Predicted Versus Measured Tritium Oxide Concentrations at SRS (U)

by

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December 1995

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ABSTRACT

Measured tritium oxide concentrations at various offsite locations are compared with concentrations predicted by three computer codes that are utilized at SRS to predict doses to the maximally exposed offsite individuals. Annual average concentrations predicted by the computer programs were compared with measured average concentrations taken from data contained in the last ten years of SRS Environmental Reports. The computer programs used for the comparison are AXAIRQ, CAP88, and MAXIGASP.

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1.0 INTRODUCTION

Various computer models are used at the Savannah River Site (SRS) to predict the dose to a hypothetical maximally exposed offsite individual from atmospheric releases of radioactivity. Different computer models are used to predict doses for routine and accidental releases. AXAIRQ is used to predict doses following a hypothetical atmospheric accident. For routine releases, MAXIGASP is used to predict the dose to the maximally exposed offsite individual. For NESHAPS compliance, CAP88 is used to determine dose to the maximally exposed offsite individual. Each of these codes applies a Gaussian plume dispersion model with special features to account for a variety of weather conditions (i.e. fumigation or meander). All three of these codes predict average annual relative air concentrations.

Each year annual average tritium oxide concentrations at several boundary locations are reported in the SRS Environmental Report (Zeigler et al. 1986, 1987, Mikol et al. 1988, Davis et al. 1989, Cummins et al. 1990, 1991, Arnett et al. 1992, 1993, 1994, 1995). The total amount of tritium oxide that is released from SRS facilities is continually monitored on-line at various potential release locations and is also reported in the Environmental Report.

Annual average tritium oxide concentrations are compared with the product of relative air concentrations predicted by AXAIRQ and MAXIGASP and the yearly amount of tritium oxide released. CAP88 displays the annual average tritium oxide concentration directly as part of the output. Differences between the programs and their conservatisms are discussed.

2.0 METHODOLOGY

Annual tritium oxide concentration results calculated using AXAIRQ, MAXIGASP, and CAP88 output are compared with data taken from SRS Environmental Reports for 1985-1994.

2.1 Computer Models Used

Though used for different purposes, all three computer models have the ability to predict annual average relative air concentrations at various locations. Each of the programs are described briefly below.

2.1.1 AXAIRQ

AXAIRQ (Simpkins 1995a and 1995b) is primarily used to predict doses to the maximally exposed offsite individual following hypothetical accidental atmospheric releases of radioactive material. AXAIRQ is based on U.S. Nuclear Regulatory Commission (NRC) Regulatory Guide 1.145 (USNRC 1982) and releases can originate from either a vent or stack. Exposure pathways within AXAIRQ include: inhalation, ground shine, and plume shine. Primary applications include Safety Analysis Reports (SARs) and Hazard Assessments (HADs).

2.1.2 MAXIGASP

MAXIGASP (Bauer 1991 and Hamby 1992), which is used to predict offsite doses for routine releases of atmospheric radioactivity, is based on U.S. NRC Regulatory Guide 1.109 (USNRC 1977). MAXIGASP is a combination of two codes developed by the NRC: XOQDOQ and GASPAR. XOQDOQ (Sagendorf et al. 1982) predicts the downwind relative air concentrations based on a given set of input parameters. GASPAR (Eckerman et al. 1980) utilizes the output from XOQDOQ to predict doses for a variety of exposure pathways (inhalation, ingestion, plume shine, and ground shine.)

MAXIGASP is used primarily to predict doses to the maximally exposed offsite individual for the annual Environmental Report and various Environmental Impact Statements (EISs). MAXIGASP contains site-specific land usage parameters (Hamby 1991).

2.1.3 CAP88

The Environmental Protection Agency (EPA) developed CAP88 (Beres 1990) to implement the mathematical models for assessing dose and risk due to radionuclide emissions to the air. CAP88 is used to demonstrate NESHAPS compliance (40CFR61). The following exposure pathways are considered: inhalation, ingestion, plume shine, and ground shine. None of the models within CAP888 have been modified for use at SRS, however, some of the

default parameters have been changed to accurately reflect conditions that are typical at SRS (i.e. humidity).

2.1.4 Annual Average Concentration Calculation

Each of the computer programs predict annual average concentrations using the same basic equation. Annual average concentrations are determined by weighting each of the calculated concentrations in accordance with the probability of the occurrence using the following equation:

$$\text{annual } (\overline{\chi/Q}) = \sum P_i \left(\frac{\chi}{Q} \right)_i \quad (1)$$

where

P_i = probability of a given set of meteorological conditions occurring
 $(\chi/Q)_i$ = sector arc average relative air concentration associated with the given set of meteorological conditions

Sector arc average relative air concentrations are determined using the following equation:

$$\left(\frac{\chi}{Q} \right)_{(x,0)} = \frac{2.032e^{-\left(\frac{h_e}{2\sigma_z^2} \right)}}{\sigma_z U x} \quad (2)$$

where

χ/Q = sector arc average relative air concentration (sec/m^3)
 x = downwind distance (m)
 h_e = effective release height (m)
 U = wind speed (m/sec)
 σ_z = standard deviation of the concentration distribution in the vertical direction (m)

Each of the computer programs uses equations (1) and (2). However, parameters within the equations may differ within each program. These difference are discussed in the results section.

2.1.5 Computer Model Input

Since each program has a different purpose, their associated inputs vary. Input data was kept as similar as possible. Table 1 shows the input parameters that were used. Parameters relating to dose are not shown since they do not affect the annual average concentration values.

Table 1. Input parameters for Code Comparison

Parameter	Input
Grid Coordinates	E 58000 and N 62000
Meteorological data file accessed	H Area
Release Height	61 m
Plume Rise	Options not activated
Diffusion Coefficients	Pasquill-Briggs (Different Formulas used for each)
Mixing Height	1000 m
Source Term	H-3, 1 Ci/yr

Meteorology from H Area for a five-year period (1987-1991) was used as input for each of the computer codes. At SRS meteorological data is collected at eight onsite towers. The most complete set of data is for H Area which is near the center of the site. Meteorological data is based on a joint frequency distribution of hourly averages for the entire five year period. The hourly averages are based on readings of the fluctuation of wind direction collected every 15 seconds. The results are grouped into seven stability categories (A-G) and six wind speed classes. Figure 1 shows the wind rose for SRS for 1987-1991. As seen in the figure, the most frequent wind direction is toward the SW.

2.2 Existing Tritium Oxide Data

Tritium oxide is sampled biweekly using silica gel samples which collect moisture from air pumped through a column. Water is removed from the silica gel by distilling over low heat. The distillate is mixed with a liquid scintillation cocktail, and a liquid scintillation counter is then used to determine the tritium oxide concentration in the atmospheric moisture. Daily atmospheric humidity values are used to convert to tritium oxide concentration in air (Cummins, et al. 1991).

Figure 1. Wind Rose Data for H Area
(Indicates frequency (%) of wind *from* the specified direction)

The tritium oxide concentrations in air at 13 perimeter locations are compared with predicted concentrations from the dose assessment computer codes. The location of each of the collection points is shown in Figure 2. Table 2 shows a list of the perimeter locations and the distance from the center of the site to each location and the corresponding sector. Measured concentrations at each location are shown in Appendix A for

1985-1994. In the Environmental Reports, the data for 1991 and 1994 displayed concentrations as tritium oxide in atmospheric moisture. A site specific humidity value of 11.4 g/m^3 (Hamby 1993) was used to convert the tritium oxide concentration in moisture to concentration in air. Appendix A also shows the computer predicted concentrations.

Tritium oxide releases over the past ten years are shown in Table 3. Releases primarily originated from the Reactor and Separations Areas and the percentage released from each is also shown in Table 3. Referring to Figure 1, Reactor Areas are noted as C, K, L, P, and R and Separations Areas are noted as F and H. Releases from other areas are negligible (<1%).

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Figure 2. Air Monitoring Surveillance Stations at SRS

Table 2. Tritium Oxide Sampling Locations

Sector	Location	Distance from Center of Site (m)
N	E. Talatha Gate	15977
NNE	Windsor Road	17825
NE	Darkhorse	17463
ENE	Highway 21/167	16603
E	Barnwell Gate	14926
SE	Patterson Mill	15518
SSE	Allendale Gate	15322
SSW	A-14	8658
WSW	D Area	10663
W	West Jackson	13061
WNW	Jackson	15258
NW	Green Pond	14484
NNW	Talatha Gate	14362

Table 3. Tritium Oxide Released at SRS

Year	Amount Released (Ci)	Released from Reactors	Released from Separations
1985	4.87E+05	54%	46%
1986	2.85E+05	46%	54%
1987	2.70E+05	37%	63%
1988	2.88E+05	38%	62%
1989	2.18E+05	60%	40%
1990	1.75E+05	45%	55%
1991	1.37E+05	55%	45%
1992	1.00E+05	47%	53%
1993	1.33E+05	29%	71%
1994	1.07E+05	22%	78%

3.0 RESULTS

Concentrations at the 13 site boundary perimeter locations are compared to output from AXAIRQ, MAXIGASP, and CAP88. The predicted annual average air concentration at the specific boundary location (for a 1 Ci release) is multiplied by the total amount of tritium oxide released for the year to determine the annual average tritium oxide concentration. This result is divided by the measured average tritium oxide concentration to determine the "predicted to measured ratio." These ratios are averaged using different combinations to study various effects.

3.1 10-Year Concentration Comparison

For each year, the ratios of predicted to measured tritium oxide concentrations from the 13 perimeter locations are averaged. The results using each of the three codes are shown in Figure 3. For each year AXAIRQ shows the greatest difference of predicted to measured tritium oxide concentrations. The 10-yr average of the ratio of differences for AXAIRQ, MAXIGASP, and CAP88 is 1.89 ± 0.56 , 1.70 ± 0.48 , and 1.40 ± 0.39 , respectively. AXAIRQ is the most conservative since the primary use of the code is for accident analysis.

Figure 3. Predicted/Measured Tritium Oxide Concentrations at SRS Boundary Locations

3.2 Explanation of Variation of Predicted Values

Several differences in code structure contribute to variations in predicted tritium oxide concentrations. The primary difference is the treatment of wind speed averages.

3.2.1 Wind Speed Averages

While each code accesses the same meteorological frequency distribution, each of the three codes uses different methodologies to calculate wind speed averages for the relative air concentration calculations. Table 4 shows the frequency distribution summed for all sectors for each of the 42 stability category and wind speed class combinations. The predominant wind speed classes are two and three. No stability class occurs considerably more than any of the others although stability classes F and G occur the least amount of time.

Table 4. Joint Frequency Distribution for H Area (all sectors)

WS	STABILITY CLASS							TOTAL
	A	B	C	D	E	F	G	
1	6%	1%	1%	1%	0%	0%	0%	9%
2	14%	6%	9%	10%	7%	1%	0%	47%
3	3%	4%	7%	10%	10%	2%	0%	37%
4	0%	1%	2%	1%	0%	0%	0%	5%
5	0%	0%	1%	0%	0%	0%	0%	1%
6	0%	0%	0%	0%	0%	0%	0%	0%
TOTAL	24%	12%	20%	23%	17%	4%	0%	100%

The meteorological data files accessed by AXAIRQ contain wind speed averages for each of the 16 sectors and 42 stability class and wind speed combinations. These 672 values are the actual harmonic average wind speeds over the five year period for the sector, stability category, and wind speed class of interest. The wind speed ranges for each of the six categories are: 0-2, 2-4, 4-6, 6-8, 8-12, and >12 m/s.

MAXIGASP contains a set of constant wind speed values that correspond to each of the six wind speed classes. The values used by MAXIGASP, which correspond to wind speed classes 1-6, are: 1, 3, 5, 7, 9, 10, and 13.05 m/s. Regardless of which sector or stability class is accessed, the same wind speed is used for a given wind speed class.

CAP88 uses a harmonic average wind speed value for each stability class and sector. Therefore, 112 (16 sectors and 7 stability categories) different values are used for the calculations. These values generally show only slight variations from stability class A-G with typical values ranging from 2.5 - 4.0 m/s.

As seen in equation 2, the wind speed is inversely proportional to the sector arc average relative air concentration. Since CAP88 wind speed values are determined by weighting the various wind speed values within a given stability class, the values are higher than the values used by AXAIRQ and MAXIGASP, therefore, resulting in lower concentrations.

3.2.2 Mixing Height

Mixing height is set to a constant value of 1000 m in MAXIGASP and CAP88. Mixing height is a user input value in AXAIRQ and the value was set at 1000 m for this comparison. The average observed mixing height for SRS in 1978 was 1260 m (Garrett 1981). Monthly observed mixing heights were under 1000 but greater than 900 for only 2 months of the year. The mixing height value of 1000 m is conservative with respect to yearly average observed values. AXAIRQ limits the value of the vertical diffusion coefficient (σ_z) to 80% of the value of the mixing height. Both CAP88 and MAXIGASP limit the vertical diffusion coefficient to a value equal to the mixing height. Since relative air concentration is inversely proportional to vertical diffusion coefficient, AXAIRQ estimates a higher value for relative air concentration. This is the primary difference between AXAIRQ and MAXIGASP.

3.2.3 Terrain

Both AXAIRQ and MAXIGASP adjust the height of the release according to terrain height at the location of the receptor. CAP88 does not account for terrain. Terrain data was provided by Oak Ridge National Lab (ORNL) for a grid surrounding the site. AXAIRQ and MAXIGASP convert this grid to a polar coordinate system centered on the release location. The terrain height at the location of the receptor is assumed to be the maximum terrain height difference between the receptor and the release location. The height of the plume is reduced by the maximum terrain height between the plume and the receptor.

MAXIGASP has a feature that allows the user to utilize terrain effects or assume flat earth. The code was executed using both methods. The predicted versus measured tritium oxide concentrations are shown in Figure 4 with and without terrain effects. The 10-year average with terrain

considered is 1.70 ± 0.48 and the 10-year average for flat earth is 1.57 ± 0.66 . These differences are slight in comparison to differences due to wind speed averaging.

Figure 4. Predicted/Measured Tritium Oxide Concentrations using MAXIGASP with Terrain Effects and for Flat Earth

3.2.4 Release Types

Over the years releases occurred from various locations and release heights. While the bulk of the releases originate from the center of the site, a few of the releases were actually closer to the boundary. Some of the releases may not have occurred at a stack height of 61 m, but at ground level. Additional analysis is needed to determine the effect of these parameters.

3.2.5 Differences in Dose Predictions

Each of the three computer codes predict dose differently and use different exposure pathways. The differences in concentration are therefore not indicative of the difference in dose for each of the programs. Both CAP88 and MAXIGASP predict doses to the maximally exposed offsite individual based on annual average concentrations as used in this study. AXAIRQ calculates dose for meteorological conditions not exceeded 99.5% of the time dependent on sector or 50% or 95% independent of sector.

4.0 CONCLUSIONS

Various dose assessment computer programs used at SRS over predict the offsite tritium oxide concentrations by a factor of 1.4 - 2.0. Since annual average concentrations are typically predicted within a factor of two to four using Gaussian plume models (Miller et al. 1987), these results show exceptional agreement. Each of the computer models follows appropriate regulatory guidance and any attempt to change currently acceptable methodology would require extensive site-specific studies and significant technical justification.

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Appendix A. Tritium Oxide Concentrations**Table A1. Air Concentrations at Various Offsite Locations**

Sector	Location	Air Concentration (pCi/m ³)				
		1985	1986	1987	1988	1989
N	E. Talatha Gate	110	64	71	51	34
NNE	Windsor	120	73	66	58	33
NE	Darkhorse	110	78	78	50	34
ENE	Highway 21/167	99	73	160	42	36
E	Barnwell Gate	97	75	57	45	33
SE	Patterson Mill	75	52	41	33	20
SSE	Allendale Gate	50	48	33	24	20
SSW	A-14	140	140	88	65	53
WSW	D Area	310	140	140	90	74
W	W. Jackson	130	73	71	50	33
WNW	Jackson	97	64	64	47	29
NW	Green Pond	120	72	75	64	31
NNW	Talatha Gate	110	76	110	86	50

Table A1. continued. Air Concentrations at Various Offsite Locations

Sector	Location	Air Concentration (pCi/m ³)				
		1990	1991	1992	1993	1994
N	E. Talatha Gate	31	26	24	29	27
NNE	Windsor	27	2*	31	26	28
NE	Darkhorse	26	2*	26	30	25
ENE	Highway 21/167	27	19	21	27	18
E	Barnwell Gate	27	19	19	26	17
SE	Patterson Mill	22	18	20	14	12
SSE	Allendale Gate	19	16	17	9	14
SSW	A-14	34	29	36	38	20
WSW	D Area	56	39	53	60	43
W	W. Jackson	33	22	26	27	19
WNW	Jackson	30	18	24	36	16
NW	Green Pond	40	18	24	32	22
NNW	Talatha Gate	44	22	23	36	31

* Data point ignored because not in range of minimum to maximum as displayed in Environmental Report.

Concentrations listed in Table A2 are multiplied by the total amount of tritium oxide released for a given year (see Table 3). This predicted tritium oxide concentration for a given year and location is compared with the actual concentrations in Table A1.

Table A2. Concentrations per Unit Release Predicted by the Computer Programs

Sector	Location	Distance (m)	AXAIRQ (pCi/m ³)	MAXIGASP (pCi/m ³)	CAP88 (pCi/m ³)
N	E. Talatha Gate	15977	4.89E-04	4.48E-04	3.80E-04
NNE	Windsor Road	17825	3.89E-04	3.37E-04	2.70E-04
NE	Darkhorse	17463	3.81E-04	3.56E-04	3.00E-04
ENE	Highway 21/167	16603	3.83E-04	3.51E-04	3.00E-04
E	Barnwell Gate	14926	3.74E-04	3.28E-04	2.80E-04
SE	Pattersons Mill	15518	2.00E-04	1.88E-04	1.60E-04
SSE	Allendale Gate	15322	1.68E-04	1.58E-04	1.30E-04
SSW	A-14	8658	5.11E-04	5.24E-04	4.30E-04
WSW	D Area	10663	5.96E-04	5.56E-04	4.80E-04
W	West Jackson	13061	3.37E-04	2.99E-04	2.70E-04
WNW	Jackson	15258	2.88E-04	2.62E-04	2.10E-04
NW	Green Pond	14484	4.35E-04	3.65E-04	2.80E-04
NNW	Talatha Gate	14362	6.48E-04	4.95E-04	3.70E-04

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Distribution List(10)

A.L. Boni, 773-A
W.H. Carlton, 773-A
J. D. Heffner, 735-16A
G.T. Jannik, 773-A
R. Lorenz, 735-16A
K.R. O'Kula, 992-1W
L.M. Papouchado, 773-A
A.A. Simpkins, 773-A
EDG Files, (3), 773-A