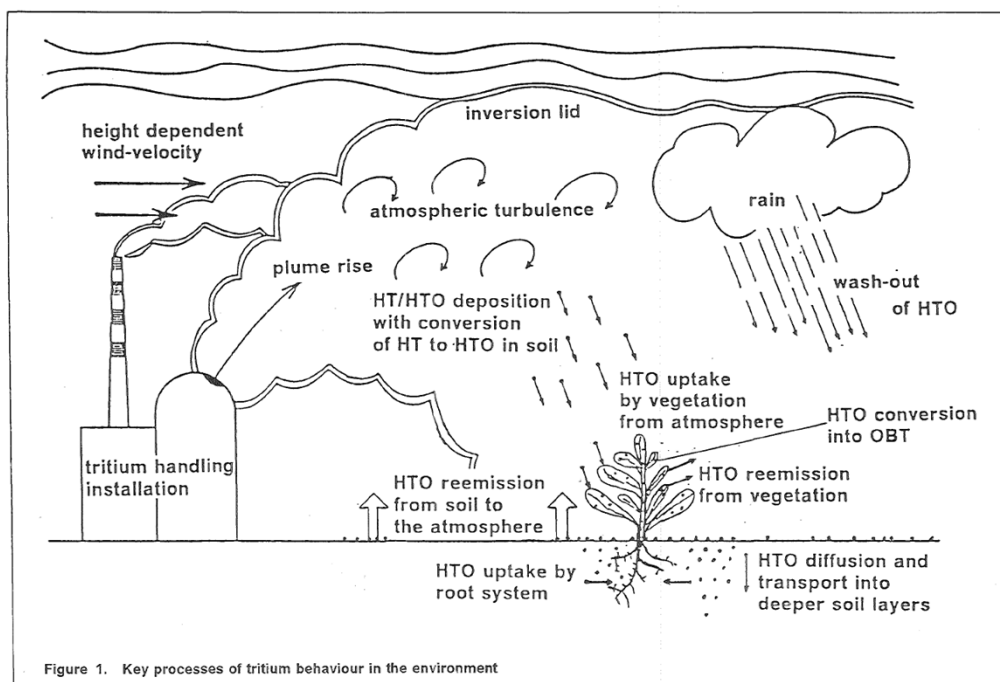


Figure 2-1. Key processes of tritium behavior in the environment. From UFOTRI Model Description [7]

Table 2-1. Tritium process descriptions in MACCS

Process	Description	Capabilities in MACCS
Atmospheric transport and dispersion	Tritium undergoes atmospheric dispersion processes using dispersion properties consistent with other types of contaminants. This process depends on plume characteristics and meteorology	MACCS contains Gaussian dispersion modeling capabilities suitable for tritium transport
Dry/wet deposition	Normal dry/wet deposition processes	MACCS contains accounting for dry/wet deposition processes
Atmosphere to plant	Tritium transfer from atmosphere to plant that is dependent on time of day, humidity, plant resistance, etc.	No detailed accounting other than dry/wet deposition (plume depletion)
Atmosphere to soil	Tritium diffusion from plume to soil, governed by soil humidity and concentration gradients	No detailed accounting other than dry/wet deposition (plume depletion)

Process	Description	Capabilities in MACCS
Soil to plant	Uptake of tritiated water by vegetation	No accounting for soil-plant uptake
Reemission	Tritium re-emitted to the atmosphere from plants and soil in evaporation (soil) and transpiration (plant) processes	No dedicated reemission physics model. May be approximated using existing MACCS short- and long-term resuspension models
Soil oxidation of HT to HTO	Oxidation by soil microbes	No accounting for soil oxidation. MACCS assumes one chemical form.
Atmospheric conversion of HT to HTO	Isotopic exchange in the atmosphere, slow process	No accounting for atmospheric conversion. MACCS assumes one chemical form.
Organically bound tritium	The conversion of tritium to organically bound tritium from plant/animal uptake and participation in biological processes (e.g., photosynthesis)	No accounting for organically bound tritium. MACCS assumes one chemical form

Source: adapted from Table 1 in [8]

2.2. Documented Tritium Releases

Insights into the potential consequences of tritium released to the atmosphere may be obtained by examining actual releases. Although tritium is released during routine emissions from nuclear facilities (e.g., Reference [9] documents yearly HTO emissions from CANDU reactors across Canada), the focus of this analysis — which is oriented towards evaluation of consequences of tritium releases arising from potential severe accidents — is on acute releases occurring over time periods ranging from minutes to hours.

Data on acute atmospheric tritium releases were compiled by Murphy Jr. and Wortham (1991) [10] to create a database of tritium concentrations found in the air, vegetation and soil surrounding the Savannah River Site after nine different inadvertent atmospheric releases. A dose of 1.6 mrem was noted as the largest potential off-site dose from any of the releases, and a population dose estimated to be near background. The atmospheric releases at the Savannah River site originated from a 60-meter-high stack with varying compositions of gaseous tritium (HT) and tritiated water (HTO). An overview of the documented releases and associated atmospheric conditions is provided in Table 2-2. The highest documented total activity released over the period of this study was 479,000 Ci of 99% gaseous tritium (Release 1). The largest tritiated water vapor activity released was approximately 168,000 Ci from Release 9 (97.8% of 172,000 Ci). This

corresponds to approximately 50 grams and 17.4 grams of tritium for Release 1 and Release 9, respectively.

Table 2-2. Overview of documented tritium releases described in [10]

Release	Source	Activity	Chemical Composition	Wind	Cloud Cover	Consequence Assessment?	Environmental Model?
1	SRS, tritium production facility, accidental release	479,000 Ci released over 4-min period	Composition approximately 99% tritium gas, 1% tritiated water	6.4-9.7 km/hr. winds	90-100%	[16]	[10]
2	SRS, tritium production facility, accidental release	182,000 Ci released with 90% released over approximately 1.5 minutes	Composition approximately 99.4% tritium gas, 0.6% tritiated water	35 km/hr	30%	No	[10]
3	SRS, tritium production facility, accidental release	33,000 Ci released over 2.5 hours	Composition approximately 99.7% tritiated water	18-26 km/hr	Sunny, Scattered	No	[10]
4	SRS, tritium production facility, accidental release	56,000 Ci released over approximately 3 minutes	Composition approximately 99% tritium gas, 1% tritium water	18 km/hr	75-100%	No	[10]
5	SRS, tritium production facility, accidental release	7,500 Ci released over approximately 2 hours 20 minutes	Composition approximately 70% HTO, 30% HT	21 km/hr	10%	No	[10]
6	SRS, tritium production facility, accidental release	57,900 Ci released over 5 days with the majority released in the first 5 hours	99% HTO	16 km/hr	Unspecified	No	[10]
7	SRS, tritium production facility, accidental release	9,285 Ci released over approximately 3 hours	54% HTO, 46% HT	21 km/hr	100%	No	[10]

Release	Source	Activity	Chemical Composition	Wind	Cloud Cover	Consequence Assessment?	Environmental Model?
8	SRS, tritium production facility, accidental release	19,422 Ci released over approximately 4.5 hours	99.9% HTO	16-23 km/hr	70%	No	[10]
9	SRS, tritium production facility, accidental release	172,000 Ci released over approximately 38 minutes	97.8% HTO	8 km/hr	Unspecified	No	[10]

For reference, the total combined inventory of tritium in the Fukushima Units 1, 2 and 3 immediately after the accident was approximately 92,000 Ci [11]. Thus, the largest documented release from SRS (approximately 500,000 Ci) is substantially larger than the total inventory from a large boiling water reactor. In contrast, the tritium inventory for a typical production reactor (at 3,000 MWth) was determined to be 70 MCi [12]. Nonetheless, in an accident scenario, it is assumed only a fraction of the total inventory would be released atmospherically. As for advanced reactor tritium inventories, they are the subject of ongoing research. For example, due to their use of lithium and beryllium salts, tritium production and transport in molten-salt reactors is being heavily investigated [13] and relying in part on information obtained from the Molten Salt Reactor Experiment [14].

2.3. Hypothetical Dose Assessments for Postulated Releases

Insights into the potential consequences of tritium released to the atmosphere may also be obtained by examining hypothetical dose assessments conducted for postulated releases, either as part of a larger consequence assessment or as a result of model benchmarking exercises.

O’Kula et al. (1991) [15] investigated the airborne release consequences of two hypothetical reactor accidents occurring at a Department of Energy (DOE) production reactor, namely, a loss-of-moderator pumping accident and loss-of-coolant accident (LOCA). In this study, tritium inventory is assumed to transport identically to noble gases and is assumed to be all tritiated water vapor. A value of 2.6E18 Bq (70 MCi) was used as the source term for a tritium only release, representing an upper bound corresponding to the entire tritium inventory in a production reactor (consistent with the information described in Section 2.2 above). The expected dose was calculated as 6.9E5 person-rem (6.9E3 person-Sv), and when compared to the site’s full-scale probabilistic risk assessment, which considered additional fission products released other than tritium, the calculated dose from tritium above represented only 7% of the total dose from a full fission product release due to full core melt [15].

Table 2-3 summarizes several model comparison efforts available in the open literature that include assessments of tritium models. The two benchmarking analyses from which Table 2-3 was developed [8][16] were undertaken as parts of efforts to assist in selecting radiological consequence computer models for use in DOE safety analyses. Blanchard et al. (1998) [8] documents a framework for selecting and applying a tritium dispersion and consequence model for accident

analysis that is both defensible and reasonable. The second study provides the “evaluations, recommendations, and insights developed by ... the Radiological Dispersion/Consequence Working Group” of the DOE Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program [16]. Table 2-3 includes only models that are generally accessible, portable, and accompanied by significant documentation, and does not include proprietary and/or research models that are not easily accessible.

Additional benchmarking assessments for tritium were identified that are largely focused on comparison and accurate quantification of longer-term environmental processes for tritium. These include a 1999 intercomparison study for model predictions of tritium concentrations in soil and food following acute airborne HTO exposure [17] and a 2022 International Atomic Energy Agency (IAEA) harmonization and intercomparison study for accidental tritium releases [18]. These two studies are not summarized in Table 2-3 because the scenarios modeled in these two studies do not lend themselves to use in a model intercomparison study including MACCS, in part because MACCS lacks a tritium-specific soil and food model. However, they are discussed here because they provide insights on potential sensitivity analyses to explore in this comparison exercise.

Table 2-3. Overview of tritium model benchmarking assessments available in open literature [8][16]

Event	Activity	Release Height	Release Duration	Other Assumptions	Models*	Comparison
HTO release	1000 Ci	Stack height	Unspecified	B/3.5, D/4.5, F/1.0	UFOTRI, MACCS	Doses to receptors at 100m, 640 m, 8 km
HTO fire release scenario	1000 Ci	Ground level	20 min-1 hour	Unspecified	MACCS, UFOTRI	Doses vs. distance and comparison to environmental model
HTO Release, Low Energy Source Term	1.0E3 Ci of HTO	60 m	1 hour	Ambient outdoor temperature of 303K	ETMOD, Hotspot, MACCS, RSAC, UFOTRI	Dose to receptor at various distances
Mixed HTO/HT Release, Medium-Energy Source Term	2.04E4 Ci of 50/50 HT/HTO	20 m	2 hours	4 MW sensible heat	UFOTRI, ETMOD, MACCS	Dose to receptor at various distances
Environmental Model	479, 000 Ci of 99/1 HT/HTO	60 m	4 minutes	6.4-9.7 km/h winds, 90-100% cloud cover, neutral stability	UFOTRI compared to field measurements	Dose to receptor at various distances

*models not listed include proprietary and/or research models not easily accessible.

2.3.1. Major Findings of the Model Defensibility and Reasonability Study [8]

Blanchard et al. examined UFOTRI (Version 4.02), MACCS (Version 1.5.11.1) and AXAIRQ models [8]. All three are Gaussian models, with UFOTRI additionally having the ability to model both vapor and gaseous tritium species. UFOTRI contains a more detailed biophysics model for tritium. In this model intercomparison, a scenario was developed that included a 1,000 Ci HTO release with three stability classes and windspeed pairings (B/3.5, D/4.5, F/1.0). Zero building wake was assumed and receptors at 100 m, 640 m, and 8 km were chosen. AXAIRQ was only able to report median and 95th percentile doses.

Results indicate that MACCS dose estimates for the closest receptor (100 m) were lower than other models for all meteorological conditions. However, UFOTRI estimates were lower than MACCS at 640 m and 8 km by up to 68% for the stable atmospheric condition. AXAIRQ predictions for the 95th percentile and median were approximately equal to the D/4.5 at 640 m and the F/1.0 dose at 8 km.

Researchers also used sampled Savannah River Site meteorology and representative receptor distances to the site boundary (11.85 km). Analysts calculated a per-unit-activity ground level release for periods of 3 to 60 minutes. For all release durations, MACCS calculated concentrations at the receptor were larger than those predicted by UFOTRI. Analysts note that the UFOTRI wind-shift capability resulted in lower concentrations, while the maximum centerline dose estimation assumes plume travel in the same direction. Plume passage contributed approximately 85-95% of the dose in the UFOTRI model.

Finally, a fire release sequence was analyzed, assuming all tritium is oxidized and released at ground level. MACCS and UFOTRI estimates for a release time ranging from 20 minutes to 1 hour indicate that MACCS estimates are conservative compared to UFOTRI. Doses were lower for a 60-minute release duration, and no significant differences in dose were found when incorporating sensible heat input (at 11.85 km). Reemission doses from tritium are larger with distance, ranging from 0 to 15% of the dose as receptors move from 100 m to 11.85 km.

2.3.2. Major Findings of the APAC Radiological Dispersion/Consequence Working Group Report [16]

O’Kula et al. [16] examined three different types of tritium release events: an HTO release with low energy, a mixed HTO/HT release with medium energy, and an environmental model response for a release from the Savannah River Site in 1974 composed of HT and HTO. While 15 models were examined, MACCS and GENII were noted as the codes most applicable to Safety Analysis Report (SAR) analyses for most accident classes and environmental conditions. ETMOD and UFOTRI were selected specifically for tritium modelling capabilities. The working group prepared a summary of the major characteristics used for bounding, deterministic analyses and best-estimate probabilistic analyses standard practices as noted in NRC Regulatory Guide 1.145, DOE Order 6430.1A, DOE Order 420.1, and DOE-STD-3009-94. Standard practice requires a Gaussian plume or puff model, with receptor distances of 30 m, 100 m, and site boundary, topography that accounts for region of transport, prescriptive meteorology of stability class D with 4.5 m/s windspeed for onsite meteorological conditions and stability class F and low windspeed (1-1.5 m/s) for offsite meteorological conditions or the median and 95th percentile for statistical sampling of onsite and offsite meteorology, respectively. Endpoint consequences are to be calculated as the plume centerline for a 2-hour exposure with a 50-year dose commitment period.

In the low energy HTO release scenario, dose to receptor at all distances were largely within an order of magnitude for all models (AI-RISK, ARAC, AXAIRQ, ETMOD, HOTSPOT, MACCS, RSAC and UFOTRI). AXAIRQ yielded the largest dose estimations. MACCS dose estimations were approximately half those estimated by AXAIRQ, noted as being the difference between horizontal and vertical dispersion models [16]. Doses calculated by UFOTRI exceeded those calculated by MACCS at 100 m for the B/3.5 and D/4.5 scenarios but were lower (0 rem) than MACCS (3.6E-8 rem) for the F/1.0 scenario. UFOTRI estimated lower doses than MACCS at both 640 m and 8 km distances. ETMOD dose calculations tracked fairly closely with MACCS but were lower for the F/1.0 scenario at all distances (ETMOD reported doses of ~0 rem for all distances).

In the mixed HTO/HT medium energy scenario, AXAIRQ calculations were again bounding, notably because of the lack of sensible heat model and the assumption that all tritium is tritiated water vapor. UFOTRI was the only model used that analyzes HT and HTO differently and was found to be the third most conservative of the models using prescribed meteorology (AI-RISK and GXQ being the most). UFOTRI dose estimations were multiple orders of magnitude higher than MACCS at all distances. ETMOD dose calculations were also multiple orders of magnitude higher than MACCS at all distances, approximately equal to UFOTRI at 100 m and 8 km, and approximately 1 order of magnitude higher than UFOTRI at 640 m.

In the environmental model scenario, only UFOTRI was used to compare to actual field measurements. Estimates from UFOTRI were higher than those measured above ground for air, vegetation, OBT, soil, and milk. When comparing calculated values in UFOTRI to measured values:

- Committed Effective Dose Equivalent (CEDE) doses at the plume centerline were 1.4 times higher,
- maximum air concentrations were approximately 3 orders of magnitude higher,
- maximum HTO and OBT concentrations in vegetation were 3.1 to 6.9 times higher,
- HTO concentrations in soil were 11.2 times higher, and
- HTO in milk was 4.9 to 36 times higher.

The analysts noted that the UFOTRI model overpredictions may be due to a number of factors including the one hour averaging time for meteorology for a very short release duration, sampling location error, dated and inaccurate documentation, and spatial heterogeneity of environmental receptors (i.e., not in the exact plume centerline).

Overall, the working group recommended a Gaussian model that accounts for variable chemical forms of tritium (or conservatively assumes all HTO) and long-term area sources of tritium. UFOTRI was the recommended model for tritium source terms, with HOTSPOT and MACCS also recommended. The analysts noted that nearly all models are capable of handling a simple inhalation dose estimation and the major differences for tritium related models are related to environmental compartment modeling for longer term transport and transformation processes.

2.3.3. Long-Term Environmental Tritium Processes Assessments

Several benchmarking assessments for tritium were identified that largely focused on comparison and accurate quantification of longer-term environmental processes for tritium, as the atmospheric transport and dispersion processes for tritium are not specific to tritium behavior [17].

Only the related processes of deposition and reemission may be expected to have some differences. For example, tritium models may use a simple deposition velocity calculation, a net flux proportional to the vapor pressure gradient between atmosphere and soil water, or net deposition modeled as a fractional rate of loss from the total amount of tritium present in the atmosphere. Instead, these longer-term environmental process model intercomparison studies focused on transport of tritium from the atmosphere into soil, vegetation and animals and the subsequent transformation of HT to HTO and organically-bound tritium (OBT) throughout. Given that the atmospheric transport processes are largely independent of tritium, substantial differences are likely to manifest in the way these processes are accounted for.

Barry et al. conducted an intercomparison study for model predictions of tritium concentrations in soil and food following acute airborne HTO exposure [17] that investigated eight tritium models including UFOTRI and UFOTRI/A, TRITRAJ, TRILOCOMO, ETMOD, TRIMOVIS, TRICAROM and TRINIRBU. Many of these models are research tools, rather than publicly available, well-documented and portable models. Two hypothetical atmospheric releases of HTO were developed for dry weather HTO releases over agricultural land 30 days before harvest. Releases were investigated for both day and night (i.e., 10 am and 12 am), with one-hour exposures of 10^4 MBq/m³ (~ 270 mCi/m³) and a given sequence of historical weather data and assumed soil properties. This study found that the most significant differences involved tritium accounting across models for the nighttime release scenarios, suggesting that the uptake by plants and the transformation of HTO to OBT by non-photosynthetic processes is dominating [17]. All models predicted higher tritium concentrations in food after a day-time release. The authors of this study note that while the processes that should be modeled are fairly well known, the method by which they are modeled is somewhat unclear.

In 2022, the International Atomic Energy Agency (IAEA) Modelling and Data for Radiological Impact Assessments (MODARIA) Program published a harmonization and intercomparison study for accidental tritium releases [18]. This study focused largely on various exchange processes for the soil-plant-atmosphere system. The model intercomparison portion focused on four models: TOCATT (France), CERES (France), SOLVEG-II (Japan), and CTEM-CLASS-TT (Canada), with both a model-measurement comparison as well as a model-model comparison. A number of realistic model scenarios were developed with the goal of experimental measurements used to generate model inputs and compare with model outputs. Key findings indicate that:

- HTO exchange at the plant-atmosphere interface is highly dependent on the stomatal resistance, implying that precise calculation of daytime versus nighttime resistance is important.
- Long term OBT concentrations are largely dependent on tissue free water tritium concentrations in plants, the impact of plant respiration on OBT formation is minor.
- Gaseous diffusion of HTO in soil has a negligible impact on behavior of HTO deposited in soil and the HTO concentration profile coupled with the root density and plant water content governs soil to plant HTO transfers.
- Translocation of exchangeable OBT and formation of non-exchangeable OBT are necessary for proper estimates of OBT behavior in leaves affect by HTO deposition.

The modeling capabilities of three of the four models evaluated in Reference [18] are largely independent of the atmospheric transport and dispersion of tritium. Specifically, the Canadian

Terrestrial Ecosystem Model (CTEM) is developed for modeling the flow of carbon through terrestrial ecosystem, SOLVEG-II was developed to research material transport in vegetated ecosystems and TOCATTA was developed for tritium and carbon-14 transfer in grassland ecosystems. Conversely, CERES was developed for atmospheric dispersion modelling and impact assessment of hazardous materials (i.e., preparedness and response) and contains a variety of dispersion calculations. CERES also has a dedicated tritium Gaussian puff model that accounts for deposition, reemission, conversion of HT to HTO and conversion of HTO to OBT.

2.3.4. Summary

Review of previous tritium dose assessments and model intercomparison exercises suggests that MACCS can perform well when computing inhalation doses compared to tritium specific codes when using standard input assumptions. This comparison study therefore relies on these assessments completed previously to inform appropriate tritium specific models to choose from as well as appropriate modeling assumptions when defining a baseline scenario. Additionally, the intercomparison studies relative to long-term environmental processes of tritium described in Section 2.3.3 helps provide insight on useful sensitivity analyses to explore in this comparison exercise. For example, these studies highlight the influence of nighttime vs. daytime releases on long-term reemission of HTO from plants.

3. TRITIUM MODEL OVERVIEW

Many of the models identified in the literature are research models not accessible in the public domain for general users or are not maintained. Based on review of previous analyses, two tritium-specific state-of-practice models were chosen for comparison against MACCS tritium modeling capabilities [19]. UFOTRI and ETMOD were chosen for this study based on:

- specific application to tritium,
- relative portability and accessibility (including documentation), and
- previous mention in regulatory documentation or the scientific literature.

A brief description of each code is provided here; additional information can be found in UFOTRI and ETMOD supporting documentation [7][21][22].

3.1. UFOTRI

UFOTRI was developed as a high-fidelity model for tritium behavior after a nuclear accident release to account for processes such as “conversion of tritium gas into HTO in the soil, re-emission after deposition and the conversion of HTO into organically bound tritium” [7]. UFOTRI is equipped with an atmospheric dispersion model similar to MACCS that describes the dispersion, deposition, and reemission processes. An additional first order compartment model describes the dynamic behavior of tritium as it moves through food chains. UFOTRI differentiates between HT and HTO, and considers relevant transfer processes between soil, plants, and animals. The simple MACCS resuspension model differs from the model used in UFOTRI regarding reemission physics. UFOTRI contains a detailed reemission physics model that accounts for reemission from soil and plants through evaporation and transpiration, respectively, using an area source model. The tritium-specific first order food chain compartment model is substantially more detailed than MACCS and includes mathematical and physical bases for plant and atmosphere exchange, soil and atmosphere exchange and transport, the formation of exchangeable and non-exchangeable tritium. The most substantial differences between UFOTRI and MACCS is the ability to model multiple chemical forms of tritium as well as the ability to account for tritium transport and transformation in the environment.

3.2. ETMOD

The Environmental Tritium Model (ETMOD) is a Canadian code designed to simulate HT and HTO transport in the atmosphere, deposition, conversion in the soil, plant uptake of HTO, reemission and subsequent dispersion, and subsequent dose [21][22]. ETMOD requires information on terrain, soil, meteorology, dosimetry, and the specific scenario of interest. ETMOD is capable of outputting tritium concentrations in soil, air, and vegetation and a wide range of related outputs (e.g., flux, time average concentrations).

This page left blank

4. ESTABLISHING A BASELINE SCENARIO

A baseline modeling scenario was developed based upon review of the existing literature and previously documented tritium releases. The baseline scenario is summarized in the following table.

Table 4-1. Baseline scenario assumptions

Activity (Ci)	Chemical Form	Release Duration	Weather	Mixing Layer Height	Wind	Stability	Release Height
5,000	HTO	1-hr	Constant, No Rain	1000 m	3 m/s	D	0 m

The upper limit for accidental tritium releases documented in the open literature is approximately 500,000 Ci release of 99% HT/1% HTO release from the Savannah River Site (See Section 2.2). This event was also included in the model evaluation exercise provided in [16]. Given that MACCS dose coefficients are consistent with tritium in the HTO form, the 1% HTO fraction of that release was selected as the benchmark scenario. The authors of this study acknowledge that a large release of HT might contribute significantly to the dose due to soil conversion and reemission of HTO from deposited HT and this is further investigated in Section 4 as part of the sensitivity analysis. The assumption made for this baseline scenario was solely due to the available dose coefficients within MACCS. Simplifying assumptions regarding release duration and meteorology were made. These simplifying assumptions are different than the meteorological conditions during the actual event but were made to allow examination of, for example, a ground-level release vs. an elevated release.

This same baseline scenario was modeled in MACCS, UFOTRI, and ETMOD. Given the unique capabilities of the tritium-specific models (and the lack of equivalent model in MACCS), additional simplifying assumptions were necessary for other environmental parameters (e.g., soil/plant properties). Wherever relevant, default values were used for each of the models. Major assumptions are summarized in Table 4-2 below.

Table 4-2. Additional scenario input assumptions

Parameter	MACCS	UFOTRI	ETMOD
Inhalation Dose Coefficients	HTO: 1.839E-11 Sv/Bq	HTO: 1.7E-11 Sv/Bq* HT: 1.7E-15 Sv/Bq *Later adjusted by 50% to account for skin absorption	HTO: 2.00E-11 Sv/Bq HT: 2.4E-15 Sv/Bq HTO skin absorption factor: 2
Air Temperature	N/A	Constant, 30°C	Constant, 30°C
Solar Radiation	N/A	Constant, 600 W/m ²	Constant, 600 W/m ²

Parameter	MACCS	UFOTRI	ETMOD
Building Dimensions	40m x 40m x 40m	40m x 40m x 40m	40m x 40m x 40m
Wake Effects	Included	Included	Included
Surface Roughness	0.03 m	Low plants, rural area, Z < 10 cm to 1 m	0.03 m
Dry Deposition Velocity	0.003 m/s	0.0005 for HT-gas 0.005 for HTO-vapor Resistance model flag selected	Unspecified (defaults were used)
Resuspension/Reemission Parameters	Default short- and long- term resuspension factors from [24]	Default values from [25] Minimal duration of reemission process: 70 hours	Unspecified (defaults were used)
Breathing Rate	2.66E-04 m ³ /s	2.66E-04 m ³ /s	2.66E-04 m ³ /s
Ingestion Model Parameters (plant parameters, soil parameters, animal parameters, product consumption rates, etc.)	N/A	Numerous, refer to [25]	Numerous, refer to [23]

5. BASELINE SCENARIO RESULTS

Results from the modeled baseline scenario for the dose at 500 m from the source are presented in Figure 5-1 and Table 5-1. For each scenario, the dose to individuals over a 7-day period and 1-year period is calculated. In MACCS, this corresponds to the short-term exposure period (EARLY phase duration) and the long-term exposure period respectively. The short-term exposure dose is further broken down into contributions due to direct inhalation and inhalation resuspension or reemission for MACCS and UFOTRI (ETMOD outputs do not differentiate between inhalation doses from the plume and from reemission). One major difference worth noting is MACCS models the dose due to resuspension inhalation using a simple resuspension factor that is independent of the radionuclide released, while UFOTRI and ETMOD estimate the dose due to reemission of HTO from the soil and plants.

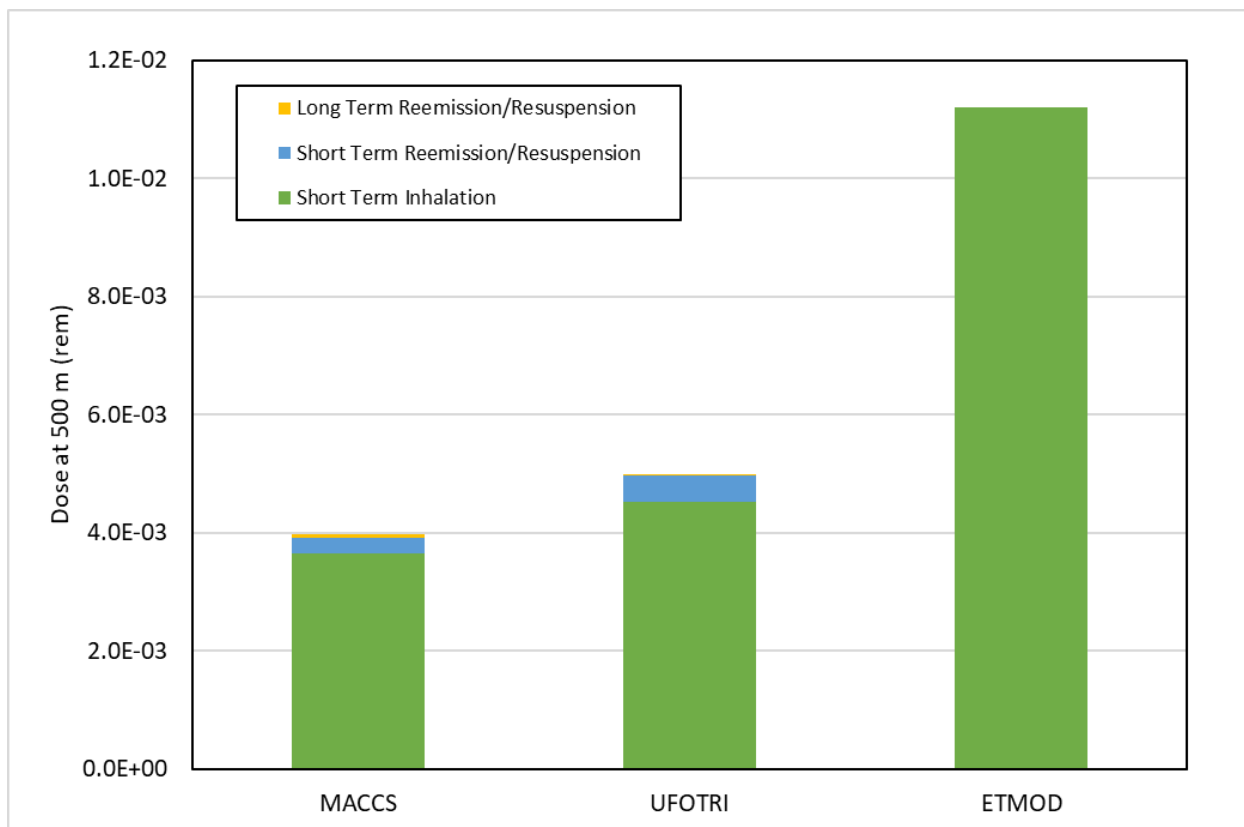


Figure 5-1. Baseline scenario modeling results at 500 m for a 1 hour, 5000 Ci release of HTO

Table 5-1. Tabular baseline scenario modeling results

Model	Short Term Inhalation	Short Term Reemission/Resuspension	Long Term Reemission/Resuspension
MACCS	3.65E-03 rem	2.74E-04 rem	6.24E-05 rem
UFOTRI	4.51E-03 rem	4.46E-04 rem	8.12E-07 rem
ETMOD	1.12E-02 rem	--	0 rem

Total inhalation dose results at 500 m are broadly similar across the models. MACCS is shown to have more agreement with UFTORI than ETMOD likely due to atmospheric transport and dispersion capabilities that are largely equivalent. For MACCS and UFOTRI, the dominant dose contribution is attributable to the inhalation during plume passage while reemission or resuspension appears to be a very small component of the total dose. Nonetheless, it is assumed that differences in the results are likely at least partly due to the following reasons:

- Each code has different default dose conversion factors for HTO and HT, as shown in Table 4-2 which has some influence on the results. Additionally, MACCS is believed to not correct for skin absorption.
- Difference in atmospheric transport and dispersion modeling capabilities/processes and their associated inputs/assumptions between the three codes.
- The use of inhalation resuspension dose in MACCS versus inhalation reemission dose in UFOTRI and ETMOD. However, when using the default resuspension factors in MACCS, the dose due to inhalation resuspension (for both short term and long-term exposure) is comparable to the inhalation dose due to reemission of HTO in UFOTRI. Since ETMOD does not delineate between inhalation dose and inhalation reemission dose exposure, it cannot be said whether this is true for ETMOD as well.

The COMIDA2 food-chain model used in MACCS is not designed to model doses from tritium releases. For that (and other) reasons, MACCS is not capable of modeling ingestion doses from tritium. However, baseline ingestion doses in UFOTRI and ETMOD were determined after a 1-year exposure period. As can be seen in Table 5-2 below, the two codes agree well with one another.

Table 5-2. Baseline scenario ingestion modeling results at 500 m for a 1 hour, 5000 Ci release of HTO

Model	Ingestion Dose
MACCS	N/A
UFOTRI	5.53E-02 rem
ETMOD	9.11E-02 rem

6. SENSITIVITY ANALYSES

Sensitivity analyses were also conducted for the influence of various parameters on modelling outputs. For this analysis, a release of 1,000 Ci was assumed for all scenarios with the remaining input assumptions being identical to those discussed in Section 4. From a model review, the most meaningful differences in output (aside from food chain contributions) might be expected from:

- The chemical speciation of tritium – HT versus HTO
- Release height – ground-level release versus an elevated release
- Receptor distance – the dose at distances closer than 500 m as well as distances farther than 500 m
- Nighttime releases - whereby plant and soil absorption and reemission may have less of an impact and thus may be more dominated by the atmospheric transport processes (which are largely the same in each model)
- Extreme summer releases – whereby extreme temperatures and solar radiation may heighten or impact plant absorption and reemission depending on if the environmental conditions are too far outside the optimal range for photosynthesis and evapotranspiration processes.

Although MACCS is currently not capable of modeling ingestion doses as described in Section 5, these sensitivity analyses described below still compare the effect these parameters have on the ingestion doses for UFOTRI and ETMOD.

6.1. Chemical Speciation

Many factors may influence the chemical form (and at which proportions) tritium will take in the environment; postulated chemical forms released into the environment include HTO and HT. This demonstration simulates different release ratios of HTO and HT sources to the environment to assess the effect of chemical speciation on modeling outputs. Currently, MACCS contains the appropriate dose coefficient information for HTO releases but not HT. In order to model releases of HTO and HT together, Kr-85 was used as a surrogate radionuclide to incorporate HT specific dose coefficients (it was assumed other factors such as half-life and lack of radioactive progeny were comparable between Kr-85 and HT). The MACCS DCF file was altered so that dose coefficients for Kr-85 were consistent with HT and then H-3 and Kr-85 were defined in MACCS as part of separate chemical groups in order to vary the release fractions between the two to represent mixtures of HTO and HT in one simulation. Specific radionuclide properties of HT (such as deposition velocity) were taken from the default inputs used in UFOTRI (see Section 4).

As can be seen in Figure 6-1 and Table 6-1 below, as the percentage of HT released compared to HTO increases, the total inhalation dose decreases. For all three models, it can be seen that there is a substantial drop as the release changes from 25% HTO/ 75% HT to 100% HT released which suggests that the doses may not decrease linearly. However, further investigation of additional mixed release scenarios (i.e. 10%, 1%, 0.1% HTO releases) is needed to confirm this. Nonetheless, for releases including some percentage of HTO, MACCS remains in alignment with the results produced by UFOTRI and ETMOD and the direct inhalation dose remains the largest contributor.

However, during a 100% HT release scenario it is shown in UFOTRI that the majority of the total inhalation dose is due to short term reemission due to the conversion of HT to HTO while MACCS reports the main dose contributor is still direct inhalation with a very small component being due to resuspension. As for long-term inhalation resuspension or reemission doses, the contribution to total inhalation dose estimations continues to be very minimal. The results suggest that when MACCS is modified to use an inhalation dose coefficient consistent with HT, MACCS is under approximating the dose given the codes current inability to model the conversion of HT to HTO and the subsequent reemission from the soil and plants. Alternatively, if the 100% HT release were to be treated as HTO in MACCS as shown by the first bar on the left (MACCS 100% HTO), MACCS can be considered the most conservative estimate between the three models for total inhalation dose.

Given the results seen here, all additional sensitivity analyses described below assess both a 100% HTO release scenario and a 100% HT release scenario.

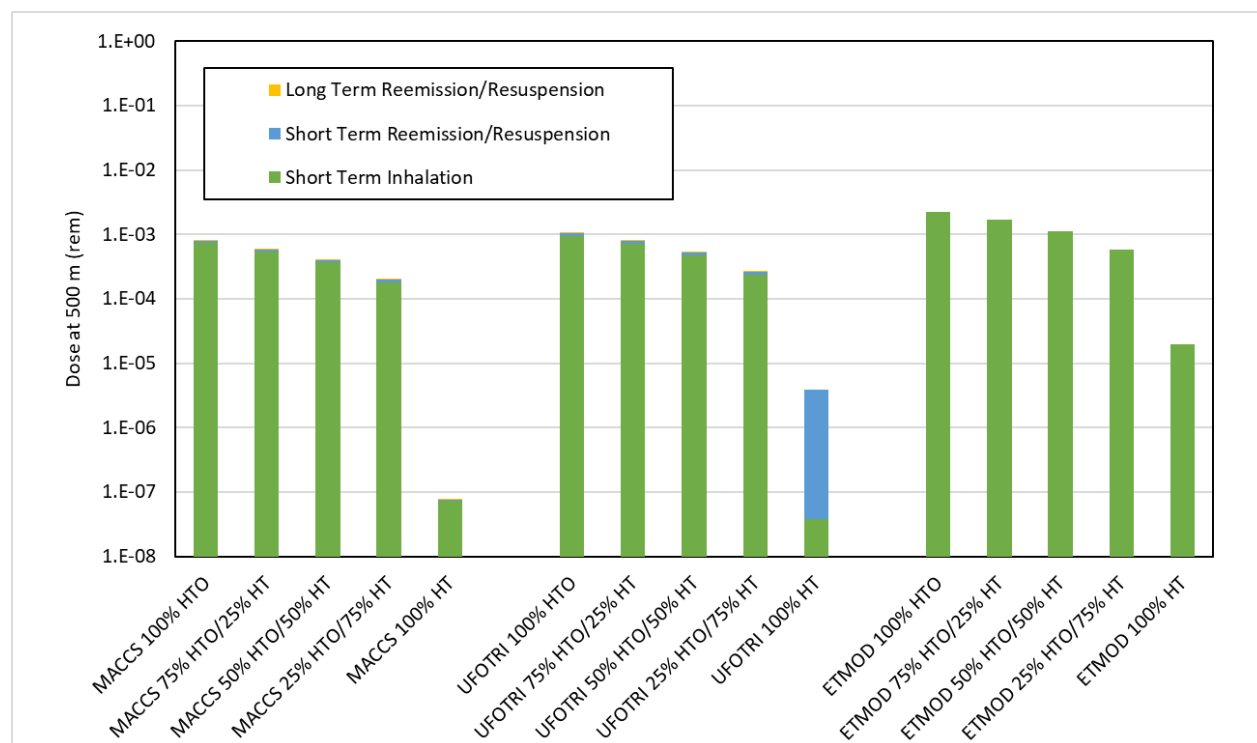


Figure 6-1. Inhalation dose chemical speciation comparison at 500 m

Table 6-1. Tabular chemical speciation comparison results

Model	Short Term Inhalation	Short Term Reemission/Resuspension	Long Term Reemission/Resuspension
MACCS			
100% HTO	7.28E-04 rem	5.48E-05 rem	1.31E-05 rem
75% HTO / 25% HT	5.46E-04 rem	4.11E-05 rem	9.36E-06 rem

Model	Short Term Inhalation	Short Term Reemission/Resuspension	Long Term Reemission/Resuspension
50% HTO / 50% HT	3.65E-04 rem	2.74E-05 rem	6.24E-06 rem
25% HTO / 75% HT	1.82E-04 rem	1.37E-05 rem	3.12E-06 rem
100% HT	7.40E-08 rem	7.47E-10 rem	2.10E-10 rem
UFOTRI			
100% HTO	9.46E-04 rem	9.36E-05 rem	9.88E-07 rem
75% HTO / 25% HT	7.12E-04 rem	7.04E-05 rem	2.09E-07 rem
50% HTO / 50% HT	4.75E-04 rem	4.70E-05 rem	1.42E-07 rem
25% HTO / 75% HT	2.37E-04 rem	2.63E-05 rem	2.66E-08 rem
100% HT	3.84E-08 rem	3.80E-06 rem	0 rem
ETMOD			
100% HTO	2.24E-03 rem	--	0 rem
75% HTO / 25% HT	1.68E-03 rem	--	0 rem
50% HTO / 50% HT	1.13E-03 rem	--	0 rem
25% HTO / 75% HT	5.73E-04 rem	--	0 rem
100% HT	2.00E-05 rem	--	0 rem

For reference, the effect of chemical speciation on ingestion dose in UFTORI and ETMOD is reported in Table 6-2 as well. It is observed that ingestion dose also appears to decrease as the percentage of HT release increases.

Table 6-2. Ingestion dose chemical speciation comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
100% HTO	N/A	1.11E-02 rem	1.83E-02 rem
75% HTO 25% HT	N/A	8.34E-03 rem	1.43E-02 rem
50% HTO 50% HT	N/A	5.61E-03 rem	1.04E-02 rem
25% HTO 75% HT	N/A	2.88E-03 rem	6.48E-03 rem
100% HT	N/A	2.33E-04 rem	2.57E-03 rem

6.2. Release Height

Since the baseline scenario and sensitivity analysis completed in Section 6.1 models a ground-level release, this sensitivity explores how an elevated release (60 m) influences the modeling outputs for each code. Table 6-3 and Table 6-4 below display the comparison between the three codes with the percentage decrease from the results shown in Section 6.1 displayed in red. For the short-term dose results, IH refers to dose due to direct inhalation and IHR refers to the dose due to inhalation resuspension or remission depending on the code. Across the three models there was approximately a 25-96% decrease across the various results due to an elevated release height demonstrating that plume downwash/trapping modeling has similar impact for each model just at different magnitudes. MACCS remains to be under approximating the dose when using dose coefficients consistent with HT. However, treating HT as HTO in MACCS produces significantly conservative estimates.

Table 6-3. Release height sensitivity inhalation dose comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
Short Term Dose (7 days) @ 500 m			
100% HTO	2.25E-04 rem (71%) 93% IH 7% IHR	7.75E-04 rem (25%) 92% IH 8% IHR	2.91E-04 rem (87%)
100% HT	2.13E-08 rem (71%) 99% IH 1% IHR	2.71E-06 rem (29%) 1% IH 99% IHR	7.77E-07 rem (96%)
Long Term Inhalation Reemission/Resuspension Dose (1 year) @ 500 m			
100% HTO	3.76E-06 rem (71%)	1.95E-07 rem (80%)	0 rem
100% HT	5.98E-11 rem (72%)	0 rem	0 rem

Table 6-4. Release height sensitivity ingestion dose comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
100% HTO	N/A	8.23E-03 rem (26%)	2.33E-03 rem (87%)
100% HT	N/A	1.71E-04 rem (27%)	3.18E-04 rem (88%)

6.3. Receptor Distance

Figure 6-2 below displays the total inhalation dose (short-term and long-term exposure) for each code as a function of distance during a 100% HTO release and a 100% HT release. For this analysis, additional distances of 100 m, 250 m, 1 km, 4 km, 8 km, and 16 km were chosen as representative distances to explore. The total inhalation dose results as a function of distance are broadly similar across the three models during a HTO releases but there is a considerable amount of deviation for HT releases. As discussed previously, this is due to MACCS producing substantially lower inhalation doses when modified to use a dose coefficient consistent with HT. Treating HT as HTO in MACCS produces significantly conservative estimates compared to UFTORI and ETMOD

for all distances. For reference, Table 6-5 and Table 6-6, displays the total inhalation doses at each distance assessed as well.

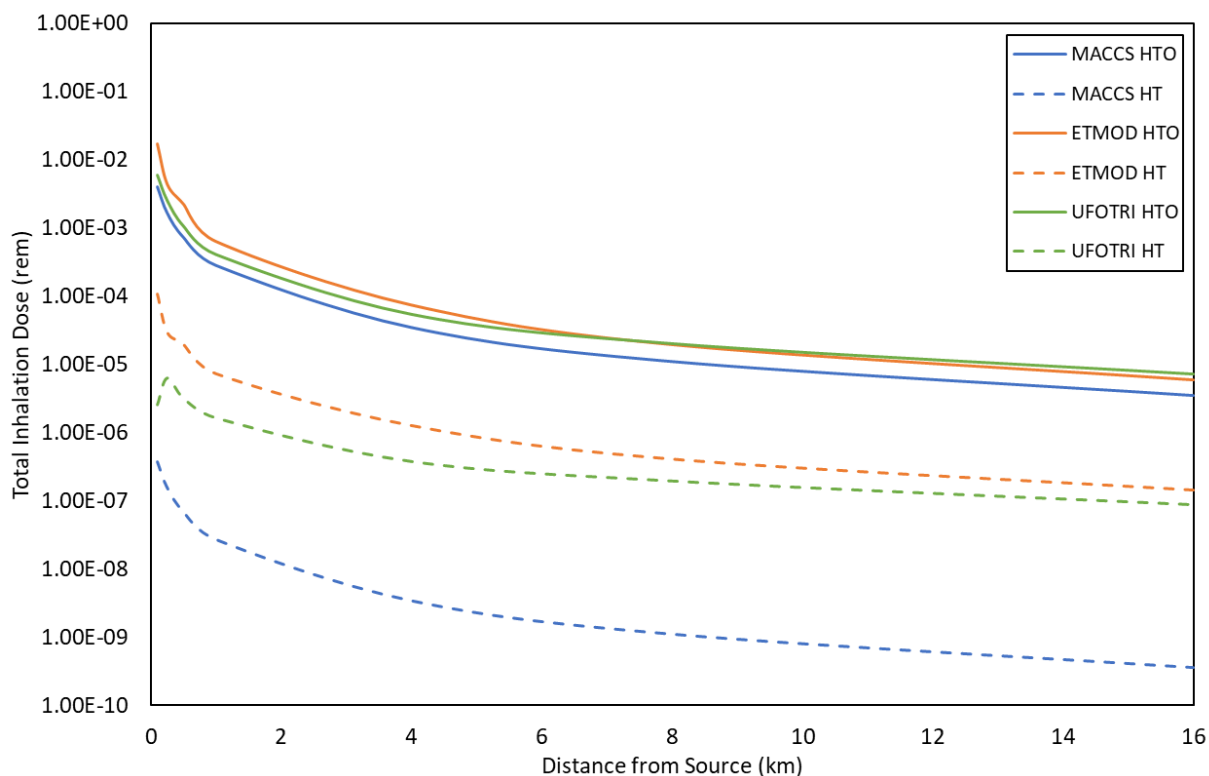


Figure 6-2. Receptor distance sensitivity comparison

Table 6-5. Tabular receptor distance sensitivity total inhalation dose comparison for a 100% HTO release

Distance	MACCS	UFOTRI	ETMOD
100 m	3.95E-03 rem	6.00E-03 rem	1.70E-02 rem
250 m	1.64E-03 rem	2.56E-03 rem	4.42E-03 rem
1000 m	2.81E-04 rem	4.09E-04 rem	6.36E-04 rem
4000 m	3.49E-05 rem	5.42E-05 rem	7.48E-05 rem
8000 m	1.11E-05 rem	2.01E-05 rem	1.97E-05 rem
16000 m	3.54E-06 rem	7.18E-06 rem	6.00E-06 rem

Table 6-6. Tabular receptor distance sensitivity total inhalation dose comparison for a 100% HT release

Distance	MACCS	UFOTRI	ETMOD
100 m	3.68E-07 rem	2.58E-06 rem	1.09E-04 rem

Distance	MACCS	UFOTRI	ETMOD
250 m	1.54E-07 rem	6.38E-06 rem	3.01E-05 rem
1000 m	2.67E-08 rem	1.65E-06 rem	7.41E-06 rem
4000 m	3.39E-09 rem	3.78E-07 rem	1.29E-06 rem
8000 m	1.10E-09 rem	1.95E-07 rem	4.16E-07 rem
16000 m	3.56E-10 rem	8.73E-08 rem	1.46E-07 rem

6.4. Nighttime Release

To simulate a nighttime release in UFOTRI and ETMOD, a temperature of 15°C and a solar radiation of 0 W/m² was specified. Table 6-7 and Table 6-8 below show the comparison between the three codes with the percentage difference from the results shown in Section 6.1 displayed in either red or green depending on if the results increased or decreased from the original estimation. MACCS does not require temperature and solar radiation as inputs, so the results reported by MACCS are identical to those in Section 6.1.

For the nighttime release the majority of the results for UFOTRI and ETMOD decrease which consequently brings them slightly closer to the results reported by MACCS. However, in UFOTRI, when considering a 100% HT release, the ingestion dose and long-term reemission dose is seen to increase. This could suggest the uptake by plants during respiration at night results in more HTO re-emitted as well as more HTO converted into OBT. MACCS remains to be under approximating the short-term inhalation dose when using dose coefficients consistent with HT. However, treating HT as HTO in MACCS produces significantly conservative estimates.

Table 6-7. Nighttime release sensitivity inhalation dose comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
Short Term Dose (7 days) @ 500 m			
100% HTO	7.83E-04 rem 93% IH 7% IHR	1.00E-03 rem (4%) 96.5% IH 3.5% IHR	2.15E-03 rem (4%)
100% HT	7.47E-08 rem 99% IH 1% IHR	1.65E-06 rem (57%) 2% IH 98% IHR	1.22E-05 rem (39%)
Long Term Inhalation Reemission/Resuspension Dose (1 year) @ 500 m			
100% HTO	1.31E-05 rem	1.68E-06 rem (70%)	0 rem
100% HT	2.10E-10 rem	0 rem	0 rem

Table 6-8. Nighttime release sensitivity ingestion dose comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
100% HTO	N/A	5.94E-03 rem (46%)	2.03E-03 rem (89%)
100% HT	N/A	2.94E-04 rem (26%)	5.18E-05 rem (98%)

6.5. Extreme Summer Release

To simulate a release during extreme summer weather, a temperature of 38°C and a 1,000 W/m² solar radiation was used to be representative of very hot conditions. Table 6-9 and Table 6-10 below show the comparison between the three codes with the percentage difference from the results shown in Section 6.1 displayed in either red or green depending on if the results increased or decreased from the original estimation. MACCS, again, does not require temperature and solar radiation as inputs, so the results reported by MACCS are identical to those in Section 6.1.

During an extreme summer release, the results for the 100% HTO release for UFOTRI and ETMOD decrease which consequently brings them slightly closer to the results reported by MACCS. However, when considering a 100% HT release, the short-term inhalation dose in UFOTRI increases and the ingestion dose in ETMOD increases. The difference between UFOTRI and ETMOD is likely due to their respective plant modeling methods and the default plant parameters and optimal temperatures specified. However, these results suggest that during extreme summer conditions, HTO reemission and the transformation of HTO to OBT is impacted either positively or negatively depending on the code. Focusing on the 100% HT short-term doses reported by UFOTRI specifically, during extreme summer conditions, the short-term inhalation dose further deviates from those reported by MACCS. However, as stated previously, treating HT as HTO in MACCS produces significantly conservative estimates.

Table 6-9. Extreme summer release sensitivity inhalation dose comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
Short Term Dose (7 days) @ 500 m			
100% HTO	7.83E-04 rem 93% IH 7% IHR	1.02E-03 rem (2%) 94% IH 6% IHR	2.19E-03 rem (2%)
100% HT	7.47E-08 rem 99% IH 1% IHR	4.72E-06 rem (23%) 1% IH 99% IHR	1.93E-05 rem (4%)
Long Term Inhalation Reemission/Resuspension Dose (1 year) @ 500 m			
100% HTO	1.31E-05 rem	3.62E-07 rem (63%)	0 rem
100% HT	2.10E-10 rem	0 rem	0 rem

Table 6-10. Extreme summer release sensitivity ingestion dose comparison at 500 m

Chemical Speciation	MACCS	UFOTRI	ETMOD
100% HTO	N/A	5.57E-03 rem (50%)	1.10E-02 rem (40%)
100% HT	N/A	2.01E-04 rem (14%)	3.65E-03 rem (42%)

7. UNIT DOSE-DISTANCE RELATIONSHIPS

The previous benchmarking exercises suggested that MACCS (with its default tritium dose coefficient and its default resuspension parameters) may, for some release and exposure scenarios, be capable of generating results that are comparable to tritium-specific codes such as UFOTRI and ETMOD (for inhalation doses from HTO releases) or bounding (for inhalation doses from HT releases). Given the fact that many accident scenarios may result in the release of only small amounts of tritium, the decision to use MACCS or a tritium specific code for modeling doses may be informed not only by the modeling fidelity available in the MACCS code, but also by the doses expected to result from a particular magnitude of tritium release. An assessment of the dose significance¹ of a tritium release can be informed by developing normalized unit dose-distance plots using a high-fidelity tritium-specific code such as UFOTRI. This section provides dose-distance curves for inhalation and ingestion from HTO and HT releases using UFOTRI for varying atmospheric conditions.

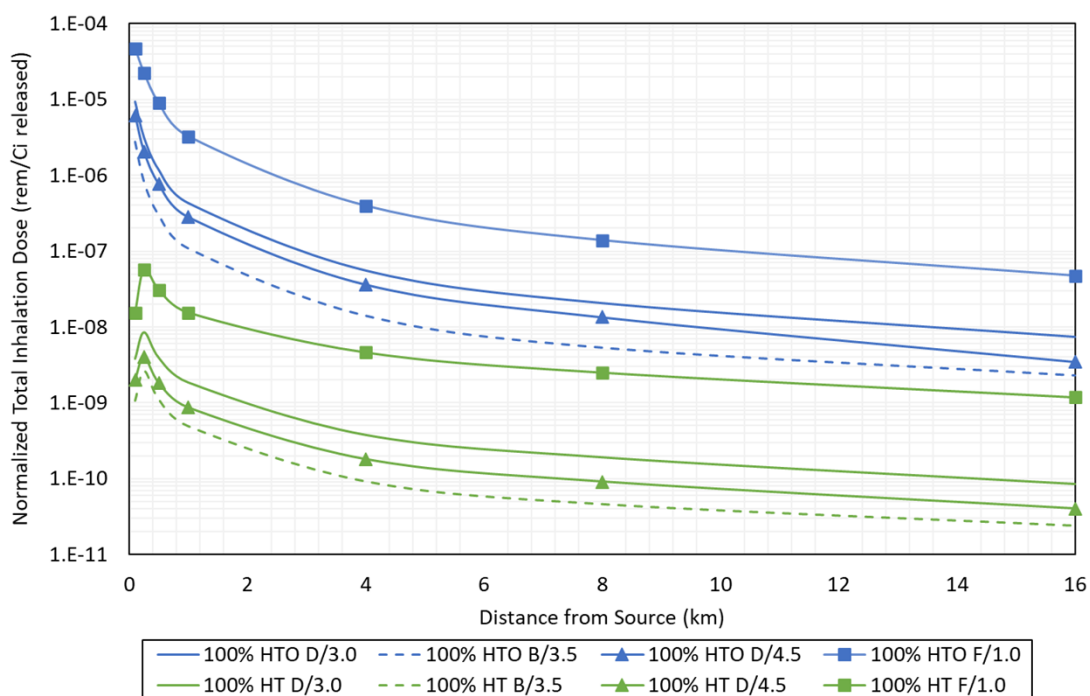


Figure 7-1. Normalized unit dose-distance plot for total inhalation in UFOTRI

Figure 7-1 shows dose-distance curves for inhalation (from both plume passage and reemission) from a unit release (rem/Ci) of either HTO or HT. These curves represent the maximum centerline doses from a unit release, and doses could be smaller off the plume centerline. Additionally, as demonstrated by varying the stability class and windspeed, atmospheric conditions and chosen input parameters will influence the results. These unit dose-distance curves utilize the

¹Although the determination of what constitutes a significant dose would be application-specific, a qualitative characterization of dose levels may be informed by a discussion in ICRP Publication 99 which states that "As a rough rule of thumb, effective doses of the order of 1 Sv, 100 mSv, 10 mSv, 1 mSv, and 0.1 mSv may be called 'moderately high', 'moderate', 'low', 'very low', and 'extremely low', respectively." [26]. In this report, doses on the order of a few rem are termed "low", doses on the order of a few hundred millirem are termed "very low", and doses on the order of a few tens of millirem are termed "extremely low".

modeling choices and input parameters discussed in Section 4 and the authors note these curves are meant as an initial demonstration. Variations in the modeling choices compared to what was used in this analysis could affect the behavior of curves shown here.

Although the exact values of these curves are uncertain due to variations in meteorological conditions and other key UFOTRI parameters, they suggest that doses from inhalation of HT or HTO releases may be low - even at distances on the order of a few hundred meters - unless large amounts of tritium are released. They suggest that, depending on the meteorological conditions, releases on the order of 1 MCi of HTO, or 100 MCi of HT, may result in low inhalation doses only out to a few hundred meters and very low doses only within a few kilometers.

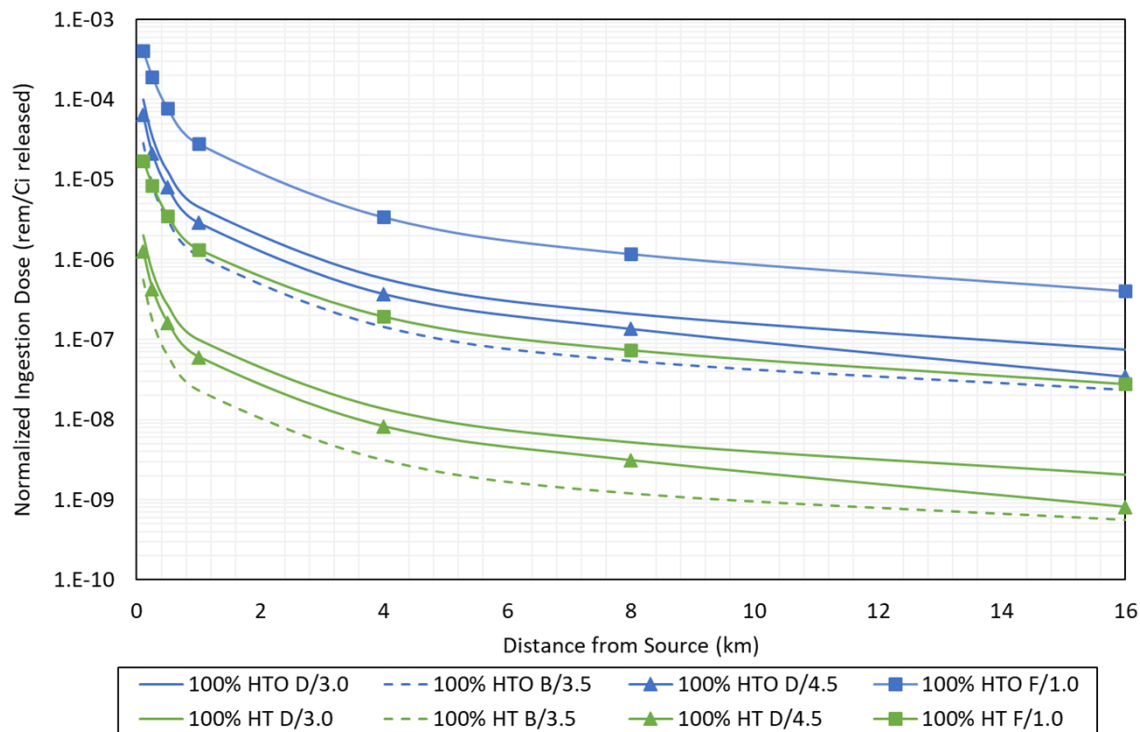


Figure 7-2. Normalized unit dose-distance plot for total ingestion in UFOTRI

Figure 7-2 shows dose-distance curves for ingestion from a unit release (rem/Ci) of either HTO or HT. These curves represent the maximum centerline doses from a unit release, and doses could be smaller off the plume centerline. As stated previously, variations in the modeling choices compared to what was used in this analysis could affect the behavior of curves shown here.

Although the exact values of these curves are uncertain due to variations in meteorological conditions and other key UFOTRI parameters, they suggest that doses from ingestion arising from HT or HTO releases may be low - even at distances on the order of a few hundred meters - unless large amounts of tritium are released. They suggest that, depending on the meteorological conditions, releases on the order of 0.01 MCi of HTO, or 1 MCi of HT, may result in low ingestion doses only out to a few hundred meters and very low doses only within a few kilometers. It may also be noted that ingestion doses may be, unlike inhalation doses, avoided simply by avoiding the consumption of contaminated food products.

8. CONCLUSIONS AND RECOMMENDATIONS

To reiterate, the purpose of this comparison study was to:

1. understand how a given tritium consequence model accounts for tritium release into the environment,
2. have a quantitative understanding of the extent to which state of practice models differ from MACCS, and
3. provide information to assist an analyst in judging whether a postulated tritium release is likely to be risk significant.

Using documented tritium analyses and previous benchmarking assessments, a baseline scenario and multiple sensitivity analyses were compared between MACCS, UFOTRI, and ETMOD. From this analysis the following observations and recommendations are made:

- Tritium does not yield significant doses from external pathways (cloudshine and groundshine) [6]. Doses from tritium would arise primarily from inhalation (from the passing cloud as well as from reemission of deposited tritium) and from ingestion of food products following deposition onto soil and plants.
- The inhalation dose coefficient for tritium in the FGR13GyEquiv DCF file supplied with MACCS is consistent with tritium in the HTO form (see Table 4-2). However, it is believed the dose coefficient for tritium in the FGR13GyEquiv DCF file has not been adjusted to account for absorption of tritium through the skin during immersion of airborne tritium given the information discussed in ICRP 119 [27].
- MACCS appears capable of modeling inhalation doses arising from tritium released as HTO. Using typical input parameters, MACCS results for modeling inhalation doses of HTO releases compared reasonably well with the tritium-specific codes, UFOTRI and ETMOD (See Figure 5-1 and Figure 6-1). Like other codes, the results from MACCS are dependent on the input variables used, including but not limited to the values selected for dispersion modeling, wet and dry deposition parameters, the resuspension model parameters, and exposure parameters such as the inhalation rate and inhalation shielding factors. Additionally, since the MACCS FGR13GyEquiv DCF file has not been adjusted for skin absorption, it is likely that MACCS would be slightly conservative relative to UFOTRI and ETMOD. While release height and various release conditions did have an influence on the results (See Sections 6.2, 6.4, and 6.5) agreement between MACCS and the tritium-specific codes remained comparable.
- MACCS inhalation doses resulting from a release of HT overestimate the dose by approximately two orders of magnitude relative to ETMOD and UFOTRI (compare, for example, the results for a MACCS 100% HTO release to the results for UFOTRI and ETMOD 100% HT release in Figure 6-1). MACCS appears to yield significantly conservative estimates of inhalation doses arising from releases of tritium as HT if the FGR13GyEquiv DCF file is used as is. However, due to the conversion of deposited HT into HTO in soil and plants followed by subsequent reemission of HTO, the degree of conservatism in MACCS results is less than would be expected from the ratio of the HT and HTO dose coefficients alone. While release height and various release conditions did have an influence on the results (See Sections 6.2, 6.4, and 6.5), MACCS results remained the most conservative estimate provided that HT is treated using the default dose coefficient.

- MACCS predicts inhalation doses of mixed releases of HTO and HT that are reasonably consistent with the tritium-specific codes UFOTRI and ETMOD provided that the initial fraction of HTO is more than a few percent (see Figure 6-1). For very low fractions of HTO in mixed releases, it appears that MACCS may yield conservative estimates since the dose coefficients use in MACCS are representative of a 100% HTO release.
- Although it is possible - with significant modification - to explicitly model mixed releases of HT and HTO using MACCS, this is not recommended because MACCS lacks a model for the conversion of HT to HTO. Use of MACCS with a tritium dose coefficient representing HT may significantly underestimate inhalation doses (See Figure 6-1). This is consistent with the findings described in O’Kula and Thoman (2007), which states “bounding estimates for tritium are obtained assuming complete oxidation of the source term...unless supporting defensible analysis is available to the contrary, the tritium release analyses should assume tritium oxide as the species released” [28].
- In general, doses from inhalation of HT or HTO releases may be low¹ - even at distances on the order of a few hundred meters - unless large amounts of tritium are released. Information is provided to assist in evaluating the magnitude of tritium release needed to yield individual inhalation doses above the very low dose (i.e., doses >1 rem) range. Atmospheric conditions (such as stability class and wind speed) and specific modeling choices can influence these determinations (See Figure 7-1).
- MACCS is not designed to model doses arising from ingestion following release and deposition of HTO, HT, or OBT. However, modeling results from UFOTRI and ETMOD, coupled with a review of selected accidental tritium releases, suggest that individual ingestion doses may be low¹ - even at distances on the order of a few hundred meters - unless large amounts of tritium are released. Information is provided to assist in evaluating the magnitude of tritium release needed to yield individual ingestion doses above the very low dose (i.e., doses >1 rem) range. Atmospheric conditions (such as stability class and wind speed) and specific modeling choices can influence these determinations (See Figure 7-2). Additionally, release height and various release conditions can further impact ingestion dose determinations (See Sections 6.2, 6.4, and 6.5).
- Inhalation doses from releases of tritium as OBT were not evaluated. It is expected that doses from OBT are more likely to arise from ingestion pathways (conversion of HT or HTO into OBT following deposition) rather than from releases of tritium as OBT. However, as described in O’Kula and Thoman (2007), atmospheric releases of special tritium compounds (STCs) may arise from “oil-based inventories in many laboratory and solid waste installations [28]. STCs have higher radiotoxicity in the body due to chemical composition characteristics indicating a large percentage of OBT.

REFERENCES

- [1] U.S. Nuclear Regulatory Commission (NRC), 2020. NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy, Volume 3- Computer Code Development Plans for Severe Accident Progression, Source Term and Consequence Analysis, Revision 1.
- [2] Andrews, N.C., Higgins, M., Taconi, A., Leute, J., 2021. Preliminary radioisotope screening for off-site consequence assessment of advanced non-LWR systems, SAND2021-11703.
- [3] Clavier, K.A., Clayton, D.J., 2022. Reviewing MACCS capabilities for assessing tritium releases to the environment. SAND2022-12016.
- [4] Canadian Nuclear Safety Commission (CNSC), 2009. Investigation of the Environmental Fate of Tritium in the Atmosphere, Part of the Tritium Studies Project. INFO-0792.
- [5] Canadian Nuclear Safety Commission (CNSC), 2010. Health Effects, Dosimetry and Radiological Protection of Tritium, Part of the Tritium Studies Project. INFO-0799.
- [6] United States Environmental Protection Agency (EPA), 1999. Cancer Risk Coefficients for Environmental Exposure to Radionuclides, Federal Guidance Report No. 13, EPA 402-R-99-001.
- [7] Raskob, W., 1990. UFOTRI: Program for assessing the off-site consequences from accidental tritium releases. KfK 4605.
- [8] Blanchard, A., O’Kula, K.R., East, J.M., 1998. Selection of a tritium dose model: defensibility and reasonability for DOE authorization basis calculations (u). WSRC-MS-98-00016.
- [9] Canadian Nuclear Safety Commission (CNSC), 2009. Tritium Releases and Dose Consequences in Canada in 2006, Part of the Tritium Studies Project. INFO-0793.
- [10] Murphy Jr., C.E., Wortham, G.R., 1991. An atmospheric tritium release database for model comparisons. WSRC-TR-91-671 Rev. 1.
- [11] Shozugawa, K., Hori, M., Johnson, T.E., Takahata, N., Sano, Y., Kavasi, N., Sahoo, S.K., Matsuo., 2020. Landside tritium leakage over through years from Fukushima Dai-ichi nuclear plant and relationship between countermeasures and contaminated water. Scientific Reports, 10, 19925. <https://doi.org/10.1038/s41598-020-76964-9>
- [12] U.S. Department of Energy (DOE), 1990. Final Environmental Impact Statement: Continued Operation of K-, L-, and P-Reactors, Savannah River Site, Aiken, South Carolina. DOE/EIS-0147.
- [13] Grabaskas, D., Fei, T., Jerden, J., 2020. Technical Letter Report on The Assessment of Tritium Detection and Control in Molten Salt Reactors: Final Report. ANL/NSE-20-15.
- [14] Haubenreich, P.N., 1971. A Review of Production and Observed Distribution of Tritium in the MSRE in Light of Recent Findings. ORNL-CF-71-8-34.
- [15] O’Kula, K.R., Olson, R.L., Hamby, D.M., 1991. Consequences of tritium release to water pathways from postulated accidents in a DOE production reactor. Fourth Topical Meeting on Tritium Technology in Fission, Fusion, and Isotopic Applications. WSRC-MS—91-395.
- [16] Evaluation of current computer models applied in the DOE complex for SAR analysis of radiological dispersion and consequences (U), 2003. Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program Radiological Dispersion and Consequence Working Group. WSRC-TR-96-0126.
- [17] Barry, P.J., Watkins, B.M., Belot, Y., Davis, P.A., Edlund, O., Galeriu, D., Raskob, W., Russell, S., Togawa, O., 1999. Intercomparison of model predictions of tritium concentrations in soil

- and foods following acute airborne HTO exposure. *Journal of Environmental Radioactivity*, 42, 191-207.
- [18] Harmonization and intercomparison of models for accidental tritium releases to the atmosphere, 2022. Report of working group 7 – Modelling and Data for Radiological Impact Assessments (MODARIA) Program. IAEA-TECDOC-1991
 - [19] Sandia National Laboratories (SNL), 2023. MACCS User Guide – Version 4.2. SAND2023-01315.
 - [20] Raskob, W., 1990. UFOTRI: Program for assessing the off-site consequences from accidental tritium releases. KfK 4605.
 - [21] Russell, S.B. and Ogram, G.L., 1988. Modelling elemental tritium deposition, conversion and reemission using Ontario Hydro's tritium dispersion code. *Fusion Technol.*, 14:2.
 - [22] Ogram, G.L., 1991. Improved ETMOD modules for HTO exchange, HT deposition, and vegetation HTO (CFFTPG-9188 / OHRD No. 91-191-K).
 - [23] Chouhan, S., 2009. ETMOD Version 2 Computer Program Abstract, Theory Manual, User's Manual, Validation Plan, validation Report and Version Tracking Record. Software User Application Documentation, Nuclear Platform Research and Development. 153-113520-SUAL-001, Revision 0.
 - [24] Bixler, N., Compton, K., Dennis, M., Eubanks, L., Haaker, R., Jones, J., Kimura, M., McFadden, K., Nosek, A., Outkin, A., Walton, F., 2022. Technical bases for consequence analyses using MACCS (MELCOR Accident Consequence Code System). NUREG/CR-720, SAND2022-12166 R.
 - [25] Raskob, W., n.d. Description of the new version 4.0 of the tritium model UFOTRI including user guide. KfK 5194.
 - [26] International Commission on Radiological Protection (ICRP), 2005. ICRP Publication 99, Low-dose Extrapolation of Radiation-related Cancer Risk. Volume 35, No. 4, *Annals of the ICRP*, ISSN 0146-6453, ISBN 008-0446590.
 - [27] International Commission on Radiological Protection (ICRP), 2012. ICRP Publication 119, Compendium of Dose Coefficients Based on ICRP Publication 60. Volume 41, Supplement 1, *Annals of the ICRP*, ISSN 0146-6453, ISBN 978-1-4557-5430-4.
 - [28] O'Kula, K.R. and Thoman, D.C., 2007. Modeling Atmospheric Release of Tritium from Nuclear Installations. WSRC-STI-2007-00027.

DISTRIBUTION

Email—Internal

Name	Org.	Sandia Email Address
Kyle A. Clavier	08855	kaclavi@sandia.gov
Daniel J. Clayton	08855	djclayt@sandia.gov
John D. Fulton	08855	jdfulto@sandia.gov
Mariah L. Smith	08855	msmith7@sandia.gov
Technical Library	1911	sanddocs@sandia.gov

Email—External

Name	Company Email Address	Company Name
Jonathan Barr	Jonathan.barr@nrc.gov	US NRC
Keith L. Compton	Keith.compton@nrc.gov	US NRC
Salman Haq	Salman.haq@nrc.gov	US NRC

This page left blank

This page left blank



Sandia
National
Laboratories

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.