Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

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Assessment of Accident Dose Models Used at the Savannah River Site

G. T. Jannik, A.M. Rivera-Giboyeaux

December 2019

SRNL-STI-2019-00695, Revision 0

SRNL.DOE.GOV

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Printed in the United States of America

Prepared for
U.S. Department of Energy

SRNL-STI-2019-00695
Revision 0

Keywords: *AXAIRQ, PUFF-PLUME, MACCS2*

Retention: *Permanent*

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EXECUTIVE SUMMARY

AXAIRQ, PUFF-PLUME, and MACCS2 are available for atmosphere modeling of accidental releases at the Savannah River Site (SRS) by qualified users. All models assume Gaussian diffusion and use site-specific or user-specified meteorological data to estimate downwind doses. However, each model was developed, maintained and applied for different purposes for use at SRS. This report briefly describes the lineage of, highlights the differing assumptions for, and compares some results from each model. The report is not intended to be an exhaustive evaluation and/or comparison of the models but to document the capabilities and assumptions of the models to gain perspective on how the models differ.

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LIST OF ABBREVIATIONS

ATG	Atmospheric Technologies Group
CW	Co-located Worker
DOE	U.S. Department of Energy
DSA	Documented Safety Analysis
EDG	Environmental Dosimetry Group
EIS	Environmental Impact Statements
E-K	Eimutis and Konicek
EPA	Environmental Protection Agency
GUI	Graphical User Interface
FGR	Federal Guidance Report
HAD	Hazard Assessment Document
ICRP	International Commission on Radiological Protection
LHS	Latin Hypercube Sampling
MACCS	MELCOR Accident Consequence Code Systems
MOI	Maximum Offsite Individual
NC&SE	Nuclear Criticality and Safety Engineering
NRC	U.S. Nuclear Regulatory Commission
P + B	Pasquill and Briggs
P-G	Pasquill-Gifford
SAR	Safety Analysis Report
SNL	Sandia National Laboratory
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
T-G	Tadmor-Gur
UTED	Unit Total Effective Dose
WSRC	Westinghouse Savannah River Company
χ/Q (chi/Q)	Relative air concentration

1.0 INTRODUCTION

AXAIRQ, PUFF-PLUME, and MACCS2 are available for atmospheric modeling of accidental releases at the Savannah River Site (SRS) by qualified users. All models assume Gaussian diffusion and use site-specific or user-specified meteorological data to estimate χ/Qs and ultimately total doses. AXAIRQ and MACCS2 are intended primarily to estimate a climatologically expected worst-case dose following a postulated accident at a nuclear facility using methods outlined in Nuclear Regulatory Commission (NRC) Regulatory Guide 1.145 (NRC, 1983). PUFF-PLUME is a deterministic model used to estimate dose in real time based on the meteorology occurring during emergency response. Some comparisons of the models have been performed in the past (Simpkins and Kurzeja, 1993; Simpkins, 1995; Blanchard et al., 1998; WSRC, 2003), but not with recent versions of the models and not with all three in the same assessment. This report is not intended to be an exhaustive evaluation and/or comparison of the models but to document the capabilities and assumptions of the models to gain perspective on how the models differ.

1.1 AXAIRQ

1.1.1 Background

AXAIRQ (Simpkins, 1995) is owned and used by the SRNL Environmental Dosimetry Group (EDG) to analyze postulated accidents involving both ground level and elevated releases. Results from AXAIRQ have historically been used for reviewing Safety Analysis Reports (SARs), Hazard Assessment Documents (HADs), and Environmental Impact Statements (EISs).

An SRNL accident dose model based on NRC Regulatory Guide 1.145 (NRC, 1983) was first developed by Pendergast and Huang (1980) and subsequently executed on the SRS IBM mainframe computer as AXAIR89Q. AXAIRQ was developed as an improved version of AXAIR89Q (Hamby, 1990). Due to the shutdown of the SRS Mainframe, AXAIRQ PC version 2011 was developed and AXAIR89Q was retired in 2012. This conversion involved source code changes from IBM FORTRAN 66 to Windows FORTRAN 95 in the various AXAIRQ modules (Farfan, 2011a and 2011b). The current AXAIRQ PC v. 2016 (Dixon and Abbott, 2016) has been updated with new files containing updated dose factors (DOE, 2011), decay factors (ICRP, 2008), and meteorological data (Viner, 2014). This conversion to a PC platform did not change the methods or capabilities of the code, therefore, it will be referred to as AXAIRQ throughout the remainder of the document.

1.1.2 Dispersion Method

AXAIRQ is a straight-line Gaussian atmospheric dispersion and dosimetry model that strictly follows the guidance provided in NRC Regulatory Guide 1.145 (NRC, 1983). Given minimal input to characterize a release, the AXAIRQ code estimates the doses via inhalation, plume shine, and ground shine exposure pathways to the onsite population, the offsite population within 50 miles (80 km), onsite individuals at user-selected locations and the offsite maximally exposed individual. The doses evaluated are typically those that would be exceeded only 0.5% of the time based on meteorological probability analysis. The resulting doses are reported by radionuclide, body organ, and pathway.

AXAIRQ provides automatic selection or generation of the following: dose conversion factors, inhalation and gamma exposure parameters, dry deposition, onsite and offsite population distributions, meteorological diffusion coefficients, relative terrain elevations, and minimum boundary distances to each compass sector.

A user can select one of two unique sets of diffusion coefficients: the Pasquill-Gifford (P-G) coefficients for both horizontal and vertical diffusion about the plume's centerline, or a combination of coefficients consisting of expressions published by Pasquill (1976) for horizontal diffusion and Briggs for vertical diffusion. The latter option was added to provide consistency with the diffusion coefficients used by PUFF-PLUME.

The P-G curves are based on experimental diffusion data that was collected over distances of a few miles from the source. For longer distances (>10 km), the P-G curves are simply extrapolations of the empirical diffusion data, which is why they are often displayed as dashed lines in the published plots.

Pasquill's expression for horizontal diffusion is a generalized function of σ_a, the standard deviation of the horizontal component (azimuth) of wind direction. AXAIRQ choses the md-point value of σ_a range used to determine Pasquill stability category as summarized by NRC Regulatory Guide 1.23, Rev. 1 (NRC, 2007).

Briggs' expressions were developed as an improvement on the already established P-G curves to account for the decreased diffusion that occurs downwind when the size and scale of turbulent eddies becomes smaller relative to plume size (generally at distances beyond 10 km). In fact, Brigg's expressions closely follow the P-G curves, but as distances increase to 10 km or more, the expressions yield smaller sigma values and therefore, more conservative concentration estimates for larger distances (out to SRS site boundary for example).

Early dispersion models developed and promulgated by the Environmental Protection Agency (EPA) and the NRC were all based on P-G, as they pre-date Briggs. To maintain consistency between all dispersion models, the Briggs coefficients were never subsequently adopted by EPA and NRC regulators.

Ingrowth of daughter radionuclides or progeny from released parent decay during plume transport may be considered at the user's discretion. Different methodologies can be used in the determination of external dose via gamma radiation using one of the following assumptions:

- Non-uniform plume upper-bound approximation
- Rigorous non-uniform plume approximation, or
- Semi-infinite uniform plume

1.2 MACCS2

1.2.1 Background

MACCS2 is a straight-line Gaussian plume model developed by the Sandia National Laboratory (SNL) for calculation of atmospheric dispersion and radiological dose consequences (Chanin et al., 1998). MACCS2 Version 1.13.1 was developed under support of NRC and uses the methods described in NRC Regulatory Guide 1.145 (NRC, 1983). The MACCS/MACCS2 codes have been used throughout the DOE Complex since the late 1980s to support probabilistic consequence assessments and as a tool for deterministic consequence calculations to support Documented Safety Analyses (DSAs). At SRS, MACCS2 is used by NC&SE to support Site DSAs.

1.2.2 Dispersion Method

MACCS2 code provides probabilistic does consequences by using multiple, straight-line Gaussian plumes. Horizontal and vertical diffusion of a plume is based in the P-G coefficients. MACCS2 was originally developed by SNL for the NRC, and that is likely the reason why the P-G curves were, and are still, used by this model. The wind direction, release duration, sensible heat, and initial radionuclide concentration may be varied. The P-G crosswind diffusion coefficients are determined by a multi-step function and both wet and dry deposition features can be modeled as independent processes. For safety analysis applications, the MACCS2 user can input hourly meteorology by selecting either the stratified random sampling mode or the latin hypercube sampling (LHS) mode to process one year of site-specific, hourly-averaged data. Based on the sampling method for the site-specific meteorological data, and application of user-specified dose and/or health effects models, total doses are calculated for various measures of consequence. The average, median, 95th, and 99.5th percentile consequences are provided in the output.

In general, MACCS2 is set up to execute in three sequential steps using the following code modules:

(1) the ATMOS module calculates air and ground concentrations, plume size, and timing information for all plume segments as a function of downwind distance;

(2) the EARLY module calculates consequences due to radiation exposure in the emergency phase (first 7 days) from the time of release; and

(3) the CHRONC module calculates long-term consequences due to exposure after the emergency phase.

Results for determining decontamination requirements and other economic impacts from the hypothetical accident are also computed. Additional input files include site meteorological data, internal dose factors, and population data to support overall execution. For the purposes of this report, the outputs from modules 1 and 2 will be used.

For ground level releases, MACCS2 uses the Tadmor-Gur (T-G) power function to determine dispersion coefficients at distances of more than 500 m. For distances of less than 500 m, or for elevated/plume heat calculations, MACCS2 uses Eimutis and Konicek (E-K) coefficients as a look up table. A look up table format is required because MACCS2 does not work well with the three-term power function (DOE, 2004). The T-G as well as the E-K table are both mathematical representations of the P-G curves that provide horizontal and vertical dispersion coefficients as a function of distance from the source. The P-G curves are based on experimental diffusion data that was collected over distances of a few miles from the source. For longer distances (>10 km), the P-G curves are simply extrapolations of the empirical diffusion data, which is why they are often displayed as dashed lines in the published plots.

1.3 PUFF-PLUME

1.3.1 Background

PUFF-PLUME is owned and maintained by SRNL's Atmospheric Technology Group (ATG). PUFF-PLUME is a segmented trajectory Gaussian atmospheric dispersion model designed to provide instantaneous estimates of downwind consequences (radiological or chemical) during the early phase of emergency response (Hunter et. al, 2017). Calculations are performed for three fixed downwind distances: 30 meters, 100 meters, and the SRS boundary, with an additional 72 equally spaced receptors extending to distance of 100 kilometers or more based on a user-supplied time increment. The PUFF-PLUME model was first developed and placed in operational use at SRS in the mid 1970's (Pendergast, 1975). Numerous changes to the model have been incorporated over the years, including the addition of algorithms for calculating wet and dry deposition for particulates and gases (Garrett and Murphy, 1981). PUFF-PLUME's dispersion algorithms have been subject to rigorous testing and verification, including comparisons to measured concentrations of tracer gas released during a series of field experiments conducted at SRS in the 1980s (Fast, 1991a and Fast, 1991b) and measurements collected following unanticipated releases from SRS facilities during emergency response.

For many years, the PUFF-PLUME software was run on Digital Equipment Corporation PDP/11 and VAX minicomputers. In 1995, the code was ported to an IBM compatible PC and compiled to run with the Windows NT operating system in 32-bit mode. In addition, a contemporary Graphical User Interface (GUI) was developed for simplifying model input and viewing model results. The GUI was originally developed with the Tcl/Tk software package; but later re-written in Python™. The current PUFF-PLUME version 13.0 runs on Windows 10 computers (Hunter and Rivera-Giboyeaux, 2019).

1.3.2 Dispersion Method

PUFF-PLUME utilizes a sequence of hourly meteorological data (observed and/or forecast) to construct downwind trajectory segments. Diffusion about each trajectory segment utilizes coefficients for rural, forested terrain derived by Smith for puff releases and Pasquill (horizontal diffusion) and Briggs (vertical diffusion) for plume releases. The Smith and Pasquill coefficients are determined by continuous functions requiring input of observed turbulence intensity. The Briggs coefficients are the commonly used discrete curves based on Pasquill stability class. The initial horizontal and vertical size of the release can be varied to represent a point, line, or volume source. The release location can be specified from a predefined list or interactively from a map of the area of interest. Terrain is assumed to be flat (but topography can be simulated by adjusting the effective release and inversion heights). Tabular and graphical output is available in less than 1 minute and includes estimates of dose, air concentration, plume width, deposition, and arrival time at each distance downwind. Radiological dose includes internal and external exposure. External dose is based on integration of infinite line sources.

Table 1-1 lists summary features of each of the three models.

Table 1-1. SRS Accident Release Model Attribute Summary

Model	AXAIRQ	MACCS2	PUFF-PLUME
Owner/Design Authority	SRNL Environmental Dosimetry Group (EDG)	Nuclear Criticality and Safety Engineering (NC&SE)	SRNL Atmospheric Technologies Group (ATG)
Primary Use	Safety Analysis Reports (SAR); Hazard Assessment Documents (HAD); Environmental Impact Statements (EIS)	Documented Safety Analysis (DSA)	Emergency Planning, and Response
Exposure Pathways	Internal/External (3 methods see Section 1.1.2)	Internal/External	Internal/External (integration of infinite line sources)
Receptors	onsite population (user-selected locations)*, offsite population within 80 km (maximally exposed individual) *not recommended at distances < 100 m	100 m and Site Boundary	30 m, 100 m, Site Boundary, and up to 72 additional receptors based on user supplied time increments for up to 12 hours of transport
Diffusion Coefficients	Set to Pasquill (horizontal) and Briggs (vertical)	Tadmor-Gur(T-G)/ (P-G) -> 500 m Eimutis and Konicek (E-K)/P-G < 500 m	Pasquill (horizontal) and Briggs (vertical)
Surface Roughness	No	Yes	Yes
Reported Dose	95th and 99.5th percentile Sector dependent	95th percentile Sector independent	Deterministic based on specified meteorology
HTO Dose Coefficients (Rem/Ci)	DOE-STD-1196	ICRP 119, Table B.1 Tritiated Water (Increased by 50% for skin absorption)	EPA Federal Guidance Report (FGR) 11
Terrain assumptions	Considers topography	Flat	Flat
Meteorological Dataset	2007-2011	2002-2006	Sequential hourly observations and/or forecasts read from a file or entered manually; up to 12 hourly values

2.0 MODEL COMPARISONS

The subsequent sections describe an attempt to align model inputs and evaluate resulting model estimates under similar input. This will provide perspective on how the differing model approaches and underlying assumptions (dose factors, deposition, statistical vs. instantaneous dose estimates) explain differences in the results. The input values for the comparison are listed in Table 2-1. In cases where variables are hard wired in the model, the output is adjusted, as appropriate, for the comparison.

Table 2-1. Input for Model Comparisons

Input Variable	Value	Notes (if applicable)
Source Term (Ci)	1 or 1.16E+08	Tritium oxide
Release Time (hrs)	2	
Release Location	233-H	
Release Height (m)	0 or 15	Only MACCS2 used a ground level release
Distance to Receptor (m)	100 (CW), 640, 800, 1000, and 11,500 for site boundary/MOI	Only MOI used in comparison of MACCS2 vs PUFF-PLUME
Breathing Rate m^3/y	10,500	AXAIRQ assumes 12,000. Output is adjusted for the comparison.

2.1 PUFF-PLUME vs AXAIRQ

AXAIRQ is mainly used in generating results for nuclear safety related documentation while PUFF-PLUME is primarily used for real-time emergency response applications. Consequently, the inputs and outputs of these two models are inherently different. For example:

1) AXAIRQ estimates the probabilistic occurrence of worst-case dispersion conditions for dose calculations based on 5-year meteorological datasets while PUFF-PLUME calculates dispersion/dose directly from a single set of meteorological observations,
2) AXAIRQ takes into consideration topography in its calculation while PUFF-PLUME assumes flat terrain,
3) AXAIRQ outputs worst-case dose at specified distances from the source based on an interpolation between two pairs of stability and wind speed classes that are exceeded only 0.5% of the total time; PUFF-PLUME, in turn, provides a deterministic estimate of downwind concentrations/doses over a series of distances from the release point based on the observed and forecast meteorological input conditions (or on the manual input of meteorological data).
4) PUFF-PLUME uses an explicit value of the horizontal component of turbulence to calculate σ_y using Pasquill, whereas AXAIRQ estimates a value based on stability class.

Even though the two models have these and other inherent differences, adjustments can be made to obtain comparable results between the two.

AXAIRQ and PUFF-PLUME have previously been compared by Simpkins and Kurzeja (1993) and Simpkins (1995). Both studies showed that the models are in close agreement (<10% difference) when consistent meteorological conditions and dispersion coefficients are used.

Rivera-Giboyeaux (2019) compared the most recent versions of AXAIRQ v. 2016 (Dixon and Abbott, 2016) and PUFF-PLUME v. 13.0 (Hunter and Rivera-Giboyeaux (2019). For this comparison, a release of 1.16E+08 Ci of tritium oxide over 2 hours from the 233-H stack at the Tritium Facilities was modeled in AXAIRQ. In an effort to standardize on a conservative scenario, the following input parameters were used in each code: A stack height of 15 meters (49 ft), a grade elevation of 308 ft (94 meters) above sea level and a mixing height of 200 meters (which is the worst-case condition allowed in AXAIRQ) were used. AXAIRQ was set to calculate results for the sector-dependent 99.5% meteorology using the Pasquill and Briggs (P+B) dispersion coefficients (which correspond to those used in PUFF-PLUME). The model was run for 5 different distances from the release location, including the site boundary (11.5 km). ATG modeled the same release conditions using PUFF-PLUME and adjusting meteorological inputs to those that best approximate the stability and wind speed class combinations that produced the AXAIRQ results for each distance. As mentioned, AXAIRQ determines the dose by interpolating between two stability-wind speed class pairs that bracket the 0.5% probability of exceedance at each specified distance. To be conservative, the stability-wind speed class pair listed in the AXAIRQ output that produces the least dispersion was used to identify the stability class and wind speed inputs needed for PUFF-PLUME. A PUFF-PLUME run was done for each of the 5 downwind distances using the appropriate inputs derived from AXAIRQ for each distance (Simpkins and Kurzeja, 1993; Rivera-Giboyeaux, 2019). The wind speed used for the PUFF-PLUME runs was first assumed to be the mid-point of the wind speed class identified in the AXAIRQ output. Small adjustments to the mid-point wind speed value were run to improve model agreement, with the constraint that the PUFF-PLUME wind speed remained within the wind speed class identified in AXAIRQ. An effective release height and effective mixing height adjustment was completed to adapt PUFF-PLUME calculations for each distance to terrain changes. The adjustment was only necessary for site boundary (11.5 km) dose estimates because terrain at the northeastern sectors of SRS (sector with the highest concentration estimates for site boundary in AXAIRQ) is higher than the grade level height of the stack. For more details on this calculations refer to Rivera-Giboyeaux (2019).

Table 2-2 demonstrates comparable results between the two models with consistent meteorological conditions and effective heights. PUFF-PLUME estimates were generally within 20% of the AXAIRQ values (or a factor of ~1.2 with AXAIR having the more conservative estimates), which is considered good agreement. Meteorological conditions listed in Table 2-2 represent the stability class and wind speed combinations that provide the best agreement with AXAIRQ estimates for each distance downwind (different meteorological conditions are shown in AXAIRQ to obtain the worst ground level dose at different distances downwind).

Table 2-2. PUFF-PLUME and AXAIRQ comparisons

Distance from release (m)	Meteorological conditions/ input	AXAIRQ dose (rem/Ci)	PUFF-PLUME dose (rem/Ci)	% Difference
100	C stab/1.5 mps	**9.57E-06**	**1.04E-05**	8.26%
640	E stab/ 1.5 mps	**1.48E-05**	**1.31E-05**	-13.16%
800	E stab/ 1 mps	**1.35E-05**	**1.13E-05**	-19.85%
1000	F stab/ 1 mps	**1.66E-05**	**1.59E-05**	-4.32%
11.5 km (site boundary)	F stab/1 (11m He)	**1.63E-06**	**1.55E-06**	-5.00%

2.2 AXIRQ vs MACCS2

AXAIRQ and MACCS2 have previously been compared by Blanchard, O'Kula, and East (1998). The results showed relatively good agreement at an offsite receptor location when similar meteorological conditions are inputted. However, there were much larger differences at 100 m and 640 m receptor locations. A comparison between AXAIRQ and MACCS2 was also performed by the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program Radiological Dispersion and Consequence Working Group (WSRC, 2003). In this comprehensive report, using an Evaporative Tritium Release scenario of 1,000 Ci of tritium oxide, AXAIRQ yielded the most bounding (i.e. conservative) offsite estimates. The MACCS2-based comparison of prescribed meteorology versus the source term characteristics and site data file showed that site statistical conditions are more bounding for the close-in receptors. However, there is a difference factor of nearly three at the Maximum Offsite Individual (MOI) distance with MACCS2 being the lower estimate. Comparing MACCS2 to AXAIRQ at the 640 m and MOI distances for the 50th and 95th percentile conditions, MACCS2 dose estimates are about half the dose estimated by AXAIRQ. These differences are due mainly to the differences in the treatment of vertical dispersion between the two codes. MACCS2 adjusts the P-G vertical diffusion coefficients with a roughness factor that is given by a ratio of the SRS roughness (160 cm) to the surface roughness that forms the original basis of the P-G coefficients (3 cm) raised to a power of 0.2, resulting in a factor of 2.22. Surface roughness is not an available option in AXAIRQ. A comparison is made here between the latest versions of AXAIRQ v. 2016 (Dixon and Abbott, 2016) and MACCS2 v. 1.13.1, which was the version used in Hope (2018) and Roberts (2016). The unit total effective dose (UTED) factors taken from Roberts (2016) were developed for use in Tritium Facilities safety basis documents and not specifically for this comparison.

A unit release of tritium oxide at ground level from H-Area for a duration of 2 hours was assessed. A breathing rate of 3.33E-04 m^3/s (10,500 m^3/y) and a dose coefficient of 1.82E-11 Sv/Bq (101 Rem/Ci) were used. A distance of 100 m was used for the collocated worker (CW) and 11,500 m for the MOI. No deposition of tritium oxide was used.

AXAIRQ runs used the 2007-2011 SRS met dataset (Viner, 2014), MACCS2 used a modified 2002-2006 dataset that was shown to be similar to the 2007-2011 dataset (Hunter, 2018).

As shown in Table 2-3, using the P+B dispersion coefficients., AXAIRQ UTED is about 3 times higher for the CW and over 11 times higher for the MOI. Using P-G dispersion coefficients, AXAIRQ is much closer to MACCS2 but still 1.7 times more for the CW and about 5 times more for the MOI.

Table 2-3. Comparison of Unit Total Effective Dose Factor (Rem/Ci) for MACCS2 and AXAIRQ

Receptor Location	MACCS2 (Tadmur-Gur) (Gifford) Rem/Ci	AXAIRQ (P+B) Rem/Ci	Factor Difference (P+B/T-G)	AXAIRQ (P-G) Rem/Ci	Factor Difference (P-G/T-G)
100 m (CW)	1.2E-04*	3.8E-04	3.2	2.0E-04	1.7
11,500 m (MOI)	7.3E-08	8.6E-07	11.7	3.7E-07	5.1

*Using MACCS2 methods, Nuclear & Criticality Safety Engineering (N&CSE) is required to use a single χ/Q value of 3.5E-03 s/m^3 for hand calculating the 100 m CW dose as specified in DOE (2014).

The differences observed between the AXAIRQ adjusted results and MACCS2 values are attributed to the 1) differences in the treatment of vertical dispersion between the two codes, 2) use of a surface roughness factor in MACCS2, but not in AXAIRQ, 3) terrain effects being used in AXAIRQ but not in MACCS2, and 4) using MACCS2 methods, N&CSE is required to use a single χ/Q value of 3.5E-03 s/m^3 for hand calculating the 100 m CW doses as specified in DOE (2014).

2.3 PUFF-PLUME VS MACCS2

A formal comparison of PUFF-PLUME vs. MACCS2 has not been done previously at SRS. For this report, a comparison was performed by comparing ATG results for a ground level tritium oxide (HTO) release of 1.16E+08 Ci over 2 hours with the results from an equivalent MACCS2 run provided by the NC&SE Analytical Support Group. For this comparison, a slightly different approach was used to examine if results from the two different models would be in good agreement when using the same model inputs because dispersion coefficients are hardwired into MACCS2 (P-G) and PUFF-PLUME (P+B) and therefore cannot be manually changed.

For ground level releases, MACCS2 uses the Tadmor-Gur power function to determine dispersion coefficients at distances of more than 500 m. For distances of less than 500 m, or for elevated/plume heat calculations, MACCS2 uses Eimutis and Konicek (E-K) coefficients as a look up table. A look up table format is required because MACCS2 cannot handle a three-term power function (DOE, 2004). The T-G as well as the E-K table are both mathematical representations of the P-G curves that provide horizontal and vertical diffusion coefficients as a function of distance from the source. To compare results from both models, the value of each diffusion coefficient (σ_y and σ_z) was obtained using both the P-G curves and the Pasquill (for σ_y) and Brigg's (for σ_z) formulations (See Table 2-4 for results at various distances). As expected, P-G curves and Briggs expressions begin to disagree with increasing distance downwind – Briggs being the more conservative of the two. Knowing by how much the dispersion coefficients differ at the distance of interest, the PUFF-PLUME results can be adjusted to normalize the diffusion calculations to that of MACCS2

Following that, assuming a smooth terrain and using F stability with 1.3 m/s winds (which represent the meteorological conditions that have been identified to produce the 95% dose) for a ground level release downwind ground level concentration at 11.5 km was estimated manually using the Gaussian Equation. The estimated concentration was then corrected by a surface roughness factor to represent the effects of SRS roughness in the dispersion coefficients. As practiced in MACCS2, the roughness adjustment factor is calculated as demonstrated in equation (1) and resulted in a χ/Q of 8.19E-06 sec/m^3.

$$\left(\frac{\boldsymbol{SRS\ roughness\ (160\ cm)}}{\boldsymbol{smooth\ surface\ roughness\ (3\ cm)}}\right)^{\mathbf{0.2}} = \mathbf{2.22} \qquad \mathbf{(1)}$$

To estimate what PUFF-PLUME's concentration value would be if calculated using the P-G curves, an additional correction is made to account for the difference in the dispersion coefficient values between the two methods- i.e. to convert concentration estimates into a P-G equivalent (concentration is inversely proportional to the sigma values). Therefore, dividing by the factor of 1.2, a χ/Q value of 7.06E-06 sec/m^3 was obtained which is approximately twice the estimate provided for MACCS2 of 2.27E-06 sec/m^3 (Table 2-5). Following that manual estimation, an actual run was completed in PUFF-PLUME using E stability sigma elevation and azimuth values (which inherently account for the site roughness) and the Pasquill and Brigg's method to convert them into sigma values. The resulting concentration was adjusted by the sigma factor of 1.2 which yielded 7.08E-6 sec/m^3. This verifies the value obtained manually for 11.5 km (Site

Boundary). Therefore, although there is some difference between the values, we can conclude that PUFF-PLUME can obtain similar concentration estimates to those obtained with MACCS2 (within a factor of 2-3) 11.5 km downwind from the source if sigma values obtained using the P-G method (instead of the default P+B equations) are used.

Table 2-4. Distance downwind and corresponding sigma values for F stability

Distance downwind (km)	P-G curves		Briggs	Pasquill	Ratio
	σ-z (m)	σ-y (m)	σ-z (m)	σ-y (m)	σ P-G /σ Pasquill and Briggs
0.5	9	18	8.7	22.1	0.8
1	15	35	15.4	42.0	0.8
6.4	40	180	43.8	151.0	1.1
8	43	230	47.1	192.5	1.1
9	45	250	48.7	208.0	1.1
10	49	280	50.0	231.0	1.2
11.5	50	300	51.7	250.0	1.2

The difference between results of both manual calculations and PUFF-PLUME runs against MACCS2 model results can be explained by various factors. First, the selection of the σ_A and σ_E values for manual input into PUFF-PLUME is somewhat subjective, i.e. sigma values are selected from a range of values that represent each stability class. The selection of σ_y and σ_z values from the P-G curves used for MACCS2 is also subjective to each user's discretion and interpolation of the logarithmic plots, which adds a source of uncertainty when using these curves. However, a more significant source of discrepancies is the process used by each model to obtain dose estimates. MACCS2 results are based on statistical dose estimations (percentile based) while PUFF-PLUME provides instantaneous downwind dose estimations, specific to the meteorological input used. An additional source of discrepancies in model results is adjustment for plume meander. MACCS2 adjusts the σ_y for meander based on the release duration using what is known as the "Gifford Model." PUFF-PLUME does not account for plume meander so the resulting dose estimates are expected to be more conservative.

Table 2-5. Comparison of Concentration Values for MACCS2 and PUFF-PLUME

Receptor Location	MACCS2 (P-G curves) Sec/m^3	PUFF-PLUME (P + B) Sec/m^3	Factor difference (PUFF-PLUME /MACCS2)	PUFF-PLUME (P-G equivalent) Sec/m^3	Factor difference (PUFF-PLUME /MACCS2)
11,500 m (MOI)	2.72E-06	8.19E-06	3	7.06E-06	2.6

3.0 CONCLUSIONS

AXAIRQ, PUFF-PLUME, and MACCS2 are all Gaussian atmospheric dispersion and dosimetry models that are available for modeling accident releases at SRS by qualified users. These models have been compared to each other in the past and have been shown to be in relatively good agreement when consistent meteorological conditions and dispersion coefficients are used. However, these models differ in their input assumptions, calculation methods, and output format.

In this report, we attempt to provide similar inputs to each model and use similar model assumptions to evaluate resulting model estimates. However, there are inherent differences in each of the model methods, assumptions, and calculations that are hardwired into the models and cannot be manually changed.

AXAIRQ and MACCS2 are probabilistic models that base their dose estimates on percentiles of concentration and associate the statistically derived worst-case dose to a set of meteorological inputs using a 5-year meteorological dataset. PUFF-PLUME, in turn, is designed to provide a single instantaneous dose estimate for each distance downwind based on manual input of meteorological data for a given time (or real-time observations and forecast for up to 12-hours).

Aside from this very basic difference in the model, additional sources of discrepancy in the estimates can be identified, for example AXAIRQ and PUFF-PLUME were set up to consider topography, but MACCS2 was not, AXAIRQ's output is sector dependent, whereas MACCS2 provides one single set of output for each distance value independent of wind sector. Therefore, AXAIRQ and MACCS2 comparison yielded larger differences in dose estimates, although they are both providing probabilistic dose estimates.

Compared against the two probabilistic models, PUFF-PLUME results were much closer to those of AXAIRQ than to MACCS2 estimates (PUFF-PLUME estimates had almost a 1:1 relationship with AXAIRQ estimates but were about three times larger than MACCS2 estimates obtained for this evaluation). This is likely because plume meander is considered in MACCS2 but not in PUFF-PLUME, as well as other differences in model inputs and assumptions.

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