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MODELLING CHRONIC ATMOSPHERIC RELEASES AT THE SRS: EVALUATION AND VERIFICATION OF XOQDOQ (U)

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SUMMARY

XOQDOQ is the atmospheric dispersion code used by the Savannah River Laboratory to estimate offsite concentrations resulting from chronic releases of radioactivity. This report documents evaluation and verification studies performed on XOQDOQ. The studies were designed to establish compliance with Site quality assurance requirements for high-impact software.

Comparisons of XOQDOQ results with that of a series of Excel® spreadsheets indicate that the code is performing as intended by the designers. Relative concentration and deposition values, χ/Qs and D/Qs, calculated by the two methods differed by no more than 0.5% in any of the test cases.

Estimates of ground-level air concentrations at the Site boundary calculated with XOQDOQ were compared with tritium concentrations measured at those locations. XOQDOQ generally overestimates tritium concentrations by a factor of 1 to 3. Other radionuclides released in recent years by the SRS have not been present in sufficient concentrations to permit evaluation efforts. However, previous studies of Kr-85, I-129, and Pu-238 have shown XOQDOQ predictions of offsite air concentrations to be adequate.

Based on this review, the performance of XOQDOQ is acceptable for continued use at the SRS. Efforts to improve the code should also be continued. Sensitivity studies of such parameters as particle size distribution, roughness length, and surface moisture would also be useful.

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INTRODUCTION

XOQDOQ is the atmospheric dispersion code used at the SRS to model offsite concentration and deposition patterns from routine releases of radioactive effluents. A comprehensive review of XOQDOQ has been conducted in association with the WSRC quality assurance requirements for software. In this report, the basic structure of the code is described, the supporting data files are documented, and the performance of the code is evaluated.

DOCUMENTATION OF XOQDOQ AS IMPLEMENTED AT THE SRS

Code History

XOQDOQ was originally developed by J. Sagendorf (National Oceanic and Atmospheric Administration) and J. Goll (U.S. Nuclear Regulatory Commission). Issue dates of the code and its revisions are as follows:

Original	June 1976
Revision 1	August 1977
Revision 2	April 1982

The version currently used at the SRS is Revision 2 which is in residence on an IBM 3380 as TENVT.TMECA.FORT(XOQDOQR2). The source code (magnetic tape OP0033) was provided by J. Hawxhurst, Meteorological Section, Meteorology and Effluent Treatment Branch, Division of Systems Integration, U.S. Nuclear Regulatory Commission, on November 15, 1982.

Site-Specific Modifications

XOQDOQ was modified by W. Pillinger on 6-29-83 and on 11-24-84. The modifications are marked in columns 73-80 of TENVT.TMECA.FORT(XOQDOQR2). The changes were primarily associated with expanding arrays and changing read/write statements to make it possible for XOQDOQ to calculate relative concentrations (1) at specific points along the SRS boundary for "maximum" and "average" individuals, and (2) within compass sector regions for population dose assessments. In addition, one other change was made; a 12th control option was invoked which constrains sector-arc average χ/Qs (relative concentrations or "chi over Q's") to values $\leq$ plume centerline χ/Qs.

Additional modifications to Version 2.0 were made by L. Bauer on 5-16-90. The subroutines called by XOQDOQ to calculate χ/Qs from short-term releases were removed from the code. XOQDOQ is not the best available code for estimating χ/Qs from purges or process upsets. This step prevented the unauthorized use of XOQDOQR2 for purge calculations. It also eliminated the need to verify code subroutines which have never been used and are not expected to be utilized in the foreseeable future. However, the complete source code, including the subroutines for purge calculations, can be retrieved from its archive location - TENVT.TMECA.FORT (XOQPURGE).

Descriptions of Input Data Files

XOQDOQ is invoked by three dose scenarios which call unique combinations of data files. All of the data files (i.e., data members) called by XOQDOQ are identified in tables located in Appendix I. The three types of data calls made by XOQDOQ involve:

1) SRS boundary data
2) Regional terrain data, and
3) SRS meteorológical data.

Boundary Data

The current boundaries of the SRS are recognized by XOQDOQ as 875 pairs of SRP Easting and Northing coordinates. These coordinates have been reviewed for accuracy and were approved for use on 7-26-90. The perimeter of the Site, as drawn by the boundary file SRSBNDRY, is shown below in Fig. 1. Complete listings and documentation for the boundary files used by XOQDOQ throughout its history have been archived as a QA record (Bauer 1990).

For certain applications of XOQDOQ, it is necessary to determine the minimum distance from the release point to the Site boundary. This calculation is performed pursuant to the methodology shown in Fig. 2. The specific example cited is a Site center release as evaluated using MAXIGASP, a computer code which calculates doses to a "maximum" or "average" individual at the Site perimeter based on concentration data generated by XOQDOQ. Though the east sector is shown in Fig. 2, analogous calculations are performed by XOQDOQ/MAXIGASP for 16 22.5° compass sectors.

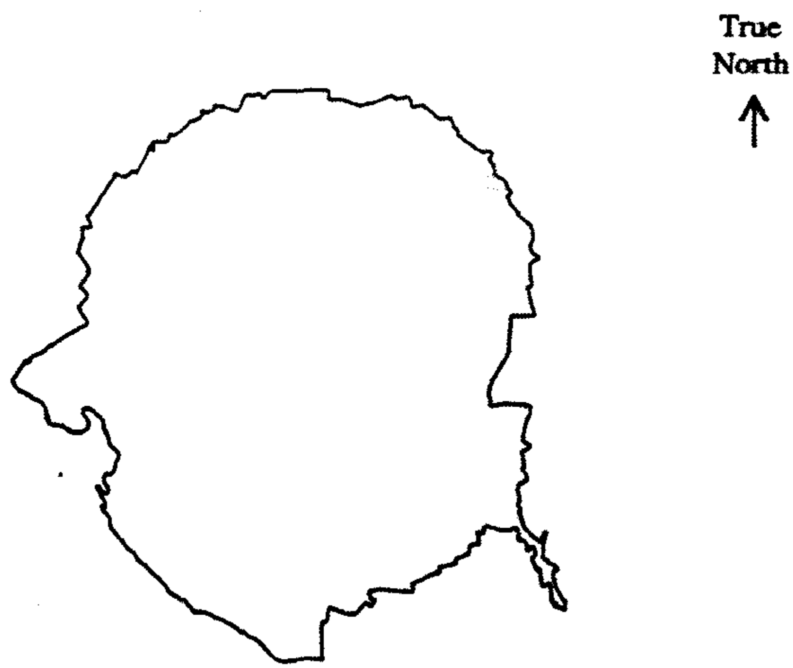
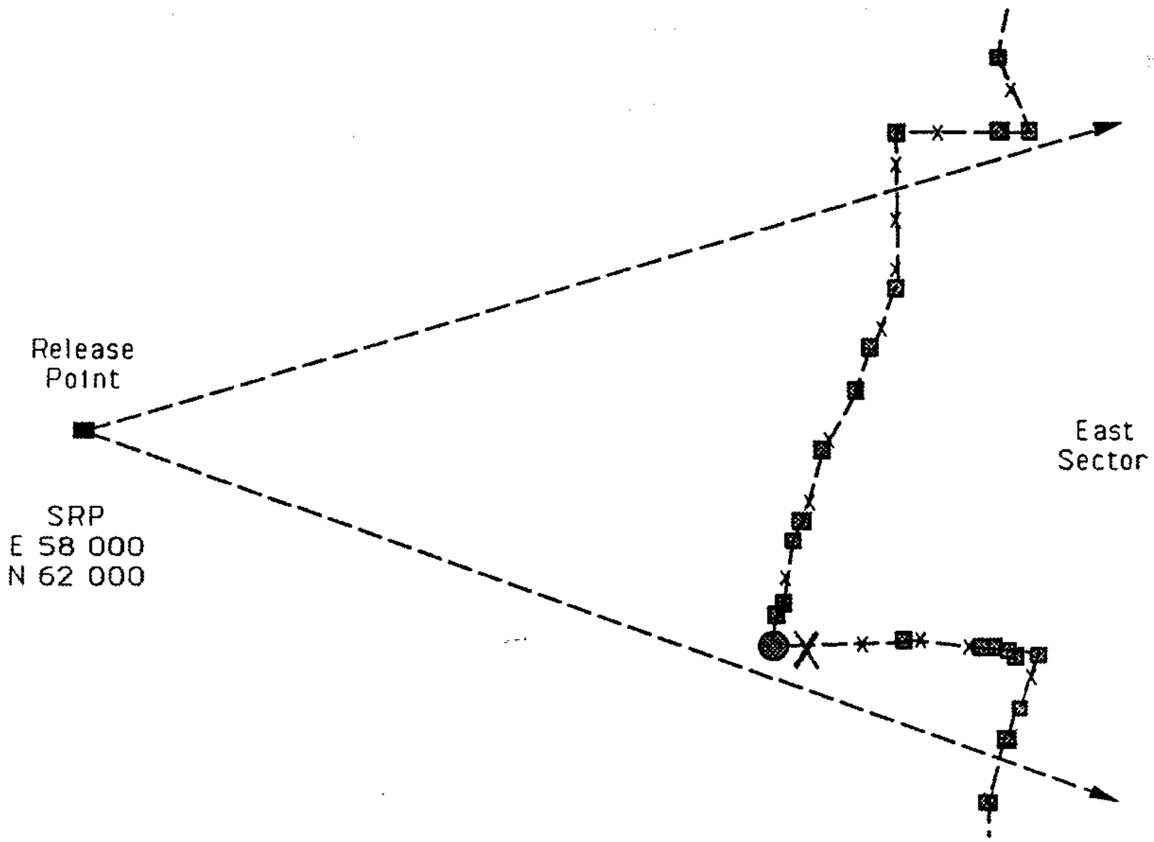


Figure 1. Current boundary file, SRSBNDRY.



LEGEND:

- - -	=	actual boundary
■	=	one of the 875 boundary points contained in TENVT.TMECA.DATA.SRSBNDRY. In the east sector, there are 17 such points.
—x—	=	one of 320 equally-spaced points about the perimeter. Fifteen such points lie within the east sector.
●	=	**the point in the east sector where the distance from the release point is the smallest. The point is selected based on the smallest distance between the release point and:** (1) any of the boundary points, (2) any of the line segments connecting the boundary points, or (3) the two intersections of the compass sector with the perimeter.
X	=	the equally-spaced point that lies nearest the point of minimum distance. To ensure that doses are calculated for the minimum distance, this point is moved to the coordinates of ●.

Figure 2. MAXIGASP's use of the boundary file SRSBNDRY.

Terrain Data

The height of the plume as it travels away from the release point may be adjusted to account for changes in terrain. Arrays of maximum changes in elevation, relative to the release point's elevation, are called to determine the reduction in plume height required for a specific compass sector and downwind location. Documentation for the original source of these data is no longer available. However, the array of elevation changes for the Site center was compared with NOAA aeronautical chart data for the southeast United States; no discrepancies were found.

Meteorological Data

XOQDOQ currently has the ability to access wind speed, wind direction, and atmospheric stability data collected from one of seven onsite meteorological towers. The towers are instrumented at 62 meters, which is approximately equal to the heights of the primary reactor and separations areas stacks. The towers are equipped with cup anemometers to measure wind speed, and with bivanes to measure the horizontal and vertical components of wind direction. Though data for many tower/time period combinations are available, wind field statistics called by XOQDOQ are most frequently based on approximately 30,000 average hourly values collected from 1982 to 1986.

XOQDOQ uses these data in the form of joint frequency distributions of wind direction, wind speed range, and atmospheric stability class for each of 16 22.5° compass sectors. The turbulence typing scheme used is the Pasquill-Gifford stability classification system.

The meteorological monitoring program in use at the SRS has been described in more detail by Hunter (1990). The collection and quality assurance of these data are the responsibility of the Environmental Transport Group (ETG). Documentation of the applicable QA procedures followed by ETG may be found in Laurinat (1987) and Hunter (1990).

Deviation from industry guidelines. NRC Reg Guide 1.111 (NRC 1977) recommends the collection of mixing height data. However, mixing height is not measured onsite and is not a user-specified variable in XOQDOQ. The maximum vertical plume dispersion (σ_z) allowed by the code is 1000 m. Regional data compiled by Garrett (1981) show that monthly average mixing heights are generally greater than this value, except during the months of December and January. Though the averages for those winter months were found to be lower than 1000 m, this is not believed to impact significantly the calculation of annual average χ/Qs.

PRINCIPAL XOQDOQ STRUCTURE AND FEATURES

Background

XQODOQ is a computer program developed for use by the Nuclear Regulatory Commission to evaluate atmospheric releases from commercial nuclear power operations (Sagendorf and Sandusky 1982). The calculations performed by XOQDOQ are those established in Reg. Guide 1.111 for the release of an effluent from a stack or vent under conditions of constant wind direction. The material in the plume is assumed to be normally distributed about the plume centerline and to be depleted by dry deposition and radioactive decay.

XOQDOQ uses gradient-transport theory as the basis for its diffusion-deposition model. The material flux in the plume is assumed to be proportional to the local concentration gradient in the x-z plane. The horizontal wind field, y, is considered to be constant. Classic Fickian diffusion equations are used to evaluate the system over time and space. Downwind relative concentrations, χ/Qs, are then determined using exact solutions for continuous point-source releases.

Key XOQDOQ Features

1. χ/Qs and D/Qs (relative deposition) values for each of 16 22.5° compass sectors at 10 radial distances out to 80,450 m.
2. Vertical plume dispersion, σ_z, to 1000 m .
3. Uniform horizontal concentration across a given compass sector.
4. Effective plume height due to:
   a. physical stack height
   b. aerodynamic downwash
   c. plume rise
      i. momentum
      ii. buoyancy
5. Plume depletion via:
   a. dry deposition
   b. radioactive decay (plume half-lives of 0.00, 2.26, or 8.00 days)

Code Structure

The structure of XOQDOQ is shown in Fig. 3. The calculations performed by major subroutines are described in the following sections. More detailed discussions of XOQDOQ's treatment of depletion, deposition, and plume rise also follow.

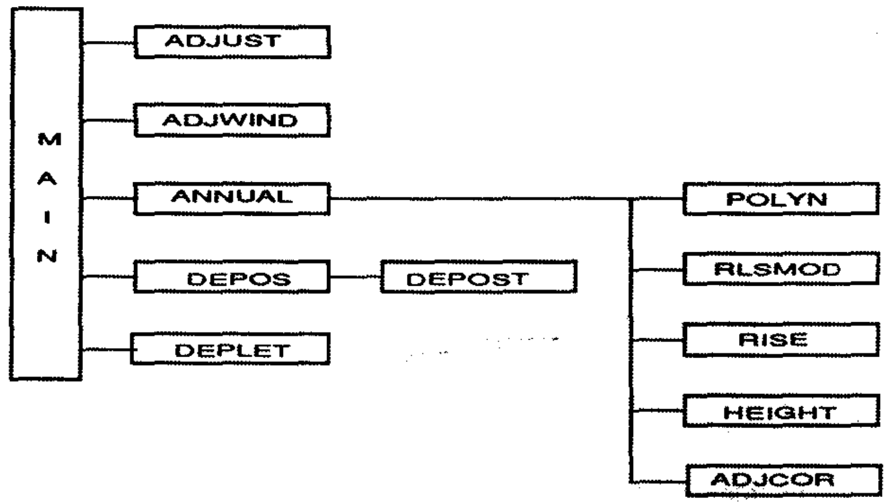


Figure 3. XOQDOQ structure.

Subroutine Descriptions

ADJUST. This subroutine adjusts effective plume heights to correct for terrain changes. Such modifications are required to establish which series of depletion/deposition curves are to be read at a given downwind location.

ADJWIND. ADJWIND provides a wind speed correction factor, CORR, when the release height does not equal the measured wind height.

$$CORR = \left(\frac{SL}{PL} \right)^{ex} \quad (1)$$

where

SL = desired wind height, m
PL = measured wind height, m
ex = 0.25 (Stability classes A, B, C, D)
0.50 (Stability classes E, F, G)

ANNUAL. ANNUAL calculates annual average ground-level and elevated χ/Qs and D/Qs for a uniform distribution of effluent across the compass sector.

For **elevated** releases the χ/Q values for specific downwind locations are calculated as follows:

$$\chi / Q(x,k) = 2.032 \sum_{ijk} \frac{JFD_{ijk} \cdot DEC_i(x) \cdot DEPL_{ij}(x,k)}{\bar{u}_i(x) \cdot \sigma_{z_j}(x) \cdot x} \cdot e^{-0.5\left(\frac{h_e}{\sigma_{z_j}(x)}\right)^2} \qquad (2a)$$

where $\chi / Q(x,k)$ = relative concentration at x meters downwind in the kth 22.5° compass sector, s/m^3

i = wind speed class, m/s

$0 \le u \le 2$	$6 < u \le 8$
$2 < u \le 4$	$8 < u \le 12$
$4 < u \le 6$	$12 < u \le 14.1$

j = atmospheric stability class

A,B, C	Unstable
D	Neutral
E,F,G	Stable

$\bar{u}_i(x)$ = mid-point of the ith wind speed class, m/s

1.0	7.0
3.0	10.0
5.0	13.15

$\sigma_{z_j}(x)$ = vertical plume spread due to ambient free-stream turbulence as determined by SR **POLYN**, m

JFD = joint frequency distribution of wind speed and atmospheric stability observations

DEC_i = plume decay factor

$DEPL_{ij}(x,k)$ = plume depletion factor as determined by SR **DEPLET** et al.

h_e = effective plume height as defined by SRs **RISE** and **HEIGHT**, m and where

$$DEC_i(x) = e^{-(0.693\, t_i / T)}$$

t_i = $x/(86400 \cdot \bar{u}_i)$, travel time, in days

T = half-life, in days, of the radioactive material

x = downwind or travel distance, in meters

$\bar{u}_i$ = midpoint of the ith wind-speed class in meters/second.

For **ground-level** releases, the larger value from the following two equations is used for specific downwind locations:

$$\chi / Q\,(x,k) = 2.032 \sum_{ijk} \frac{JFD_{ijk} \cdot DEC_i(x) \cdot DEPL_{ij}(x,k)}{\sqrt{3} \cdot \bar{u}_i(x) \cdot \sigma_{z_j}(x) \cdot x} \qquad (2b)$$

-or-

$$\chi / Q\,(x,k) = 2.032 \sum_{ijk} \frac{JFD_{ijk} \cdot DEC_i(x) \cdot DEPL_{ij}(x,k)}{\bar{u}_i(x) \cdot \sqrt{(\sigma_{z_j}^2(x) + cD^2/\pi)}} \qquad (2c)$$

where $\chi / Q\,(x,k)$ = relative concentration at x meters downwind in the kth 22.5° compass sector, s/m^3

c = defined constant, 0.5

D = building height used to evaluate dispersion due to building wake effects

Subroutine **ANNUAL** also calculates relative concentration and deposition for 10 downwind segments in each of the 16 compass sectors. The computed value represents an average value for the downwind directional sector bounded by the range of the region. The method used by ANNUAL to calculate a segment average χ/Q is shown in Eq. 3. Eq. 3 is also used to calculate segment average D/Qs.

$$\overline{\frac{\chi}{Q}}_{seg}(k) = \frac{R_1 \cdot \chi/Q(R_1, k) + R_2 \cdot \chi/Q(R_2, k) + R_3 \cdot \chi/Q(R_3, k)}{R_1 + R_2 + R_3} \qquad (3)$$

where

$\overline{\frac{\chi}{Q}}_{seg}(k)$ = average χ/Q for the segment in compass sector k

$\chi/Q(R_n, k)$ = χ/Q at downwind distance R_n for the compass sector k

R_1, R_3 = downwind distance of the segment boundaries

DEPOS. This subroutine calculates D/Qs (relative deposition per unit area) pursuant to Eq. 4. DEPOS uses the same distance information as ANNUAL.

$$\overline{\frac{D}{Q}}(x,k) = \frac{RF(x,k) \sum_{ij}^{N=7} D_{ij} f_{ij}(k)}{(2\pi/16)\, x} \qquad (4)$$

where

$\overline{\frac{D}{Q}}(x,k)$ = average relative deposition per unit area at a downwind downwind distance x and direction k, in meters^{-2}

D_{ij} = the relative deposition rate from Figures 7 through 10 of Regulatory guide 1.111 (USNRC, 1977) for the ith wind-speed class (since plume height is dependent on wind speed) and the jth stability class, in meters.

$f_{ij}(k)$ = joint probability of the ith wind-speed class, jth stability class, and kth wind-direction sector

x = downwind distance, in meters

π = 3.14159265

RF(x,k) = correction factor for air recirculation and stagnation at distance x and kth wind direction

DEPOST. DEPOST solves the polynomial regression equations for the deposition curves of Regulatory Guide 1.111 (NRC 1977). The deposition curves have been reproduced in Appendix II.

DEPLET. DEPLET solves the polynomial regression equations for the depletion curves of Regulatory Guide 1.111 (NRC 1977). The depletion curves have been reproduced in Appendix II.

POLYN. This subroutine calculates values of vertical plume spread, σ_z, as a function of downwind distance using equations of the form:

$$\sigma_{z_j}(x) = ax^b + c \qquad (5)$$

where σ_{z_j} = vertical standard deviation of material in the plume due to ambient free-stream turbulence for stability category j

x = downwind distance

a,b,c = coefficients, derived by Eimutis and Konicek (1972), which are functions of stability class and distance

(σ_z is limited to 1000 meters.)

RLSMOD. RLSMOD is invoked for mixed-mode releases. RLSMOD evaluates the need for an entrainment factor, E_t, by computing the ratio of the plume exit velocity to the wind speed. If a mixed-mode release is indicated, the proportion of the plume considered to be elevated and the proportion considered to be ground level are determined by the following relationships:

$$E_t = 1.0 \qquad \text{for } W_o/\bar{u} \le 1.0 \qquad (6a)$$

$$E_t = 2.58(W_o/\bar{u}).- 1.58(W_o/\bar{u}) \qquad \text{for } 1.0 < W_o/\bar{u} \le 1.5 \qquad (6b)$$

$$E_t = 0.3 - 0.06(W_o/\bar{u}) \qquad \text{for } 1.5 < W_o/\bar{u} \le 5.0 \qquad (6c)$$

$$E_t = 0.0 \qquad \text{for } W_o/\bar{u} > 5.0 \qquad (6d)$$

where

E_t = fraction of the time when the release is ground level

W_o = the plume exit velocity

$\bar{u}$ = average wind speed at the vent height

RISE. Plume rise, h_{pr}, is calculated using the formulae of Briggs (1969). Plume rise due to momentum and buoyancy is considered, and the lesser value is selected for use. However, as SRS atmospheric releases are considered to be ambient temperature plumes, plume rise may be considered to be exclusively a function of momentum. The specific empirical relationships recognized by RISE for h_{pr} as a function of momentum are:

For stability classes A, B, C, D, the smaller value of

$$1.44\left(\frac{w}{u}\right)^{2/3} \cdot \left(\frac{x}{d}\right)^{1/3} \cdot d \quad , m \tag{7a)*}$$

$$3\left(\frac{w \cdot d}{u}\right) \quad , m \tag{7b)*}$$

where w = effluent exit velocity, m/s
u = wind speed at release height, m/s
x = downwind distance, m
d = stack diameter, m

For stability classes E, F, G, the smallest value of

$$1.44\left(\frac{w}{u}\right)^{2/3} \cdot \left(\frac{x}{d}\right)^{1/3} \cdot d \quad , m \tag{7a)*}$$

$$3\left(\frac{w \cdot d}{u}\right) \quad , m \tag{7b)*}$$

$$4\left(\frac{F_m}{S}\right)^{0.25} \quad , m \tag{7c}$$

$$1.5\left(\frac{F_m}{u}\right)^{1/3} \cdot S^{-1/6} \quad , m \tag{7d}$$

where F_m = momentum flux parameter, m^4/s^2

$$F_m = \left(\frac{w \cdot d}{2}\right)^2 \tag{7e}$$

S = restoring acceleration per unit vertical displacement for adiabatic motion in the atmosphere, s^{-2}

E	$8.75 \times 10^{-4}/s^2$
F	$1.75 \times 10^{-3}/s^2$
G	$2.45 \times 10^{-3}/s^2$

---

* If w < 1.5 u, plume rise is adjusted for downwash by subtracting the following correction factor, C:

$$C = 3\left(1.5 - \frac{w}{u}\right) \cdot d \quad , m$$

HEIGHT. An effective plume height, $\mathbf{h_e}$, is calculated by XOQDOQ using Eq. 8. HEIGHT linearly interpolates an $\mathbf{h_t}$ for a given downwind distance X, based on the highest elevation between the source and X -- anywhere in the compass sector in which X falls.

$$h_e = h_s + h_{pr} - h_t \quad (h_e \geq 0) \tag{8}$$

h_e = effective plume height, m
h_s = physical stack height, m
h_{pr} = plume rise, m
h_t = terrain height, m

ADJCOR. ADJCOR keeps track of the cross-over heights which each plume passes for each direction, wind-speed class, and stability category. It determines which depletion and deposition adjustment factors derived in **ADJUST** should be used. XOQDOQ's treatment of depletion and deposition are described more fully on pages 15 and 17, respectively.

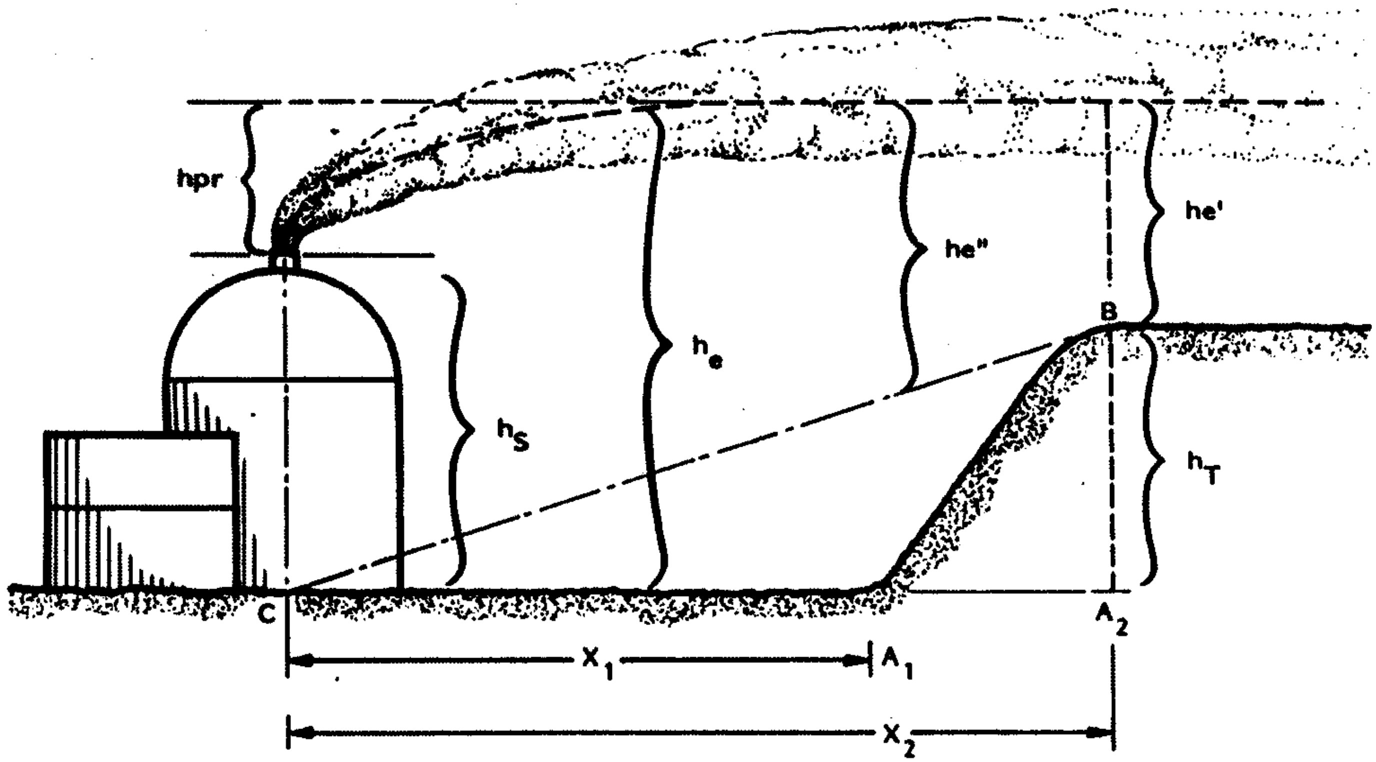
Treatment of Plume Rise, Depletion and Deposition

Plume Rise

Though XOQDOQ can accommodate plume rise due to momentum and buoyancy, only momentum is applicable to the SRS stacks as they are characterized by ambient temperature plumes. Plume rise due to momentum is addressed in XOQDOQ through the use of empirical relationships developed by Briggs (1969). Although these relationships are somewhat dated, they are still widely used and little improvement over them has been observed in the last 10 years (Netterville 1990).

The formulae of Briggs are based on the effective stack height method in which plume rise is artificially decoupled from dispersion. The principal site-specific parameters upon which plume rise depends are effluent exit velocity, wind speed, stack diameter, and stack height.

At the user's option, XOQDOQ will adjust plume height to reflect changes in topography. The impact this feature has on effective stack height is shown in Fig. 4 (Sagendorf et al. 1982).



h_S = HEIGHT OF STACK (RELEASE Pt)

hpr = HEIGHT DUE TO PLUME RISE

he = EFFECTIVE STACK HEIGHT

he', he" = EFFECTIVE STACK HEIGHT WITH TERRAIN CORRECTION

h_T = TERRAIN HEIGHT ABOVE PLANT GRADE

X_1, X_2 = DISTANCE TO TERRAIN FEATURES

Figure 4. "Effective" stack height in XOQDOQ.

Depletion

Plume depletion by XOQDOQ is automatic whenever 8-day decayed χ/Qs are calculated. The methodology is based on work by Markee (1967) in connection with the CERT (Controlled Environmental Radioiodine Tests) Project conducted at the NRTS (National Reactor Testing Station) in Idaho.

Plume depletion via ground surface adsorption was assumed by Markee to be a function of eddy diffusivity and wind velocity. By establishing vertical profiles of these variables, Markee was able to estimate vertical plume concentration profiles for a variety of release conditions applicable to the NRTS. The results of those studies were used by the NRC to develop depletion factors for general use. Depletion curves for release heights of 0, 30, 60, and 100 meters, expressed as a function of atmospheric stability class, were published in Reg Guide 1.111 (NRC 1977). Those figures have been reproduced in Appendix II.

The applicability of these depletion factors to non-NRTS conditions has not been established. Also, there is no provision in the NRC approach to accommodate site-specific parameters such as mixing height.

Implementation in XOQDOQ. XOQDOQ decreases the total mass in the plume at progressive downwind distances by solving the polynomial regression equations of the depletion curves described above. Because depletion factors are a function of plume height, XOQDOQ uses subroutines ADJCOR and ADJUST to track the plume and modify the depletion factors as terrain features (and therefore effective plume heights) change with increasing distance. This often dictates that more than one set of depletion curves be used. The downwind distances at which it is necessary to change from one set of curves to another are referred in XOQDOQ as cross-over points.

XOQDOQ's treatment of depletion is shown in Fig. 4 for a 60-m release. The depletion factors of Reg Guide 1.111 would be adjusted by XOQDOQ as follows for a downwind distance of X:

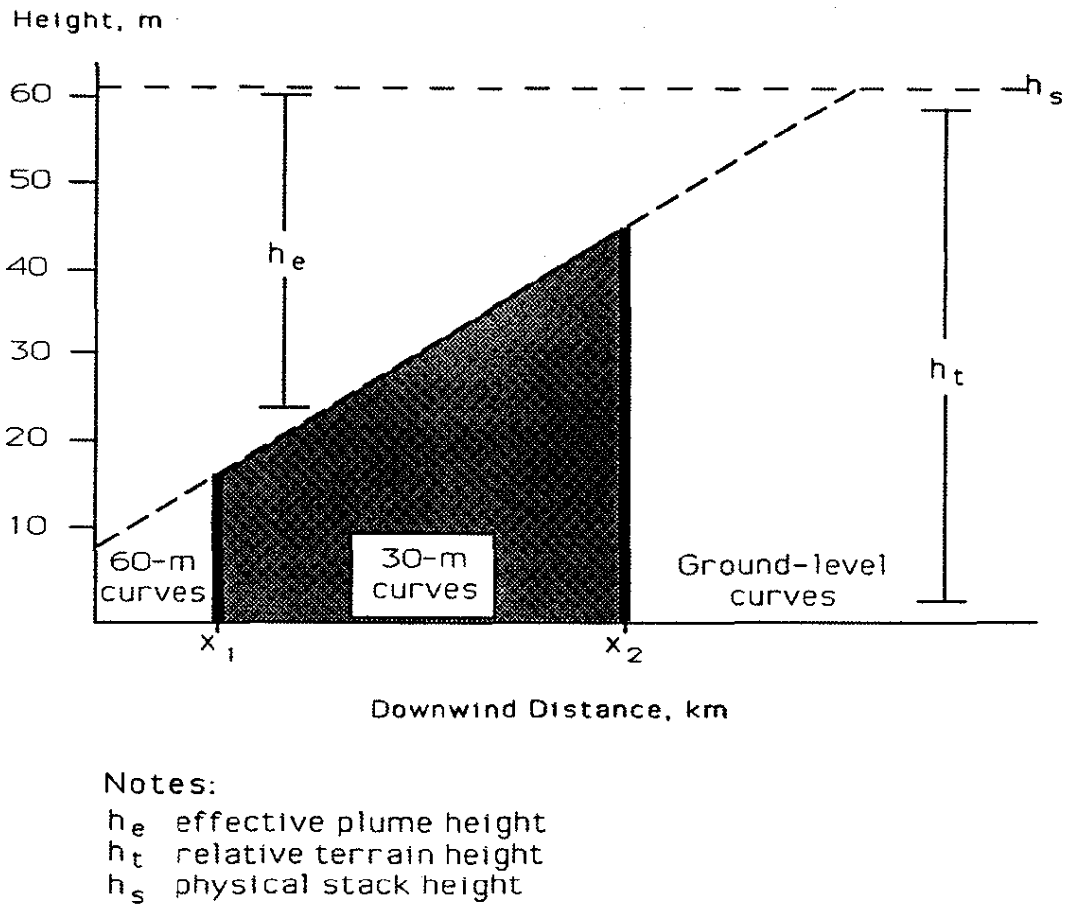


Figure 5. XOQDOQ treatment of cross-over points.

$X < x_1$	Stability-class-specific depletion factors taken from their respective 60-m curves. No adjustments are required.
$x_1 \leq X < x_2$	Once the plume passes a cross-over point, depletion factor adjustments are required. Depletion factors for distances in this range are adjusted by adding to them the difference between the 60-m and 30-m depletion factors evaluated at the cross-over point, x_1.
$X \geq x_2$	At this point, the depletion factors are adjusted by adding to them the difference in the 60- and 30-m curves at x_1 as well as the difference between the 30-m and ground-level curves at x_2.

Deposition

Relative deposition is calculated in XOQDOQ based on deposition velocities (v_ds) measured by Pelletier and Zimbrick (1970) as a function of wind speed. The data were collected in support of the CERT project, and are therefore specific to the vegetation, wind velocity, temperature, and humidity profiles of the desert NW.

The deposition curves developed by the NRC from the Pelletier and Zimbrick data have not been shown to be equally applicable to all sites. Also, the NRC position does not address the roles of such parameters as particle size distribution, solubility, roughness length for particulates or surface area, surface moisture and stoma openings for gases.

Implementation in XOQDOQ. XOQDOQ uses the deposition curves of Reg Guide 1.111 (NRC 1977) to determine relative deposition rates, m^{-1}. Deposition rates are considered to be functions of the distance from the source, release height and atmospheric stability. The deposition rate curves have also been reproduced in Appendix II.

XOQDOQ estimates relative deposition per unit area, m^{-2}, by multiplying the relative deposition rate by the fraction of the release transported into the sector. This value must then be divided by the arc length of the sector at the distance of interest.

As was required for the depletion factors, XOQDOQ makes adjustments in the deposition factors to account for changes in plume height. The adjustments made at the cross-over points can be categorized as follows using the example presented in Fig. 4.

$X < x_1$ — Stability-class-specific deposition factors taken from their respective 60-m curves. No adjustments are required.

$x_1 \leq X < x_2$ — Once the plume passes a cross-over point, deposition factor adjustments are required. Deposition factors for distances in this range are adjusted by multiplying them by the ratio of the 60-m and 30-m depletion factors evaluated at the cross-over point, x_1.

$X \geq x_2$ — At this point, the deposition factors are adjusted by multiplying them by the ratio of the 60- and 30-m curves at x_1 as well as by the ratio of the 30-m and ground-level curves at x_2.

EVALUATION AND VERIFICATION STUDIES

Evaluation Study Results

Tritium

Estimates of ground-level air concentrations at the Site boundary calculated with XOQDOQ have been compared with measured concentrations of tritium at those locations. Perimeter HTO concentrations for the period 1985 - 1988 (du Pont 1986, 1987, 1988; WSRC 1989) were used to make the comparisons. XOQDOQ's performance was analyzed on a compass-sector-specific basis. The results of the evaluation for 1988 are shown in Figure 6.

As seen in the figure, XOQDOQ generally overestimates HTO concentrations in air by a factor of 1.1 to 3. A few instances of under-predictions were noted for the WSW sector in data from earlier years, but data for that sector are confounded by the effects of D-Area tritium releases.

It is concluded from the ratios of predicted-to-measured values for 1985 - 1988 that XOQDOQ is performing acceptably with respect to its ability to estimate Site boundary HTO ground-level air concentrations.

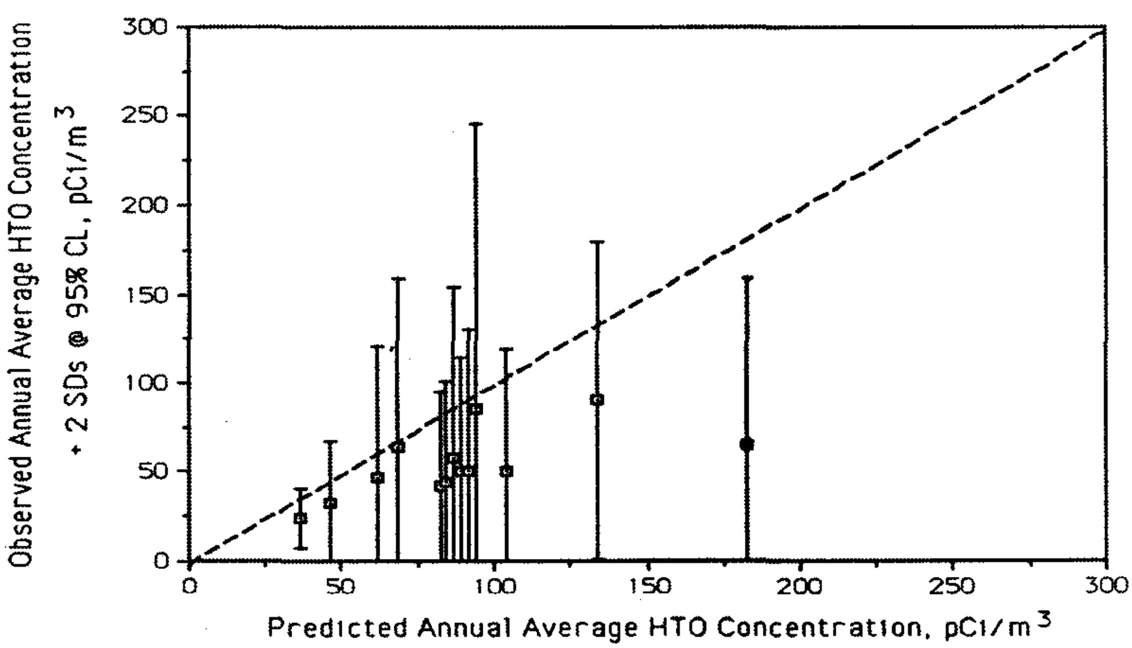


Figure 6. Predicted v. observed HTO concentrations for 1988.

Krypton-85, Iodine-129 and Plutonium-238

Other radionuclides released by the SRS in recent years have not been present in sufficient concentrations in the offsite environment to permit evaluation efforts. However, previous studies of Kr-85, I-129 and Pu-238 have shown XOQDOQ predictions of offsite air concentrations and deposition patterns to be adequate (Marter 1984).

Verification Efforts

Methodology

The calculations performed by XOQDOQ were replicated on Microsoft Excel® spreadsheets to determine the precision of XOQDOQ ouput. The verification runs were divided into two general categories: specific downwind locations and downwind segments. Verification calculations were weighted toward the more commonly used values for XOQDOQ parameters; however, the complete range of release conditions potentially encountered by SRS release conditions were included in the test matrices.

The test conditions for the verification runs are shown in Tables 1a, 1b, 2a, and 2b. Hard copies of the XOQDOQ and Excel® output from the 72 test cases identified in the tables have been archived as QA records.

Results

As seen in Tables 3a and 3b, Excel® spreadsheet- and XOQDOQ-generated values differed by less than 0.5 % for all cases and all distances. In addition to the test cases reported here, many other informal tests of XOQDOQ were conducted; no discrepancies were found.

Generally, DOQ values exhibited better agreement than XOQ values, and segment results were better than point-specific results. These findings reflect differences in computational complexity, and should not be interpreted as evidence of a systematic bias in XOQDOQ or the Excel® simulations.

Table 1a. Matrix for specific downwind locations: releases from SRS center.

Parameter Specifications for Test Cases (n=20)
H-Area Met Data (1982-1986)

	Downwind Distance, m					Release Height, m*				Plume Decay, d			Terrain Included		Exit Velocity, m/s**				
Sector	32180	8045	16090	80450	64360	20	0	62	40	0.00	2.26	8.00	Yes	No	5	0	3	7	9
1. SOUTH					■		■					■		■		■			
2. SSW				■		■					■		■				■		
3. SW			■						■	■			■					■	
4. WSW		■					■					■		■					■
5. WEST	■							■				■	■					■	
6. WNW		■				■					■			■			■		
7. NW			■					■				■	■			■			
8. NNW				■				■		■			■		■				
9. NORTH					■	■					■		■			■			
10. NNE				■			■					■		■			■		
11. NE			■			■					■			■				■	
12. ENE		■					■				■		■						■
13. EAST	■					■				■				■				■	
14. ESE		■						■			■		■				■		
15. SE			■			■						■		■		■			
16. SSE				■					■			■	■		■				
17. WNW					■			■				■	■			■			
18. WSW				■				■				■	■				■		
19. WEST			■					■				■	■					■	
20. NORTH		■						■				■		■		■			

* Range of vertical bldg. areas tested: 0 - 10,000 m^2.
** Range of stack diameters tested: 0-5 m.

Tested by: L.R. Bauer

Table 1b. Matrix for specific downwind locations: non-Site center releases.

Parameter Specifications for Test Cases (n=16)
Test of Non-H-Area Met Files and Terrain Data Calls

	Downwind Distance, m					Release Height, m*		Plume Decay, d			Terrain Included		Release Area (82-86 Met Data)					Exit Velocity, m/s***				
Sector	32180	8045	16090	80450	64360	0	62	0.00	2.26	8.00	Yes	No	D	F	K	P	M**	5	0	3	7	9
21. SOUTH					■	■				■	■		■							■		
22. SSW				■			■		■		■			■							■	
23. SW			■			■		■			■				■					■		
24. WSW		■				■				■	■					■				■		
25. WEST	■						■			■	■						■	■				
26. WNW					■		■		■		■					■			■			
27. NW				■			■			■	■				■				■			
28. NNW		■					■	■			■			■								■
29. NORTH				■			■		■		■		■						■			
30. NNE					■	■				■	■			■							■	
31. NE	■						■		■		■				■				■			
32. ENE				■		■			■		■					■			■			
33. EAST		■				■		■			■						■		■			
34. ESE	■						■	■			■					■				■		
35. SE		■				■				■	■				■					■		
36. SSE			■			■				■	■			■					■			

* Range of vertical bldg. areas tested: 0 - 10,000 m^2.
** M-Area releases evaluated using A-Area met data.
*** Range of stack diameters tested: 0-5 m.

Tested by: L.R. Bauer

Table 2a. Matrix for downwind segments: releases from SRS center.

Parameter Specifications for Test Cases (n=20)
H-Area Met Data (1982-1986)

	Downwind Distance, mi					Release Height, m*				Plume Decay, d			Terrain Included		Exit Velocity, m/s**				
Sector	5-10	10-20	20-30	30-40	40-50	20	0	62	40	0.00	2.26	8.00	Yes	No	5	0	3	7	9
1. SOUTH																			
2. SSW																			
3. SW																			
4. WSW																			
5. WEST																			
6. WNW																			
7. NW																			
8. NNW																			
9. NORTH																			
10. NNE																			
11. NE																			
12. ENE																			
13. EAST																			
14. ESE																			
15. SE																			
16. SSE																			
17. WNW																			
18. WSW																			
19. WEST																			
20. NORTH																			

* Range of vertical bldg. areas tested: 0 - 10,000 m^2.
** Range of stack diameters tested: 0-5 m.

Tested by: L.R. Bauer

Table 2b. Matrix for downwind segments: non-Site center releases.

Parameter Specifications for Test Cases (n=16)
Test of Non-H-Area Met Files and Terrain Data Calls

	Downwind Distance, mi					Release Height, m*		Plume Decay, d			Terrain Included		Release Area (82-86 Met Data)					Exit Velocity, m/s***				
Sector	5-10	10-20	20-30	30-40	40-50	0	62	0.00	2.26	8.00	Yes	No	D	F	K	P	M**	5	0	3	7	9
21. SOUTH																						
22. SSW																						
23. SW																						
24. WSW																						
25. WEST																						
26. WNW																						
27. NW																						
28. NNW																						
29. NORTH																						
30. NNE																						
31. NE																						
32. ENE																						
33. EAST																						
34. ESE																						
35. SE																						
36. SSE																						

* Range of vertical bldg. areas tested: 0 - 10,000 m^2.
** M-Area releases evaluated using A-Area met data.
*** Range of stack diameters tested: 0-5 m.

Tested by: L.R. Bauer

Table 3a. Results of the verification runs for relative concentration values*.

Test Case No.	"Chi over Q's", s/m**3 Specific Downwind Location XOQDOQ	Excel	Downwind Segment XOQDOQ	Excel
1.	1.052E-09	1.052E-09	8.666E-10	8.667E-10
2.	1.748E-09	1.749E-09	3.475E-09	3.475E-09
3.	1.874E-08	1.878E-08	6.392E-09	6.392E-09
4.	6.116E-08	6.112E-08	1.229E-08	1.229E-08
5.	3.059E-09	3.058E-09	1.094E-08	1.094E-08
6.	3.600E-08	3.601E-08	9.388E-09	9.389E-09
7.	8.707E-09	8.705E-09	2.149E-09	2.149E-09
8.	1.588E-09	1.588E-09	2.562E-09	2.562E-09
9.	2.854E-09	2.854E-09	2.408E-09	2.409E-09
10.	1.486E-09	1.490E-09	2.799E-09	2.799E-09
11.	1.830E-08	1.825E-08	5.450E-09	5.450E-09
12.	6.318E-08	6.316E-08	1.349E-08	1.349E-08
13.	6.812E-09	6.816E-09	2.628E-08	2.628E-08
14.	2.531E-08	2.541E-08	5.575E-09	5.574E-09
15.	8.384E-09	8.386E-09	1.956E-09	1.956E-09
16.	3.975E-10	3.978E-10	7.213E-10	7.212E-10
17.	9.031E-10	9.036E-10	7.524E-10	7.524E-10
18.	1.040E-09	1.044E-09	1.822E-09	1.822E-09
19.	7.482E-09	7.483E-09	2.379E-09	2.379E-09
20.	2.486E-08	2.487E-08	5.951E-09	5.951E-09
21.	2.348E-09	2.348E-09	1.944E-09	1.944E-09
22.	8.281E-10	8.278E-10	1.356E-09	1.356E-09
23.	2.896E-08	2.893E-08	8.360E-09	8.360E-09
24.	6.529E-08	6.539E-08	1.160E-08	1.160E-08
25.	3.976E-09	3.982E-09	1.629E-08	1.629E-08
26.	1.355E-09	1.356E-09	1.151E-09	1.151E-09
27.	8.440E-10	8.441E-10	1.492E-09	1.492E-09
28.	2.870E-08	2.866E-08	7.913E-09	7.914E-09
29.	8.477E-10	8.480E-10	1.424E-09	1.424E-09
30.	2.231E-09	2.228E-09	1.838E-09	1.838E-09
31.	4.840E-09	4.843E-09	1.814E-08	1.814E-08
32.	2.443E-09	2.443E-09	4.132E-09	4.132E-09
33.	9.163E-08	9.166E-08	1.984E-08	1.984E-08
34.	3.718E-09	3.701E-09	1.400E-08	1.400E-08
35.	3.241E-08	3.243E-08	5.814E-09	5.815E-09
36.	6.061E-09	6.064E-09	1.431E-09	1.430E-09

* XOQDOQ-Excel comparisons were also made for the nearest distance to the site boundary for all 16 22.5-degree compass sectors; no discrepancies were found.

Table 3b. Results of the verification runs for relative deposition values.

	"D over Q's", m**-2			
	Specific Downwind Location		Downwind Segment	
Test Case No.	XOQDOQ	Excel	XOQDOQ	Excel
1.	3.646E-12	3.649E-12	2.932E-12	2.932E-12
2.	4.011E-12	4.012E-12	7.848E-12	7.848E-12
3.	1.036E-10	1.034E-10	2.662E-11	2.662E-11
4.	2.035E-10	2.035E-10	4.918E-11	4.918E-11
5.	1.398E-11	1.400E-11	6.651E-11	6.650E-11
6.	1.577E-10	1.576E-10	2.985E-11	2.985E-11
7.	5.775E-11	5.775E-11	1.515E-11	1.515E-11
8.	4.941E-12	4.943E-12	9.862E-12	9.862E-12
9.	6.554E-12	6.556E-12	5.270E-12	5.270E-12
10.	5.566E-12	5.565E-12	1.082E-11	1.082E-11
11.	8.357E-11	8.356E-11	2.207E-11	2.207E-11
12.	2.582E-10	2.581E-10	4.739E-11	4.738E-11
13.	3.196E-11	3.196E-11	1.281E-10	1.281E-10
14.	1.859E-10	1.857E-10	3.818E-11	3.818E-11
15.	4.172E-11	4.175E-11	1.137E-11	1.137E-11
16.	2.742E-12	2.743E-12	4.945E-12	4.945E-12
17.	6.013E-12	6.014E-12	4.835E-12	4.834E-12
18.	7.321E-12	7.319E-12	1.427E-11	1.427E-11
19.	3.991E-11	3.991E-11	1.605E-11	1.605E-11
20.	1.413E-10	1.412E-10	2.433E-11	2.433E-11
21.	4.890E-12	4.892E-12	3.971E-12	3.971E-12
22.	4.093E-12	4.091E-12	7.040E-12	7.040E-12
23.	7.997E-11	7.998E-11	1.766E-11	1.766E-11
24.	2.998E-10	3.000E-10	4.855E-11	4.855E-11
25.	3.215E-11	3.217E-11	1.071E-10	1.071E-10
26.	5.598E-12	5.595E-12	4.501E-12	4.501E-12
27.	4.413E-12	4.417E-12	8.792E-12	8.791E-12
28.	1.347E-10	1.346E-10	4.435E-11	4.435E-11
29.	4.335E-12	4.333E-12	8.636E-12	8.637E-12
30.	6.485E-12	6.485E-12	5.214E-12	5.214E-12
31.	3.050E-11	3.049E-11	1.130E-10	1.130E-10
32.	4.950E-12	4.948E-12	9.861E-12	9.860E-12
33.	3.475E-10	3.478E-10	5.628E-11	5.629E-11
34.	1.758E-11	1.760E-11	8.329E-11	8.329E-11
35.	1.713E-10	1.715E-10	2.831E-11	2.832E-11
36.	2.619E-11	2.620E-11	5.468E-12	5.468E-12

CONCLUSIONS AND RECOMMENDATIONS

Gaussians models are the recognized standard method for regulating radioactive species. The suitability of such models has been established by experimental data, and there is a scientific consensus that the theoretical bases are sound (NCRP 1984).

Based on this review, XOQDOQ's performance is adequate for continued use at the SRS. Efforts to improve and monitor the code should also be continued. Sensitivity studies of user-specified parameters and a review of the potential importance of such variables as particle size distribution, roughness length, and surface moisture would also be useful.

As with most commonly used dispersion codes, a weakness in XOQDOQ is its treatment of plume rise. If there is increased interest in using the plume rise capabilities of XOQDOQ, additional study of this phenomenon is warranted.

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