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7. Abstract

This report documents the program user's guide of a general purpose atmospheric dispersion code named GXQ. GXQ is an IBM Compatible microcomputer based program for calculating atmospheric dispersion coefficients using Hanford site specific joint frequency data. It uses the Gaussian straight line model to calculate either an atmospheric dispersion coefficient (X/Q') or a maximum normalized air concentration (X/Q). Several options are available to the user which alter the standard Gaussian model to allow for plume depletion, building wake, plume meander, sector averaging, gravitational settling and plume rise. Additional options control handling of the joint frequency data and output. Combinations of the above allow calculation of X/Q' in accordance with Nuclear Regulatory Commission Regulatory Guide 1.145.

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GXQ 4.0 Program Users' Guide

B. E. Hey

December 19, 1994

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**Consequence Analysis
Westinghouse Hanford Company**

MASTER

CONTENTS

1.0	SOFTWARE	1-1
1.1	INTENDED USE	1-1
1.2	CONFIGURATION CONTROL	1-1
2.0	HARDWARE AND SOFTWARE REQUIREMENTS	2-1
3.0	EXECUTION	3-1
4.0	METHODOLOGY	4-1
4.1	X/Q, DEPLETION, SOURCE TERM AND WIND SPEED MODELS	4-1
4.1.1	CONTINUOUS PLUME	4-2
4.1.2	INSTANTANEOUS PUFF	4-3
4.1.3	PLUME DEPLETION	4-4
4.1.4	SOURCE TERM CONSIDERATIONS.	4-5
4.1.5	WIND SPEED AND VERTICAL PROFILE	4-7
4.2	DIFFUSION COEFFICIENTS AND ADJUSTMENT MODELS	4-8
4.2.1	PASQUILL GIFFORD DIFFUSION COEFFICIENTS	4-8
4.2.2	BUILDING WAKE/AREA SOURCE	4-9
4.2.3	PLUME MEANDER	4-11
4.2.4	STACK FLOW	4-13
4.2.5	ENTRAINMENT	4-14
4.3	EFFECTIVE PLUME HEIGHT AND ADJUSTMENT MODELS	4-15
4.3.1	PLUME RISE	4-15
4.3.2	GROUND EFFECTS	4-24
4.3.3	STACK DOWNWASH	4-25
4.3.4	GRAVITATIONAL SETTLING	4-26
4.4	DISTRIBUTIONS	4-27
4.4.1	ANNUAL AVERAGE	4-27
4.4.2	FREQUENCY OF EXCEEDANCE.	4-29
4.4.3	POPULATION WEIGHTING	4-31
5.0	INPUT DESCRIPTION	5-1
6.0	ERROR AND WARNING MESSAGES	6-1
7.0	EXAMPLE USAGE	7-1
8.0	REFERENCES	8-1
APPENDICES:		
A	INDEPENDENT REVIEW CHECKLIST	A-1

LIST OF TABLES

4-1	Rural Roughness Power Coefficients As a Function of Atmospheric Stability Class	4-7
4-2	Constant Values for Diffusion Coefficient Evaluation	4-8
5-1	Typical GXQ Input File	5-1

LIST OF FIGURES

3-1	GXQ Program Flow Diagram	1-1
3-2	Subroutine XQSUB Flow Diagram	1-2
3-3	Subroutine FHE Flow Diagram	1-3

LIST OF TERMS

NOMENCLATURE

A	area (m^2)
d	release or stack diameter (m)
F_b	buoyancy flux (m^4/s^3)
F_m	momentum flux (m^4/s^2)
g	gravitational constant ($9.8 m/s^2$)
h_e	effective plume height (m)
h_a	anemometer height (m)
h_m	mixing layer height (m)
h_s	stack height (m)
H_b	building height (m)
M	plume meander correction factor
s	stability parameter (s^{-2})
t_{rd}	release duration (s)
T	temperature (K)
q_h	convective heat release rate (w)
Q	puff release quantity
Q'	continuous release rate (s^{-1})
R	velocity ratio
u_a	wind speed at anemometer (m/s)
u_e	wind speed at effective plume height, h_e , (m/s)
u_s	wind speed at stack height, h_s , (m/s)
$\bar{u}$	average of u_e and u_s (m/s)
v_d	particle deposition velocity (m/s)
v_g	particle gravitational fall velocity (m/s)
V	plume volume flow rate (m^3/s)
W_b	building width (m)
w	plume vertical velocity (m/s)
x	release to receptor distance (m)
y	lateral offset of receptor from centerline (m)
z	height of receptor (m)

GREEK LETTERS

β	Beta, entrainment coefficient
Δ	Delta, difference
π	Pi, 3.1415927
σ	Sigma, Pasquill-Gifford diffusion coefficient (m)
Σ	Sigma, adjusted diffusion coefficient (m)
θ	Theta, potential temperature (K)
χ	Chi, air concentration (m^{-3})

SUBSCRIPTS

0	initial or original
a	anemometer or ambient
c	critical or crossover point
f	final
max	maximum
v	virtual
x	windward coordinate
y	lateral coordinate
z	vertical coordinate

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1.0 SOFTWARE

1.1 INTENDED USE

GXQ, Version 4.0 is an IBM¹ compatible microcomputer-based program for calculating atmospheric dispersion using site specific joint frequency data. It uses the Gaussian straight line model for both instantaneous and continuous releases. Several models are available to the user that modify parameters within the Gaussian plume model to account for phenomena such as plume depletion, building wake, plume meander, gravitational settling, and plume rise. Additional controls alter the handling of joint frequency data and output.

GXQ has three modes of operation. These modes allow (1) calculation of a centerline X/Q' based on site specific meteorology, (2) an offset X/Q' based on atmospheric stability class and wind speed, and (3) an x-y plot file based on atmospheric stability class and wind speed.

GXQ is an expert program. This means that it is intended to be used by individuals who are knowledgeable of the limits and applicability of the models implemented. Although some error checking is provided, it is possible to select one or more models that may not be analytically compatible with each other, or may not be applicable to the problem. This is by design. GXQ implements the following models in a straight forward and flexible manner. It is up to the user to ensure that the models selected are compatible and applicable to the problem. The user is advised to consult the referenced or similar texts to understand the model limitations.

The flow diagram for GXQ is provided in Figures 1-1 through 1-3. The three flow paths shown in Figure 1-1 represent the three modes of GXQ operation discussed above. Regardless of the mode of operation, the core subroutine XQSUB is called in all three. Figure 1-2 shows the calculational steps taken within XQSUB. If a plume elevation adjustment model is selected then XQSUB also calls FHE. Figure 1-3 shows the calculational steps taken within FHE.

¹a trademark of International Business Machines Corporation.

Figure 3-1. GXQ Program Flow Diagram

Figure 3-2. Subroutine XQSUB Flow Diagram

Figure 3-3. Subroutine FHE Flow Diagram

1.2 CONFIGURATION CONTROL

This section fulfills the configuration control requirements of Section 4.3 "Software Configuration Control" of the *Safety Analysis and Regulation Work Procedures* (WHC 1992). Code test requirements of WHC (1992) are satisfied in *GXQ 4.0 Program Verification & Validation* (Hey 1994).

The GXQ code is controlled by the Westinghouse Hanford Company code custodian. The custodian is responsible for maintaining a validated version of the code and documentation and for reporting any changes in code status or errors identified to registered users. The code source listing, as well as verification case results, are provided in *GXQ 4.0 Program Verification and Validation* (Hey 1994).

The code can be obtained directly from the code custodian. Copies obtained elsewhere can not meet Westinghouse Hanford Company software configuration control procedures and should, therefore, not be used for quality or safety affecting applications. Any errors identified in the code or its results should be communicated to the Westinghouse Hanford Company code custodian. Improvements in the code may also be requested of the code custodian. However, changes to the code are solely at the discretion of the code custodian. The code custodian will ensure that all quality affecting errors and/or changes to the code are documented and communicated to the registered users'. Code recompilations incorporating changes will be documented, verified and assigned a unique version number.

This report comprises all the necessary code documentation needed by the user for code use. Copies should be obtained from Westinghouse Hanford Central Files. A GXQ registered users' list is maintained by and available from the GXQ code custodian upon request.

An electronic back-up copy of all GXQ source code is maintained and in the possession of the code custodian. Since the code is written for the personnel computer, the user is responsible for maintaining on his/her machine the latest version of the software as communicated by the code custodian. Backup and recovery of the software on the users' machine is solely the responsibility of the user.

Nothing in the Westinghouse Hanford Company software configuration control procedures or GXQ code description or verification shall eliminate the need for independent review of code calculated results.

2.0 HARDWARE AND SOFTWARE REQUIREMENTS

GXQ is written in the FORTRAN 77 computer language (i.e., with some Lahey Fortran enhancements for system date and time access) by the Westinghouse Hanford Company under contract to the U.S. Department of Energy. The source code was compiled and linked using Lahey Fortran², Version 5.01. Approximately 200 kb of free memory are required on an IBM personal computer or compatible personal computer with math co-processor and DOS³, Version 3.0, or later.

²trademarks of Lahey Computer Systems, Incorporated.

³a trademark of International Business Machines Corporation.

3.0 EXECUTION

The GXQ program is contained in a single executable file named GXQ.EXE. The program is distributed along with several auxiliary files consisting of Hanford joint frequency data, Hanford 50-mile population data, utility batch files, and typical GXQ input files. The GXQ program and its auxiliary files should be installed in a single directory. Since the joint frequency and population input files used by GXQ are the same as those used by GENII Version 1.485 (Napier 1988), it is sometimes convenient to put the GXQ program in the same directory with GENII, should that program already be installed on the users' personal computer. GXQ is executed using the following example command lines,

GXQ

or

GXQ > myfile.out

or

GXQ > lpt1:

The first example executes GXQ and sends the output to the terminal device (i.e., to the screen). The second example redirects the output to a file called myfile.out. The third example redirects the output to parallel port 1 which is usually connected to a printer.

A simple batch file called G.BAT is also provided for the users' convenience. This batch file executes GXQ using the argument names as input files with a .IN extension and puts the output in files of the same argument name with a .OUT extension. The user is free to modify this batch file as necessary. An example usage of the batch file is as follows,

G myfile1 myfile2

The input is taken from MYFILE1.IN and MYFILE2.IN and placed in output files MYFILE1.OUT and MYFILE2.OUT. All files are assumed to be located in the current directory.

4.0 METHODOLOGY

4.1 X/Q', DEPLETION, SOURCE TERM AND WIND SPEED MODELS

This section discusses the Gaussian model used for atmospheric transport calculations and adjustment factors to account for plume depletion and source terms. This section also discusses the vertical wind speed profile model used.

4.1.1 CONTINUOUS PLUME

The Gaussian straight line continuous plume model is employed by GXQ for calculating atmospheric dispersion. The atmospheric dispersion coefficient X/Q' is given by,

$$\frac{X}{Q'} = \frac{f(y)g(z)}{2\pi\sigma_y\sigma_z\bar{u}}$$

where:

4.1-1

$f(y)$ = horizontal correction term
 $g(z)$ = vertical correction term.

This equation can be found in Hanna (1982), Turner (1970), and Slade (1968). Also, it is the equation used by the GENII code. The horizontal correction term is given by,

$$f(y) = \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]$$

4.1-2

The vertical correction term is given by,

$$g(z) = F_{\text{ref}} \exp \left[-\frac{1}{2} \left(\frac{h_e - z}{\sigma_z} \right)^2 \right] \quad 4.1-3$$

where h_e is the effective plume height. The effective plume height is equal to the stack height, h_s , plus any change in height, Δh , due either to plume rise, stack downwash or gravitational settling (see Section 4.3).

$$h_e = h_s + \Delta h \quad 4.1-4$$

The plume trapping reflection parameter, F_{ref} , is given by,

$$F_{\text{ref}} = 1 + \exp \left(\frac{-2zh_e}{\sigma_z^2} \right) + \sum_{N=1}^5 \exp \left(\frac{2(h_e - Nh_m)(Nh_m - z)}{\sigma_z^2} \right) + \exp \left(\frac{2Nh_m(h_e - Nh_m - z)}{\sigma_z^2} \right) \\ + \exp \left(\frac{2(h_e + Nh_m)(-Nh_m - z)}{\sigma_z^2} \right) + \exp \left(\frac{-2Nh_m(h_e + Nh_m - z)}{\sigma_z^2} \right) \quad 4.1-5$$

Note that in Equation 4.1-5 both the receptor height, z , and the effective plume height, h_e , are assumed to be less than the mixing height, h_m .

Uniform vertical mixing is assumed when the vertical diffusion coefficient reaches 80% of the mixing height. The normalized X/Q' is then,

$$\frac{X}{Q'} = \frac{f(y)}{\sqrt{2\pi} \sigma_y h_m \bar{u}} \quad 4.1-6$$

The continuous plume model is selected in GXQ by setting $ipuff=0$.

4.1.2 INSTANTANEOUS PUFF

Equation 4.1-1 gives the time integrated normalized exposure to a continuous point source release of atmospheric contamination. Dividing the integrated exposure by the release duration gives the average air concentration of the contaminant at the receptor. It assumes no diffusion in the windward or x direction. For receptors that have a plume travel time that is short in comparison to the release duration, the average and peak air concentration during plume passage is approximately the same and is given by,

$$\frac{\bar{x}}{Q} = \frac{f(y)g(z)}{2\pi\sigma_y\sigma_z\bar{u}t_{rd}} \quad 4.1-7$$

For receptors that have a plume travel time that is long in comparison to the release duration there can be significant windward diffusion. Hence, use of Equation 4.1-7 for deriving peak air concentration is overly conservative. Because the peak air concentration should not exceed that "seen" for an instantaneous "puff" release, the maximum normalized air concentration is limited to that of the puff release beyond the transition point. The transition point at which the peak air concentration of the plume exceeds the puff occurs at the point where the following equation is satisfied.

$$\sigma_x = \frac{\bar{u}t_{rd}}{\sqrt{2\pi}} \quad 4.1-8$$

Because little data exists as to diffusion in the windward direction, it is assumed to be the same as that given by the lateral diffusion coefficient (i.e., $\sigma_x = \sigma_y$).

The peak normalized air concentration for an instantaneous puff release is given by

$$\left(\frac{\bar{x}}{Q}\right)_{\max} = \frac{f(y)g(z)}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \quad 4.1-9$$

This equation is given in Turner (1970) eq. 5.21; Slade (1968), eq. 3.113, 3.154, and 3.155; as well as other atmospheric dispersion texts. The maximum concentration occurs at time $t = x/u$ when the center of the puff is passing overhead.

As a result of the large uncertainties and relatively small differences between the dispersion coefficients for steady-state versus instantaneous, the puff dispersion coefficients are assumed to be the same as for the continuous model. The instantaneous puff model is selected in GXQ by setting $ipuff=1$.

4.1.3 PLUME DEPLETION

The plume depletion correction factor is based on the so called "source depletion model." A discussion of the model can be found in Slade (1968) in Equation 5.48. The model does not alter the plume shape but reduces its concentration uniformly assuming dry deposition. The integral formula is solved numerically using Simpson's One-Third Rule on logarithmic intervals (Rittmann, 1984).

$$\frac{Q'_x}{Q'_0} = \exp \left[\frac{-v_d}{\sqrt{2\pi}} \int_{0.1}^x \frac{g(z=0)}{u_e \sigma_z} dx \right]$$

where:

4.1-10

Q'_x = depleted source term at distance x

Q'_0 = original source term

v_d = deposition velocity (m/s)

Both the elevation corrected wind speed, u_e , and the vertical correction term, $g(z)$, can be a function of plume height, h_e , which in turn is a function of the plume travel distance, x . Equation 4.1-10 is applicable to a plume that is either rising or falling. The receptor is always assumed to be at ground level, thus $z=0$.

The source depletion model is selected in GXQ by setting $idep=1$.

4.1.4 SOURCE TERM CONSIDERATIONS

The atmospheric dispersion coefficient, X/Q' , is a ratio of the air concentration, X , to the release rate, Q' . Q' is also called the source term. In many cases the X/Q' is input into another program such as GENII in order to calculate dose, etc. In other cases the source term and dose conversion factors are known constant values for a given scenario and it is a simple matter to take the product of these numbers to arrive at the desired result. However, there are cases where the source term is not a constant, independent of atmospheric parameters. One such case is evaporation from a pool which is a function of wind speed and other parameters. Two options are provided in GXQ to give the user the ability to calculate X or other dependent results.

Constant Source Term

A common application of the X/Q' is to multiply it by a constant in order to determine a dose, ground contamination, etc. Setting $isrc=1$ in GXQ causes the calculated X/Qs to be multiplied by a scaling factor c as follows,

$$P = \left(\frac{X}{Q'} \right) c \quad 4.1-11$$

where P is the product of the two numbers. The scaling factor c could represent several parameters which are independent of atmospheric dispersion. A typical use of this option is given in the equation below for calculating a dose to man due to the release of a respirable quantity of radioactive material.

$$D = \left(\frac{X}{Q'} \right) Q' R F T \quad 4.1-12$$

where D is a dose (rem), X/Q' is the atmospheric dispersion coefficient (s/m^3), Q' is the source term (Ci/s), R is a breathing rate (m^3/s), F is a dose conversion factor (rem/Ci) and T is the exposure duration (s). This same calculation can be accomplished in GXQ by setting $c=(Q' R F T)$.

Power Function Source Term

Another application of the X/Q' is to use it in conjunction with a source term which is also dependent on wind speed. Setting $isrc=2$ in GXQ causes the calculated X/Qs to be adjusted as follows,

$$P = \left(\frac{X}{Q'} \right) c \bar{u}^a \quad 4.1-13$$

where c is a scalar and a is an exponent. A typical use of this option is given in the equation below for calculating an air concentration at a downwind receptor resulting from pool evaporation (used in the EPI code). This equation is taken from Clement (1981) and is applicable to spilled pools of chemicals where the rate of release is taken to be the evaporation rate.

$$X = \left(\frac{X}{Q'} \right) 105.2 \left(\frac{u^{0.78} M^{2/3} A v}{T} \right)$$

where:

$$\frac{X}{Q'} = \text{atmospheric dispersion coefficient (s/m}^3\text{)} \quad 4.1-14$$

u = wind speed (m/s)

M = liquid molecular weight (g/mole)

A = surface area of spill (m^2)

v = vapor pressure of liquid (mm Hg)

T = temperature of liquid (K)

This same calculation can be accomplished in GXQ by setting $a=0.78$ and $c=(105.2 M^{2/3} A v)/T$.

Since both the evaporation source term and dispersion increase with wind speed it is convenient to combine the two models when it is desirable to determine a bounding scenario.

4.1.5 WIND SPEED AND VERTICAL PROFILE

The anemometer height, h_a , corresponding to the meteorological data is taken from the input provided by the user (*mode* = 2 or 3) or taken from the joint frequency file (*mode* = 1). If the anemometer height differs from the calculated effective height of the plume, h_e (see Equation 4.1-4), then the wind speed at the plume effective height can be calculated using a power law function given by Equation 4.9 of Hanna (1982). This equation is repeated below.

$$u_e = u_a \left(\frac{h_e}{h_a} \right)^p \quad 4.1-15$$

where power coefficient p represents rural roughness factors. Power coefficients for rural areas are also taken from Hanna (1982). The power coefficient for Stability Class G is estimated from trends in the data shown in Table 4-1. Below 10 m and above 200 m in height there is no further adjustment to u_e .

Table 4-1. Rural Roughness Power Coefficients As a Function of Atmospheric Stability Class.

STABILITY CLASS							
	A	B	C	D	E	F	G
Rural p	0.07	0.07	0.10	0.15	0.35	0.55	0.60

The vertical wind profile adjustment model is selected in GXQ by setting *iwind*=1.

Unless specified otherwise, the wind speed, u , used in the Gaussian plume model (Section 4.1) and various adjustment models (Sections 4.2 and 4.3) is set equal to either the anemometer wind speed or to the average of the wind speed representing the release point and the wind speed at the plume effective height given by equation 4.1-15. In GXQ the following logic is used.

$u = u_a$ if *iwind*=0 (i.e., no wind adjustment model selected),
 $u = u_s$ if *iwind*=1 and no plume height adjustment model selected,
 $u = (u_s + u_e)/2$ if *iwind*=1 and a plume height adjustment model is selected.

4.2 DIFFUSION COEFFICIENTS AND ADJUSTMENT MODELS

This section discusses the diffusion coefficients used in the Gaussian model. Also discussed are the various adjustment models for diffusion coefficients to account for building wake, area sources, plume meander, stack flow and entrainment. GXQ will allow any number of these models to be selected simultaneously. However, only the model providing the largest adjustment to the diffusion coefficient, either lateral or vertical, is used in the final calculation. No attempt is made to combine the effects of more than one model unless one model happens to dominate in the lateral and another dominates in the vertical.

4.2.1 PASQUILL GIFFORD DIFFUSION COEFFICIENTS

Empirical formulae for horizontal and vertical diffusion coefficients were taken from Napier (1988) and are based on the Pasquill-Gifford-Turner curves. The formulae are given below.

$$\sigma_y = A_y x^{0.9031} \quad 4.2-1$$

$$\sigma_z = A_z x^{B_z} + C_z$$

where: 4.2-2

A, B, C = fitting parameters
 x = downwind distance (m)

The empirical diffusion coefficient fitting parameters are given in Table 4-2 for three distance ranges as follows, (1) less than 100 m, (2) 100 to 1000 m, and (3) greater than 1000 m.

Table 4-2. Constant Values for Diffusion Coefficient Evaluation.

Stability Class	A_y	Az Distance Range			Bz Distance Range			Cz Distance Range		
		1	2	3	1	2	3	1	2	3
A	0.3658	0.192	0.00066	0.00024	0.936	1.941	2.094	0	9.27	-9.6
B	0.2751	0.156	0.0382	0.055	0.922	1.149	1.098	0	3.3	2
C	0.2089	0.116	0.113	0.113	0.905	0.911	0.911	0	0	0
D	0.1471	0.079	0.222	1.26	0.881	0.725	0.516	0	-1.7	-13
E	0.1046	0.063	0.211	6.73	0.871	0.678	0.305	0	-1.3	-34
F	0.0722	0.053	0.086	18.05	0.814	0.74	0.18	0	-0.35	-48.6
G	0.0481	0.032	0.052	10.83	0.814	0.74	0.18	0	-0.21	-29.2

4.2.2 BUILDING WAKE/AREA SOURCE

This section discusses the models available in GXQ to evaluate situations which involve a greater degree of initial dispersion than accounted for in the point source Gaussian plume model.

NRC RG 1.145 Model

Two building wake models are implemented in GXQ. The first is identical to the model described by Equations 1, 2 and 3 in NRC (1982). The formulae and procedure implemented in GXQ are described below.

$$\frac{\chi}{Q'} = \frac{f(y)g(z)}{2\bar{u}(\pi\sigma_y\sigma_z + A/2)} \quad 4.2-3$$

$$\frac{\chi}{Q'} = \frac{f(y)g(z)}{2\bar{u}(3\pi\sigma_y\sigma_z)} \quad 4.2-4$$

$$\frac{\chi}{Q'} = \frac{f(y)g(z)}{2\bar{u}\Sigma_y\sigma_z}$$

where:

$$A = W_b \times H_b \quad 4.2-5$$

W_b = building width (m)
 H_b = building height (m)
 Σ_y = meander corrected diffusion coefficient
 (see NRC plume meander model description).

The χ/Q' chosen is given by

$$\frac{\chi}{Q'} = \text{MIN}(\text{eq. 4.2-5}, \text{MAX}(\text{eq. 4.2-3}, \text{eq. 4.2-4})) \quad 4.2-6$$

The NRC building wake model is selected in GXQ by setting $i_{wake}=1$.

MACCS Model

The second building wake model is a simple alteration of the Gaussian plume model. It assumes the release point to be at the ground level and in the middle of the downwind face of the building. By selecting this model and entering values for the building width and height, the plume horizontal and vertical dimensions (σ_y and σ_z) are initialized such that the plume concentrations at the sides and roof line of the building from which the release occurs is ten (10) percent of plume centerline concentrations (i.e., building edges are 2.15σ from the plume centerline). The formulae are taken from Equation 2.2 of the *MELCOR Accident Consequence Code System (MACCS) Model Description* (NRC 1990).

$$\sigma_y(x=0) = \frac{W_b}{4.3} \quad 4.2-7$$

$$\sigma_z(x=0) = \frac{H_b}{2.15} \quad 4.2-8$$

The adjustment to the diffusion coefficients is made using the virtual distance method. This method involves calculating the virtual distance, x_{vy} , corresponding to $\sigma_y(x=0)$ and, x_{vz} , corresponding to $\sigma_z(x=0)$ and adding these distances to the distance from the release point to receptor, (x). These adjusted "virtual distances" are then used to calculate subsequent diffusion coefficients using the following equations,

$$\Sigma_y = \sigma_y(x_{vy} + x) \quad 4.2-9$$

$$\Sigma_z = \sigma_z(x_{vz} + x) \quad 4.2-10$$

The MACCS building wake model is selected in GXQ by setting *iwake*=2.

Area Source

The MACCS building wake model can also be used to simulate an area source by setting the building width equal to the source diameter and setting the building height equal to zero.

4.2.3 PLUME MEANDER

Three plume meander models are available in GXQ. Each of these are discussed below.

NRC RG 1.145 Model

The first model is based on the empirical model given by the NRC (1982). When selected, it is applied to the horizontal diffusion coefficient for the atmospheric stability class and wind speed and before any interpolation. The procedure is given below.

For $1 \text{ m/s} \leq u \leq 2 \text{ m/s}$:

M =	6	Stability Class	G
	4		F
	3		E
	2		D

For $2 \text{ m/s} < u \leq 6 \text{ m/s}$:

M =	$(u/6)^{(-\ln(6)/\ln(3))}$	Stability Class	G
=	$(u/6)^{(-\ln(4)/\ln(3))}$		F
=	$(u/6)^{(-\ln(3)/\ln(3))}$		E
=	$(u/6)^{(-\ln(2)/\ln(3))}$		D

For $x < 800 \text{ m}$:

$$\Sigma_y = M \sigma_y(x) \quad 4.2-11$$

For $x \geq 800 \text{ m}$:

$$\Sigma_y = (M-1) \sigma_y(800) + \sigma_y(x) \quad 4.2-12$$

The NRC plume meander model is selected in GXQ by setting $ipm=1$.

One-fifth Power Law

The second plume meander model is based on the One-fifth Power Law formulae (NRC 1990). When selected, an effective horizontal diffusion coefficient is calculated from a user supplied release duration, t_{rd} , according to the following equation.

$$\sigma_{ey} = \sigma_y \left(\frac{t_{rd}}{t_{600}} \right)^\alpha$$

where:

4.2-13

σ_{ey} = effective horizontal diffusion coefficient

$\alpha = 0.2$ when $10 \text{ min} \leq t_A \leq 1 \text{ hr}$

$\alpha = 0.25$ when $1 \text{ hr} < t_A \leq 100 \text{ hr}$

t_{600} = measurement averaging time (600 seconds assumed)

The One-fifth power law plume meander model is selected in GXQ by setting $ipm=2$.

Sector Average

The third model assumes that there is no horizontal cross wind variation in concentration within the sector. This is called the sector average model. The formula can be found in Hanna (1982), Equation 4.18, among other texts.

$$\frac{\chi}{Q'} = \frac{4\sqrt{2} g(z)}{(\pi^{3/2}) \times \sigma_z \bar{u}} \quad 4.2-14$$

If the vertical diffusion coefficient exceeds 80% of the mixing height, uniform vertical mixing is assumed throughout the mixing layer. The normalized sector averaged concentration is then,

$$\frac{\chi}{Q'} = \frac{8}{\pi \times h \bar{u}} \quad 4.2-15$$

The sector average model is selected in GXQ by setting $ipm=3$.

4.2.4 STACK FLOW

As the release point to receptor distance x approaches zero, the values for σ approach zero as well. Thus, the calculated atmospheric dispersion coefficient (X/Q') and normalized air concentration (X/Q) using the Gaussian model approaches infinity. In reality the effluent air concentration, X , should not exceed the initial effluent concentration at the release point.

To correct this deficiency in the mathematical model, the diffusion coefficients at the point of release are chosen to represent the initial plume dimensions (Rittmann 1984). For the case of a puff release, the initial windward plume spread $\sigma_x(x=0)$ is based on the spatial length of the plume. For both puff and continuous releases, the initial lateral plume spread $\sigma_y(x=0)$ is based upon the stack diameter or initial plume width. The initial vertical plume spread $\sigma_z(x=0)$ is based on the exhaust flow rate in such a way that the initial puff/plume concentration is obtained at $x=0$. This dimension is essentially the vertical rise of the plume in the time it takes the plume to travel downwind one stack diameter. This model is applicable to releases having an initial vertical velocity. The above adjustment is accomplished through the following equations.

$$\sigma_x(x=0) = \frac{\bar{u} t_{rd}}{\sqrt{2\pi}} \quad 4.2-16$$

$$\sigma_y(x=0) = \frac{d}{\sqrt{2\pi}} \quad 4.2-17$$

$$\sigma_z(x=0) = \frac{F_{ref}(z=h_s)V_0}{\sqrt{2\pi} \bar{u} d} \quad 4.2-18$$

where:

$F_{ref}(z=h_s)$ = reflection factor evaluated at stack height

As in the MACCS building wake model, the virtual distance method also is used in the exhaust flow rate adjustment.

The stack flow adjustment model is selected in GXQ by setting $iflow=1$.

4.2.5 ENTRAINMENT

The method of Pasquill (1976) is used to account for the initial dispersion of plumes caused by turbulent motion of the plume and turbulent entrainment of ambient air. With this method, the adjusted vertical dispersion Σ_z is calculated as follows.

$$\Sigma_z = \left[\sigma_z^2 + \left(\frac{\Delta h}{3.5} \right)^2 \right]^{1/2} \quad 4.2-19$$

where σ_z is the vertical dispersion due to ambient turbulence and Δh is the plume rise due to momentum and/or buoyancy. The lateral plume spread is parameterized using a similar expression.

$$\Sigma_y = \left[\sigma_y^2 + \left(\frac{\Delta h}{3.5} \right)^2 \right]^{1/2} \quad 4.2-20$$

where σ_y is the lateral dispersion due to ambient turbulence. In both equations, Δh represents the rise of the plume due either to buoyant or momentum effects. Thus, this adjustment model is meant to be used in conjunction with a plume rise model.

The method of Pasquill is also employed by the ISC2 code (EPA 1992). Accounting for entrainment might be more conservative for elevated releases when receptors are close to the release point.

The entrainment model is selected in GXQ by setting *ientr*=1.

4.3 EFFECTIVE PLUME HEIGHT AND ADJUSTMENT MODELS

4.3.1 PLUME RISE

Two procedures for calculating plume rise are available in GXQ. The first (*irise=1*) is strictly a buoyancy rise model based on Briggs' equation for a buoyant plume in a crosswind. A similar procedure is used in the MACCS code (NRC 1990) with some minor differences. The second (*irise=2*) also uses the Briggs' relationships but includes momentum rise. This procedure is similar to that used in the ISC2 code (EPA 1992).

Both models require the value of the Briggs buoyancy flux parameter, F_b (m^4/s^3), given by,

$$F_b = g w_0 d^2 \left(\frac{\Delta T}{4T_0} \right) \quad 4.3-1$$

where $\Delta T = T_0 - T_a$, T_0 is the initial plume temperature (K), and T_a is the ambient air temperature (K). The initial plume vertical velocity, w_0 (m/s), is given by,

$$w_0 = \frac{4V_0}{\pi d^2} \quad 4.3-2$$

where V_0 (m^3/s) is the initial plume volumetric flow rate.

Buoyancy flux can also be calculated from the convective heat emission rate, q_h (W), using the following formula,

$$F_b = 8.79 \times 10^{-6} q_h \quad 4.3-3$$

The initial plume temperature T_0 , volume flow rate V_0 , and convective heat emission rate q_h are related through the following relationship,

$$T_0 = \frac{T_a}{1 - \frac{q_h}{355,000 V_0}} \quad 4.3-4$$

Equation 4.3-4 assumes a plume specific heat of 1 kJ/(kg K) which is a good approximation for air at normal temperatures (i.e., less than 500 K).

For determining plume rise due to the momentum of the plume, the momentum flux, F_m (m^4/s^2), is calculated based on the following formula,

$$F_m = w_0^2 d^2 \frac{T_a}{4T_0} \quad 4.3-5$$

For stable atmospheric conditions it is also necessary to know the value of the stability parameter, s . In GXQ the stability parameter is defined as follows (Randerson 1984, eq. 8.14),

$$s = \frac{g}{T_a} \left[\frac{\partial T_a}{\partial z} + \frac{g}{c_p} \right] \quad 4.3-6$$

where the dry adiabatic lapse rate $g/c_p = 0.0098$ K/m. For stability class E, F and G the ambient temperature lapse rate $\delta T_a/\delta z = 0.005$, 0.0275 and 0.0625 K/m respectively. These midpoint values are identical to those used in the MACCS code, with the exception that MACCS does not consider the G stability class. The $\delta T_a/\delta z$ for the G stability class is taken from Sagendorf (1982).

Near surface wind speeds increase with altitude. Because plume rise is a function of wind speed, and wind speed is a function of altitude, iteration is necessary to converge on an effective plume height and corresponding wind speed. In the following discussions of plume rise models, iteration is performed in the following manner. As the plume experiences a change in elevation, the wind speed calculated at the stack level, u_s , and the effective plume height, u_e , is used to calculate an average wind speed. Iteration on effective plume height and average wind speed continues until the difference between the last two calculated effective plume heights becomes less than 1 m or five iterations are completed. This procedure is followed any time an elevation corrected wind speed is selected ($iwind=1$) and a plume rise/fall model ($irise=1$, $irise=2$, $iwash=1$ or $igrav=1$) results in an elevation different than the release height. This procedure is slightly different than that implemented in MACCS, which limits the number of iterations to two.

GXQ Implementation of MACCS Buoyancy Rise Formulae

This section discusses the GXQ implementation of the plume rise formulae used by the MACCS code. The implementation is similar to that of the MACCS code (NRC 1990) with three exceptions. First, the distance dependent buoyancy rise formulae (Equation 4.3-7) is applied to all stability classes. This is done because; 1) the formulae is applicable to all stability classes, 2) its use ensures conservatism when modeling plume rise under stable conditions, and 3) it provides a smoother transition to peak rise under stable conditions. This difference is not great since the distance dependent plume rise equation for stable conditions is limiting only at plume travel times of less than 20 seconds. MACCS assumes that the plume rise under stable conditions is at its maximum, regardless of the plume travel time. The second difference is that iteration on effective plume height and average wind speed continues until the difference between the last two calculated effective plume heights becomes less than 1 m or five iterations are completed. MACCS performs two iterations, regardless of convergence which results in an underestimated plume rise. The third difference is the treatment of G stability class by GXQ. MACCS does not currently include provisions for stability class G.

Briggs' asymptotic prediction for the rise of buoyant bent-over plumes before ambient stratification or turbulence is given below. The equation is discussed in Randerson (eq. 8.58 1984) as well as other texts. Assumptions made are that the effluent is a heated gas with a heat capacity and mean molecular weight close to that of air, and that initial effluent density and vertical velocity within the plume are constant.

$$\Delta h = 1.6 \left(\frac{F_b^{1/3} x^{2/3}}{\bar{u}} \right) \quad 4.3-7$$

For Pasquill stability conditions of E, F, and G the buoyant rise of the plume is assumed to be limited by

$$\Delta h = 2.6 \left(\frac{F_b}{\bar{u} s} \right)^{1/3} \quad 4.3-8$$

This equation can be found in NRC (1990, pages 2-7 and 2-8).

For Pasquill stability conditions of A through D buoyant rise is terminated when any of the following conditions are met (NRC 1990).

1. $\Delta h = 300 (F_b/\bar{u}^3)$,
2. the plume has travelled downwind for one hour (i.e. $\Delta h = 1.94E+7 F_b/(\beta_b \bar{u})$).

In all cases the effective plume height, h_e , is not allowed to exceed the mixing layer height, h_m .

When wind speeds are high, a buoyant plume that is released into a strong building wake will be unable to escape from the wake. Escape of a buoyant plume from a building wake is governed by a liftoff criterion. The criterion states that plume rise occurs only when the stack-level wind speed is less than a critical wind speed u_c that is calculated using the following formula.

$$u_c = \left(\frac{9.09 F_b}{H_b} \right)^{1/3} \quad 4.3-9$$

If the building height is set to zero then the lift-off criterion is assumed to be not applicable.

The MACCS plume rise model is selected in GXQ by setting *irise*=1.

GXQ Implementation of ISC2 Buoyancy and Momentum Plume Rise Formulae

This section discusses the GXQ implementation of the plume rise formulae used by the ISC2 code. The implementation is similar to that of the ISC2 code (EPA 1992) with three exceptions. First, in GXQ the average wind speed between the release height and the effective plume height is used in the distance dependent plume rise and distance to final rise equations. Iteration on effective plume height and average wind speed continues until the difference between the last two calculated effective plume heights becomes less than 1 m or five iterations are completed. Use of a height averaged wind speed is generally conservative since a higher wind speed decreases the distance dependent plume rise and increases the distance to final plume rise. In contrast, ISC2 bases all plume rise calculations on the stack level wind speed. The second difference is in the value used for the stability parameter, s . There is considerable difference between the values chosen for this parameter between the various codes. GXQ uses Equation 4.3-6 and the MACCS midpoint ambient temperature lapse rate values for E and F stability and the XOQDOQ value for G stability. The largest difference in the stability parameter is for E stability class. The MACCS/GXQ value for s results in a computed buoyancy rise approximately 10% higher than would be calculated by the ISC2 default value. The third difference is that GXQ treats G stability class whereas ISC2 does not.

The following equations are taken from the ISC2 Users' Guide (EPA 1992). They are reproduced here for the readers' convenience.

Unstable or Neutral - Crossover Between Momentum and Buoyancy

The approach used in the ISC2 code is to determine whether the plume rise is momentum or buoyancy dominated. This is accomplished by calculating a crossover temperature difference, $(\Delta T)_c$, as follows,

for $F_b < 55$,

$$(\Delta T)_c = 0.0297 T_0 \frac{w_0^{1/3}}{d^{2/3}} \quad 4.3-10$$

and for $F_b \geq 55$,

$$(\Delta T)_c = 0.00575 T_0 \frac{w_0^{2/3}}{d^{1/3}} \quad 4.3-11$$

If the difference between the initial plume and ambient temperature, ΔT , exceeds $(\Delta T)_c$, plume rise is assumed to be buoyancy dominated, otherwise plume rise is assumed to be momentum dominated.

Unstable or Neutral - Buoyancy Rise

For situations where ΔT exceeds $(\Delta T)_c$ as determined above, buoyancy is assumed to dominate. The distance to final rise, x_f , is calculated as follows,

for $F_b < 55$,

$$x_f = 49F_b^{5/8} \quad 4.3-12$$

and for $F_b \geq 55$,

$$x_f = 119F_b^{2/5} \quad 4.3-13$$

The final plume rise, Δh_f (m), is determined by substituting x_f defined above into equation 4.3-7 yielding the following equations for final buoyant rise,

for $F_b < 55$,

$$(\Delta h)_f = 21.425 \frac{F_b^{3/4}}{u} \quad 4.3-14$$

and for $F_b \geq 55$,

$$(\Delta h)_f = 38.71 \frac{F_b^{3/5}}{u} \quad 4.3-15$$

Unstable or Neutral - Momentum Rise

For situations where the initial plume gas temperature is less than or equal to the ambient air temperature, the assumption is made that the plume rise is dominated by momentum. If ΔT is less than $(\Delta T)_c$ from equation 4.3-10 or 4.3-11, the assumption is also made that the plume rise is dominated by momentum. The final plume rise is calculated from,

$$\Delta h_f = 3d \frac{w_0}{u} \quad 4.3-16$$

Stable - Crossover Between Momentum and Buoyancy

For cases with initial plume gas temperature greater than or equal to ambient temperature, it must be determined whether the plume rise is dominated by momentum or buoyancy. The crossover temperature difference, $(\Delta T)_c$, is determined as follows,

$$(\Delta T)_c = 0.019582 T_0 w_0 \sqrt{s} \quad 4.3-17$$

If the difference between the initial plume and ambient temperature, ΔT , exceeds or equals $(\Delta T)_c$, plume rise is assumed to be buoyancy dominated, otherwise plume rise is assumed to be momentum dominated.

Stable - Buoyancy Rise

For situations where ΔT exceeds $(\Delta T)_c$ as determined above, buoyancy is assumed to dominate. The distance to final rise, x_f , is calculated as follows,

$$x_f = 2.0715 \frac{\bar{u}}{\sqrt{s}} \quad 4.3-18$$

Final plume rise is determined by substituting x_f defined above into equation 4.3-7 which yields the final buoyant rise equation 4.3-8 (i.e., same as MACCS).

Stable - Momentum Rise

For situations where the initial plume gas temperature is less than or equal to the ambient air temperature, the assumption is made that the plume rise is dominated by momentum. If ΔT is less than $(\Delta T)_c$ from equation 4.3-17, the assumption is also made that the plume rise is dominated by momentum. The final plume rise is calculated from,

$$\Delta h_f = 1.5 \left(\frac{F_m}{\bar{u} \sqrt{s}} \right)^{1/3} \quad 4.3-19$$

Equation 4.3-16 for unstable - neutral momentum rise is also evaluated. The lower result of these two equations is used as the resulting plume height.

All Conditions - Buoyancy Rise - Distance Less Than Distance to Final Rise

Where gradual rise is to be estimated for unstable, neutral, or stable conditions, if the distance downwind from source to receptor, x , is less than the distance to final rise, x_f , equation 4.3-7 is used to calculate the buoyant plume rise. This height will be used only for buoyancy dominated conditions; should it exceed the final rise for the appropriate condition, the final rise is substituted instead.

All Conditions - Momentum Rise - Distance Less Than Distance to Final Rise

For momentum dominated conditions, the following equations are used to calculate a distance dependent momentum plume rise,

Unstable Conditions

$$\Delta h = \left(\frac{3F_m x}{\beta_m^2 \bar{u}^2} \right)^{1/3} \quad 4.3-20$$

where x is the downwind distance (m), with a maximum value defined by $x_{\max}$ as follows,

$$\begin{aligned} x_1 &= \frac{4d(w_0 + 3\bar{u})^2}{w_0 \bar{u}} && \text{for } F_b = 0 \\ x_2 &= 49F_b^{5/8} && \text{for } 0 < F_b \leq 55 \\ x_2 &= 119F_b^{2/5} && \text{for } F_b > 55 \\ x_{\max} &= \max(x_1, x_2) \end{aligned} \quad 4.3-21$$

Stable Conditions

$$\Delta h = \left[3F_m \frac{\sin(x\sqrt{s}/\bar{u})}{\beta_m^2 \bar{u} \sqrt{s}} \right]^{1/3} \quad 4.3-22$$

where x is the downwind distance, with a maximum value defined by $x_{\max}$ as follows,

$$x_{\max} = 0.5 \frac{\pi \bar{u}}{\sqrt{s}} \quad 4.3-23$$

The jet entrainment coefficient, β_m , is given by,

$$\beta_m = \frac{1}{3} + \frac{\bar{u}}{w_0} \quad 4.3-24$$

As with the buoyant gradual rise, if the distance dependent momentum rise exceeds the final rise for the appropriate condition, then the final rise is substituted instead.

As in the MACCS buoyant rise model, the liftoff criterion is also applied to the ISC2 buoyant rise model. The ISC2 plume rise model is selected in GXQ by setting *irise*=2.

4.3.2 GROUND EFFECTS

Briggs' plume rise equations described above specifically apply to the release from a stack with negligible radius. The buoyant rise from a pool fire will be less than the Briggs value due to ground effects. Mills (1987) provides a modified formulae for a burning pool of diameter d . The calculated plume rise is modified as follows,

$$h_e = \sqrt[3]{h_b^3 + \left(\frac{d}{2\beta_b}\right)^3} - \frac{d}{2\beta_b}$$

where:

4.3-25

h_b = effective release height via the Briggs methodology (m)

d = diameter of release (m)

β_b = entrainment coefficient for buoyant plume rise, 0.6.

A combination of the Briggs plume rise model (see Section 4.3.1) and Mills modification could be applied to model ground elevation fire scenarios. The entrainment model discussed in Section 4.2.5 might also be applied to account for the enhanced mixing of a rising plume.

The Mills adjustment model is selected in GXQ by setting $igrnd=1$.

4.3.3 STACK DOWNWASH

Two downwash correction models are implemented in GXQ. The first model is applicable to wind blowing past a fixed obstacle, such as a smokestack. It depends upon the ratio of efflux velocity to cross-flow velocity at the top of the stack. The second model is applicable to buoyant plumes and is dependent upon the Froude number. Both models can be found in Randerson (1984), equations 8.117 and 8.118.

$$h_e = h_s - 2(1.5 - R)d$$

where:

d = stack diameter(m)

R = velocity ratio

4.3-26

$$= \frac{w_0}{u_s} \quad \text{for momentum rise}$$

$$= 0.45 w_0 \left[\frac{d}{2 F_b} \right]^{1/3} \quad \text{for buoyancy rise.}$$

When momentum or buoyancy exceeds a certain value, downwash can be neglected. This occurs at approximately $R > 1.5$ at which point downwash is turned off.

The GXQ code uses the maximum velocity ratio to determine which downwash correction to apply.

The stack downwash model is selected in GXQ by setting $iwash=1$.

4.3.4 GRAVITATIONAL SETTLING

The basic assumption of the Gaussian plume model is that particulates in the plume are small enough not to be significantly affected by gravity as they travel downwind. If the plume contains larger particles, however, the gravitational settling may be approximated by tilting the plume downward. This is done by adjusting the effective plume height as follows,

$$h_e = h_s - \frac{v_g x}{u}$$

4.3-27

where:

v_g = gravitational fall velocity (m/s)

This equation can be found in Miller (1984), equation 3.10. The adjusted effective plume height is not allowed to fall below zero.

The gravitational settling model is selected in GXQ by setting $igrav=1$.

4.4 DISTRIBUTIONS

One of the most useful aspects of using the GXQ code is to have it determine a bounding or average atmospheric dispersion coefficient for the scenario being evaluated (i.e., $mode=1$). This is done by evaluating many possible values for the dispersion coefficient and time weighting them to obtain either an average value, useful for a chronic release evaluation or probabilistic risk analysis; or, a bounding value which bounds most, if not all possible values, useful for a design basis type of analysis. In addition to time weighting, it is also useful to population weight the dispersion coefficient when a macroscopic analysis is being performed (i.e., $ipop=T$).

The data available to GXQ to perform these functions are contained in two files named JOINTFRE.IN and POP.IN. JOINTFRE.IN contains joint frequency data or the frequency that atmospheric conditions can be defined by a joint combination of wind speed and stability class. Joint frequency data is provided for each of 16 compass sectors in units of percent. POP.IN contains population data for each of 16 compass sectors and 10 radial intervals, for a total of 160 points. In the discussions below the indices i, j, k and m represent individual stability class, wind speed, sector and radial interval bins respectively. Capital I, J, K and M represent the number of respective bins. Currently, the JOINTFRE.IN and POP.IN files are set up so that $I=7, J=8, K=16$ and $M=10$.

4.4.1 ANNUAL AVERAGE

The annual average X/Q' (i.e., $ifox=F$) for a particular sector is calculated by summing the frequency weighted X/Q s for all atmospheric stability classes and wind speed bins in the JOINTFRE.IN file for a particular sector. The annual average X/Q' for sector k is calculated using the following equation,

$$\left(\frac{X}{Q'}\right)_k = \sum_{j=1}^J \sum_{i=1}^I \left(\frac{X}{Q'}\right)_{ijk} \frac{f_{ijk}}{100} \quad 4.4-1$$

where f_{ijk} is the annual frequency in percent that atmospheric conditions fall within stability class i , wind speed j , and sector k . This X/Q' is suitable for evaluating the consequences in sector k for a chronic, year long release. The cumulative frequency that the wind is in the direction of sector k is given by,

$$C_k = \sum_{j=1}^J \sum_{i=1}^I f_{ijk} \quad 4.4-2$$

Setting $inorm=T$ causes equation 4.4-1 to be modified as follows,

$$\left(\frac{X}{Q'}\right)_k = \sum_{j=1}^J \sum_{i=1}^I \left(\frac{X}{Q'}\right)_{ijk} \frac{f_{ijk}}{C_k} \quad 4.4-3$$

This value represents the annual average X/Q' of all conditions having a wind speed in the direction of sector k . This X/Q' could be used to evaluate the consequences of an acute release under average meteorological conditions in the direction of sector k .

If an annual average overall site X/Q' is desired (i.e., $isite=T$), then the operation started in equation 4.4-1 continues with the inclusion of all 16 sectors as follows,

$$\frac{X}{Q'} = \sum_{k=1}^K \sum_{j=1}^J \sum_{i=1}^I \left(\frac{X}{Q'}\right)_{ijk} \frac{f_{ijk}}{100} \quad 4.4-4$$

This value represents the average X/Q' for the entire site as if the receptor were in all 16 sectors simultaneously. The code divides this X/Q' by 16 when $ipop=F$ since in the absence of population weighting, the receptor can only exist in one sector. If population weighted (discussed in Section 4.4.3), the above equation is not normalized by 16. The resultant population weighted X/Q' could then be used to evaluate the macroscopic consequences of a chronic release to the entire surrounding population. Note that setting $inorm=T$ in addition to $isite=T$ has no effect since by definition

$$\sum_{k=1}^K C_k = 100 \quad 4.4-5$$

4.4.2 FREQUENCY OF EXCEEDANCE

The frequency of exceedance X/Q' (i.e., $ifox=T$), as its name implies, refers to atmospheric conditions which are less dispersing for a specific (usually small) fraction of time. This is accomplished by sorting the sector k X/Q s calculated for each stability class and wind speed bin such that the following equation is satisfied,

$$\left(\frac{X}{Q}\right)_{k,l} > \left(\frac{X}{Q}\right)_{k,l+1} \quad 4.4-6$$

where the index l includes all combinations of stability class and wind speed and $L=I+J$. Additionally, there is a frequency, $f_{k,l}$, associated with each $(X/Q)_{k,l}$. If the percent of time the X/Q' is to be exceeded is specified as C_x , then an indice ll is found such that

$$C_{k,ll} < C_x < C_{k,ll+1} \quad 4.4-7$$

If $inorm=F$, the cumulative frequency for sector k , $C_{k,ll}$, is calculated as follows,

$$C_{k,ll} = \sum_{l=1}^{ll} \left(\frac{f_{k,l} + f_{k,l-1}}{2} \right)$$

where:

4.4-8

$$f_{k,0} = 0$$

$f_{k,l}$ = joint frequency that conditions are characterized
by stability class and wind speed interval l
in sector k (%)

$C_{k,ll}$ as defined in equation 4.4-8 represents the cumulative frequency that $(X/Q)_{k,ll}$ is exceeded, including those times the wind is not blowing in the direction of sector k . The X/Q' associated with C_x is found by linear interpolation such that

$$\left(\frac{X}{Q'}\right)_{k,ll} > \left(\frac{X}{Q'}\right)_{k,x} > \left(\frac{X}{Q'}\right)_{k,ll+1} \quad 4.4-9$$

If $inorm=T$ then equation 4.4-8 is modified as follows,

$$C_{k,ll} = \sum_{l=1}^{ll} \left(\frac{f_{k,l} + f_{k,l-1}}{2} \right) \frac{100}{C_k} \quad 4.4-10$$

The above equation for calculating the cumulative frequency is that used in the GENII code (Napier 1988); and, for consistency, the GXQ code has that capability as well. $C_{k,ll}$ as defined in equation 4.4-10 represents the cumulative frequency that the sector k $(X/Q)_{k,ll}$ is exceeded, excluding those times the wind is not blowing in the direction of sector k . C_k is defined in equation 4.4-2.

If a bounding overall site X/Q' is desired (i.e., $isite=T$), then the procedure described above includes all 16 sectors such that the indice l includes all combinations of stability class, wind speed and sector and $L=I+J+K$. Calculations similar to equations 4.4-6 through 4.4-9 are solved. X/Q s are sorted such that,

$$\left(\frac{X}{Q} \right)_l > \left(\frac{X}{Q} \right)_{l+1} \quad 4.4-11$$

If the percent of time the X/Q' is to be exceeded for the overall site is specified as C_x , then an indice ll is found such that

$$C_{ll} < C_x < C_{ll+1} \quad 4.4-12$$

where the cumulative frequency for the overall site, C_{ll} , is defined as,

$$C_{ll} = \sum_{l=1}^{ll} \left(\frac{f_l + f_{l-1}}{2} \right) \quad 4.4-13$$

C_{ll} as defined in equation 4.4-13 represents the cumulative frequency that the

overall site $(X/Q)_{ll}$ is exceeded. The X/Q' associated with C_x is found by linear interpolation such that

$$\left(\frac{X}{Q'}\right)_{ll} > \left(\frac{X}{Q'}\right)_x > \left(\frac{X}{Q'}\right)_{ll+1} \quad 4.4-14$$

Again, setting $inorm=T$ in addition to setting $isite=T$ has no effect.

4.4.3 POPULATION WEIGHTING

Population weighting is performed when $ipop=T$. In this case the X/Q' for each sector, stability class, and wind speed bin, $(X/Q)_{ijk}$ is calculated as follows,

$$\left(\frac{X}{Q'}\right)_{ijk} = \sum_{m=1}^M \left(\frac{X}{Q'}\right)_{ijkm} P_{km}$$

where:

4.4-15

M = number of radial intervals

P_{km} = population contained in sector k , radial interval m .

The radial intervals are defined by their midpoint distances specified in the population file POP.IN. An annual average or frequency of exceedance X/Q' which has been population weighted is then calculated as discussed in Sections 4.4.1 and 4.4.2.

5.0 INPUT DESCRIPTION

GXQ obtains data from at least one and as many as three files located in the current directory. The first input file is named GXQ.IN and provides user supplied options, model parameters and receptor locations. A typical GXQ input file is shown in Table 5-1. The second input file is named JOINTFRE.IN and is the same joint frequency file used by the GENII code developed by Pacific Northwest Laboratories (PNL) (Napier 1988). PNL has created several joint frequency files for the Hanford Site. For GXQ operating modes that use joint frequency data, it is first necessary to copy and rename the appropriate joint frequency file to the current directory with the file name JOINTFRE.IN. The third input file is named POP.IN and is the same population file used by the GENII code. PNL has created four population files for the Hanford Site, all of which are compatible with GXQ. GXQ also expects to find midpoint distances (m) in line 26 of POP.IN. This is different from GENII which obtains midpoint distances from file DEFAULT.IN. For GXQ operating modes which use population data, it is first necessary to copy and rename the appropriate population file to the current directory with the file name POP.IN.

In the discussion that follows, X/Q' refers to both atmospheric dispersion coefficient and peak normalized air concentration.

Table 5-1. Typical GXQ Input File.

```

Input title line
c GXQ Version 3.2 Input File
c   mode
c     1
c
c   MODE CHOICE:
c mode = 1 then X/Q based on Hanford site specific meteorology
c mode = 2 then X/Q based on atmospheric stability class and wind speed
c mode = 3 then X/Q plot file is created
c
c   LOGICAL CHOICES:
c   ifox inorm icdf ichk isite ipop
c     t   f     f     f     f     f
c ifox = t then joint frequency used to compute frequency to exceed X/Q
c       = f then joint frequency used to compute annual average X/Q
c inorm = t then joint frequency data is normalized (as in GENII)
c       = f then joint frequency data is un-normalized
c icdf  = t then cumulative distribution file created (CDF.OUT)
c       = f then no cumulative distribution file created
c ichk  = t then X/Q parameter print option turned on
c       = f then no parameter print
c isite = t then X/Q based on joint frequency data for all 16 sectors
c       = f then X/Q based on joint frequency data of individual sectors
c ipop  = t then X/Q is population weighted
c       = f then no population weighting
c

```

c X/Q AND WIND SPEED ADJUSTMENT MODELS:

c ipuff idep isrc iwind
0 0 0 0

c DIFFUSION COEFFICIENT ADJUSTMENT MODELS:

c iwake ipm iflow ientr
0 0 0 0

c EFFECTIVE PLUME HEIGHT ADJUSTMENT MODELS:

c (irise igrnd)iwash igrav
0 0 0 0

c ipuff = 1 then X/Q calculated using puff model
c = 0 then X/Q calculated using default continuous plume model
c idep = 1 then plume depletion model turned on (Chamberlain model)
c isrc = 1 then X/Q multiplied by scalar
c = 2 then X/Q adjusted by wind speed function
c iwind = 1 then wind speed corrected for plume height
c iwake = 1 then NRC RG 1.145 building wake model turned on
c = 2 then MACCS virtual distance building wake model turned on
c ipm = 1 then NRC RG 1.145 plume meander model turned on
c = 2 then 5th Power Law plume meander model turned on
c = 3 then sector average model turned on
c iflow = 1 then sigmas adjusted for volume flow rate
c ientr = 1 then method of Pasquill used to account for entrainment
c irise = 1 then MACCS buoyant plume rise model turned on
c = 2 then ISC2 momentum/buoyancy plume rise model turned on
c igrnd = 1 then Mills buoyant plume rise modification for ground effects
c iwash = 1 then stack downwash model turned on
c igrav = 1 then gravitational settling model turned on
c = 0 unless specified otherwise, 0 turns model off

c PARAMETER INPUT:

release height hs(m)	reference anemometer height ha(m)	mixing height hm(m)	frequency to exceed Cx(%)	
0	10	1000	.5	
initial plume width Wb(m)	initial plume height Hb(m)	release duration trd(hr)	deposition velocity vd(m/s)	gravitational settling velocity vg(m/s)
0	0	0	0.001	0.001
ambient temperature Tamb(C)	initial plume temperature T0(C)	initial plume flow rate V0(m3/s)	release diameter d(m)	convective heat release rate(1) qh(w)
20	22	1	1	0

c (1) If zero then buoyant flux based on plume/ambient temperature difference.

```

c  X/Q      Wind
c  scaling  Speed
c  factor   Exponent
c  c(?)     a(?)
c
c  1         .78
c
c RECEPTOR DEPENDENT DATA (no line limit)
c FOR MODE   make      RECEPTOR DEPENDENT DATA
c 1 (site specific)    sector distance receptor-height
c 2 (by class & wind speed) class windspeed distance offset receptor-height
c 3 (create plot file)  class windspeed xmax imax ymax jmax xqmin power
c
c RECEPTOR PARAMETER DESCRIPTION
c sector = 0, 1, 2... (all, S, SSW, etc.)
c distance = receptor distance (m)
c receptor height = height of receptor (m)
c class = 1, 2, 3, 4, 5, 6, 7 (P-G stability class A, B, C, D, E, F, G)
c windspeed = anemometer wind speed (m/s)
c offset = offset from plume centerline (m)
c xmax = maximum distance to plot or calculate to (m)
c imax = distance intervals
c ymax = maximum offset to plot (m)
c jmax = offset intervals
c xqmin = minimum scaled X/Q to calculate
c power = exponent in power function step size
0 100 0

```

The file is read in free format; therefore, values need only be separated by a blank space or comma. It is important that all variables be assigned values in the input file, even if they are not used. It is also important that integer and logical variables be assigned integer and logical values respectively.

Lines that begin with the letter C are comments and are ignored. This input file is written with many such comments annotating input variables for readability. No comment lines are allowed in lines containing receptor dependent data. A line-by-line description of the input file follows.

Line 1

The first line of the input file is the title line. This line can contain 80 characters of descriptive information.

Line 2

The second line contains the integer variable *mode*.

Integer variable *mode* determines the operational mode of GXQ. It also determines the form of receptor dependent data required. Mode options are described below.

- Mode=1* A peak centerline X/Q' is calculated based on Hanford site-specific meteorology. Wind speed, atmospheric stability class and their joint frequency (JF) are all obtained from file JOINTFRE.IN. The reference anemometer height is also obtained from JOINTFRE.IN (fifth variable of third record). JF data can be used to either calculate a frequency of exceedance X/Q' (*ifox=t*) or an annual average X/Q' (*ifox=f*).
- Mode=2* An offset X/Q' is calculated for the user defined atmospheric stability class and wind speed.
- Mode=3* An offset X/Q' is calculated over a rectangular grid for the user defined atmospheric stability class and wind speed. This mode is specifically intended to be used in producing an isopleth plot file suitable for input to SURFER or other plotting packages.

Line 3

The third line contains the logical variables *ifox*, *inorm*, *icdf*, *ichk*, *isite*, and *ipop*. These logical variables are defined as follows:

- ifox* Controls how JF data is used. *Ifox=t* causes a frequency of exceedance X/Q' to be calculated. A false value causes an annual average X/Q' to be calculated. This flag operates only in *Mode 1*.
- inorm* The JF data contained in file JOINTFRE.IN contains frequency in percent that atmospheric conditions are within a specific sector, stability class, and wind speed interval. The sum of the frequencies for all sectors totals to 100 percent. *Inorm* controls normalization of the JF data contained in file JOINTFRE.IN. *Inorm=t* causes the joint frequency data for the specified sector to be normalized. Thus, a X/Q' calculated for an individual sector has a frequency or average based on normalized JF data for that sector. If an overall site X/Q' is desired (*isite=t*), then normalization should not make any difference as the JF data is already normalized across all sectors. This flag operates only in *Mode 1*.
- icdf* Controls printing of the cumulative distribution used in an *ifox=t* calculation to file CDF.OUT. *Icdf=t* will cause the file to be created if *mode=1*. A false value turns it off. The cumulative distribution data is useful when it is desired to know the wind speed and atmospheric stability class most closely corresponding to a frequency of exceedance X/Q , which was found by interpolation. This flag operates only in *Mode 1*.
- ichk* Controls printing of parameter values that are used in the X/Q' equations. If *ichk=t*, then printing to standard output is turned on. A false value turns printing off. This flag is useful for checking and understanding the calculated X/Q . This flag is operable in all modes but is not normally used in *Mode 1* due to the large amount of data generated in this mode.
- isite* Controls the way JF data is used in subsequent calculations. If *isite=t*, an overall site X/Q' is calculated based on JF data for

all 16 sectors contained in file JOINTFREE.IN. If *isite=f*, then only the JF data for an individual sector is used. If *isite=t*, then receptor dependent data must contain data in multiples of 16 lines (i.e., either *isec=0* or *isec=1* through 16). If *isec* equals zero then all sixteen sectors are evaluated at distance *x*. If 16 sectors are specified, the distances need not be the same for each sector. This flag operates only in *Mode 1*.

ipop Controls population weighting. If *ipop=t* then a population weighted X/Q' is calculated based on joint frequency data contained in file JOINTFREE.IN, population data contained in POP.IN, sector (*isec*) and distance (*x*). If *ipop=f*, then no population weighting is applied. This flag operates only in *Mode 1*.

The population contained within the bounds of *x* for the corresponding sectors is also tallied. Maximum distances for each of the 16 sectors should be provided. Usually, *ipm=3* to turn sector averaging on and simulate a uniform population distribution in each sector.

Line 4

The fourth line contains the integer variables *iflow*, *iwake*, *ipm*, and *ientr*. These integer variables are defined as follows:

iflow Determines whether the plume flow rate adjustment is used to modify the diffusion coefficients. If *iflow=1*, then the diffusion coefficients are adjusted so that the normalized concentration at *t=0* is equal to the effluent concentration. If *iflow=0* turns it off. This model uses release duration (t_{rd}), release diameter (*d*), and plume volume flow rate (V_0) as inputs. The model is useful for estimating near field concentrations.

iwake Controls application of building wake, initial puff volume and area source models. If *iwake=1* then the NRC (1982) wake model is implemented. If *iwake=2* then the MACCS (Chanin 1990) building wake model is turned on. *Iwake=0* turns it off. For a puff release the MACCS wake model can be used to establish an initial hemispherical cloud size by setting W_b to the diameter of the cloud and H_b to the height of the cloud. For an area source release the MACCS wake model can be used to simulate an area source by setting W_b to the diameter of the release area and H_b to zero.

ipm Controls application of plume meander models. *Ipm=1* implements the NRC (1982) plume meander model. *Ipm=2* implements the One-fifth Power Law plume meander model (Miller 1984). *Ipm=3* implements sector averaging over a 22.5 degree compass sector. *Ipm=0* turns plume meander off. These models are particularly meant for long-term or population weighted releases.

ientr Determines whether the entrainment model for vertically rising plumes is used to adjust the diffusion coefficients. If *ientr=1*, then the entrainment model is used. *Ientr=0* turns it off. This

model is intended to be used with a plume rise model since it operates on the difference between the effective plume height (h_e) and the stack height (h_s).

Line 5

The fifth line contains the integer variables *irise*, *igrnd*, *iwash*, and *igrav*. These integer variables are defined as follows:

- irise* Controls application of the momentum and buoyancy plume rise models. *Irise=1* turns the MACCS buoyancy rise model on. *Irise=2* turns the ISC2 momentum/buoyancy model on. *Irise=0* turns the plume rise model off. Both models use the convective heat rate (q_h) for calculating buoyancy flux unless $q_h=0$, in which case the initial temperature difference between the plume and ambient is used. The entrainment model should also be considered since the plume rise model only accounts for the increase in effective height of the plume and not the additional dispersion induced by the relative motion of the plume. If the scenario being modeled is a ground level fire, then the Briggs' buoyant rise model as modified by Mills' should be considered (see *igrnd* below). Input line 9 contains parameters needed for the plume rise models.
- igrnd* Controls application of the modification formulae proposed by Mills for applying the Briggs' buoyant rise model to a ground level fire. If *igrnd=1*, then the Mills' modification is utilized to decrease the amount of plume rise based on the fire radius. *Igrnd=0* causes Mills' modification to not be used. The input needed for this modification formulae is the release diameter (d).
- iwash* Controls application of a stack downwash model. *Iwash=1* turns the stack downwash model on while *iwash=0* turns it off. This model uses release diameter (d), plume initial temperature (T_0), ambient temperature (T_a), convective heat emission rate (q_h), and plume volume flow rate (V_0) as input. The effect of the model is to lower the effective plume height of elevated stack releases.
- igrav* Controls application of a gravitational settling model. *Igrav=1* turns the model on while *igrav=0* turns it off. This model uses the gravitational settling velocity (v_g) supplied by the user to decrease the effective stack release height. The equation is found in Miller (1984).

Line 6

The sixth line contains the integer variables *idep*, *isrc*, *ipuff*, and *iwind*. These integer variables are defined as follows:

- idep* Controls plume depletion using the Chamberlain model (Slade 1968). *Idep=1* turns plume depletion on while *idep=0* turns it off. This model uses deposition velocity (v_d) and is not normally used for short distances where plume depletion is negligible.
- isrc* Causes the standard Gaussian X/Q' equation to be multiplied by the user specified scaling factor *c* if *isrc=1*. If *isrc=2* then the

X/Q' equation is multiplied by $(c u^a)$. The intent of this option is to allow the user to scale the X/Q' or evaluate scenarios where both the source term and atmospheric dispersion are functions of wind speed. Operation of the code in *mode=1* facilitates the determination of an average or bounding condition of the combined effects.

ipuff *Ipuff=1* specifies the use of the Gaussian puff model whereas *Ipuff=0* specifies the Gaussian continuous plume model. If *ipuff=1* then a puff of release duration (t_{rd}) is assumed. The code will then calculate the peak normalized air concentration in units of $1/m^3$ based on either the puff or plume model, whichever is lower. For receptors located close to the release point, the continuous plume is the better model since its assumption of no windward diffusion is most valid when plume travel time is short. For receptors located far from the release point, the puff model is more appropriate since windward diffusion can have a large effect on peak air concentration. The intent of this option is to give the user the ability to estimate peak air concentrations which are important for toxic releases. For radiological releases, the continuous plume model should always be used since it is the integrated (i.e., cumulative) dose that is of interest.

iwind Causes the input wind speed to be adjusted for elevation. If *iwind=1* then the wind speed is adjusted according to the one-fifth power law from the anemometer height (h_a) to the effective plume height (h_e). *Iwind=0* causes the input wind speed to remain unmodified.

Line 7

The seventh line contains the real number variables h_s , h_a , h_m , and C_x . These are defined as follows:

h_s stack height (m). This input parameter is used to determine the effective plume height, h_e , (equation 4.1-4). It is also the height at which the stack or release level wind speed, u_s , is calculated. The stack level wind speed is used in the iteration procedure discussed in Section 4.3.1. If no plume height adjustment models are implemented, then $h_e=h_s$. This parameter is used in all modes and models of GXQ.

h_a anemometer height (m) corresponding to meteorological wind data. This input parameter is only used in modes 2 and 3. When *mode=1*, h_a is read from the joint frequency file, JOINTFRE.IN. It is used in the vertical wind speed adjustment model, equation 4.1-15, as the height corresponding to the wind speed data provided either in JOINTFRE.IN (*mode=1*) or from receptor input data (*mode=2 or 3*).

h_m mixing height (m) (1000 meters typical). This input parameter is used in the plume trapping reflection equation 4.1-5. It applies to all modes and models of GXQ.

C_x frequency the computed X/Q' will be exceeded. This input parameter is used in equations 4.4-7 and 4.4-11 which apply only when $mode=1$ and $ifox=t$.

Line 8

The eighth line contains the real number variables W_b , H_b , t_{rd} , v_d and v_g . These are defined as follows:

W_b building width (m). This input parameter is used to specify an initial plume width (and length when $ipuff=1$) using equation 4.2-7 which applies only when $iwake=1$.

H_b building height (m). This input parameter is used to specify an initial plume height using equation 4.2-8 which applies only when $iwake=1$.

t_{rd} release duration (hr). This input parameter is used by the instantaneous puff model (equations 4.1-7 and 4.1-8), the one-fifth power law plume meander adjustment (equation 4.2-13), and the flow adjustment model (equation 4.2-16). These models are activated when $ipuff=1$, $ipm=2$ or $iflow=1$.

v_d dry deposition velocity (m/s). This input parameter is used by the plume depletion model described in equation 4.1-10. This model is activated only when $idep=1$.

v_g gravitational settling velocity (m/s). This input parameter is used by the gravitational settling model described in equation 4.3-27. This model is activated only when $igrav=1$.

Line 9

The ninth line contains the real number variables T_a , T_0 , V_0 , d and q_h . These are defined as follows:

T_a ambient temperature ($^{\circ}C$), used in the plume rise and stack downwash models. This input parameter is used to determine the buoyancy flux (equation 4.3-1), the momentum flux (equation 4.3-5), the stability parameter (equation 4.3-6), and as a comparison to the crossover temperature difference given by equations 4.3-10, 4.3-11 and 4.3-17. These models are activated when $irise=1$ or $iwash=1$.

T_0 initial plume temperature ($^{\circ}C$), used in the plume rise and stack downwash models. It is important that the user specify a plume temperature consistent with q_h and V_0 , if provided (see equation 4.3-4); because, the crossover temperature difference, ΔT_c , and the plume to ambient temperature difference, ΔT , with which it is compared are dependent upon the user supplied initial plume temperature.

V_0 initial plume volume flow rate (m^3/s). This input parameter, along with release diameter, d , is used in the calculation of initial vertical plume velocity w^0 (equation 4.3-2) which is used

to determine plume rise (equations 4.3-1, 5, 10, 11, 16, 17, 21 and 24) and stack downwash (equation 4.3-26). V_0 is also used in the exhaust flow rate adjustment model (equation 4.2-18). These models are activated when $irise=1$, $irise=2$, $iwash=1$ or $iflow=1$.

d release diameter (m). This input parameter represents either the stack diameter for a stack release; or, the release diameter for a ground level release. In both cases it is a parameter used in the calculation of plume rise (equations 4.3-1, 2, 5, 10, 11, 16 and 21). It is also used in the Mills' adjustment for buoyant plume rise (equation 4.3-25) and stack downwash (equation 4.3-26), and in the exhaust flow rate adjustment model (equation 4.2-17 and 18). These models are activated when $irise=1$, $irise=2$, $igrnd=1$, $iwash=1$ or $iflow=1$.

q_h convective heat emission rate (w). This input parameter is used in the plume rise and stack downwash models. It performs two functions. When $q_h=0$, buoyancy flux is based on the initial plume temperature T_0 . For non-zero values of q_h the buoyancy flux is based on that value. The plume rise and stack downwash models are activated when $irise=1$ or 2 or $iwash=1$.

Line 10

The tenth line contains the real number variables c and a . These are defined as follows:

c scaling factor. This input parameter is applied to X/Q' as a constant c if $isrc=1$ or $isrc=2$ (equations 4.1-11 and 4.1-13).

a wind speed exponent. This input parameter is applied to X/Q' as $c \cdot u^a$ if $isrc=2$.

Line 11 and beyond

These input lines contain the receptor location data and are format free (i.e., delineated by commas or blanks). As many lines as are desired can be entered. The type of receptor data is determined by the program mode which is entered in line 2. For detailed information on the meaning of the mode variable see the discussion given for input line 2 above. Receptor location data are described below.

For $Mode=1$ the eleventh and following input lines contain the integer variable $isec$ and the real number variables x and z . These are defined as follows:

$isec$ sector identifier, $isec=0$ means all 16 compass sectors, $isec=1$ means S, and $isec=2$ means SSW. The sector is represented by the index, k , in the discussions in Section 4.4.

x release point to receptor distance (m). This input parameter is used to compute the horizontal and vertical diffusion coefficients (equations 4.2-1 and 4.2-2), the plume depletion factor (equation

4.1-10), distance dependent plume rise (equations 4.3-7, 4.3-20 and 4.3-22), and gravitational settling (equation 4.3-27).

z receptor "flagpole" height (m). This input parameter is used to calculate the vertical offset and reflection factor (equations 4.1-3 and 4.1-5).

For *Mode=2* the eleventh and following lines contain the integer variable *iclass* and the real number variables u_a , x , y and z . These are defined as follows:

iclass atmospheric stability class, where *iclass=1* means Pasquill stability class A, and *iclass=2* means class B, etc. The choice of stability class determines the value of the horizontal and vertical diffusion coefficients (equations 4.2-1 and 4.2-2), the vertical wind speed profile (equation 4.1-15), the plume meander adjustments (Section 4.2.3), and plume rise (Section 4.3.1).

u_a wind speed (m/s) corresponding to the reference anemometer height, h_a , given on input line 6. This input parameter is used in the calculation of an elevation corrected wind speed (equation 4.1-15) if *iwind=1*, or as the mean wind speed, $\bar{u}$, representative of ambient conditions.

x defined above

y receptor lateral offset from centerline of plume (m). This input parameter is used in equation 4.1-2 to simulate off-centerline receptors.

z defined above

For *Mode=3* the eleventh and following lines contain the integer variable *iclass* and the real number variables u , x_{max} , x_{int} , y_{max} , y_{int} , x_{qmin} and *power*. These are defined as follows:

u_a defined above

x_{max} maximum distance (m)

x_{int} number of distance intervals

y_{max} maximum offset (m)

y_{int} number of offset intervals

x_{qmin} minimum X/Q' value calculated. Variable x_{qmin} reduces the size of the plot file somewhat by excluding dispersion coefficients that are below this cutoff.

power grid density parameter. For example, if *power=1*, then the grid density is uniform. If *power=2*, then grid density varies as the square of distance and offset. Variable *power* allows a higher

density grid at the release point where the dispersion function is changing rapidly.

6.0 ERROR AND WARNING MESSAGES

The GXQ computer program does perform limited input data checking as an aid to the user. The data checking results in two levels of significance. The first is flagged as an error. An error is flagged to prevent a math error (i.e., divide by zero) or whenever it is concluded that no useful result can be obtained. This error always results in orderly program termination. The second is flagged as a warning but allows continued program execution. A warning brings to the users' attention, items for consideration. All other error messages originate from the system or are FORTRAN runtime errors. Most often these errors are caused by unmatched data types between the GXQ input file and the coded variable. System and runtime errors are not addressed here.

The following section provides a brief explanation and recommended solution for each of the coded error or warning messages incorporated into GXQ. If further information or explanation is necessary to interpret these errors, the WHC code custodian should be contacted. Additionally, any apparent errors in the code or its results should be brought to the attention of the code custodian for GXQ.

ERROR #1 - Could not open gxq.in file

The GXQ input file GXQ.IN was not found in the current directory. Ensure that the file GXQ.IN is in the directory from which GXQ execution is taking place.

ERROR #2 - Xmax or ymax less than or equal to zero

The maximum downwind distance xmax or offset ymax selected for Mode 3 is less than zero. Enter a positive value.

ERROR #3 - Could not open jointfre.in file

The joint frequency file JOINTFRE.IN for Mode 1 operation was not found in the current directory. Ensure that the file JOINTFRE.IN is in the directory from which GXQ execution is taking place.

ERROR #4 - Could not open pop.in file

The population file POP.IN was not found in the current directory. Ensure that the file POP.IN is in the directory from which GXQ execution is taking place.

ERROR #5 - Distance is less than or equal to zero

The downwind distance selected is less than or equal to zero. Although this number can be a small value, it can not be zero. Select a positive value.

ERROR #6 - Stability class must be between 1 and 7

Seven Pasquill atmospheric stability classes are defined. These are assigned the letters A through G. GXQ uses the integers 1 through 7. Make sure that only these integers are used for stability class.

ERROR #7 - Wind speed must be greater than zero.

The wind speed entered was less than or equal to zero. Depending upon the mode of operation, the wind speed could have been obtained from either file GXQ.IN or JOINTFRE.IN. Ensure that a positive value of wind speed is selected.

ERROR #8 - Selected frequency above joint freq. range.

Selected frequency is _____,Cx
Maximum sector frequency is _____,cd(n)

For Mode=1 operation with ifox=T, the selected frequency to exceed is above the total sector wind frequency. Thus, an interpolation can not be performed. This is caused by either selecting a frequency that is too high or by unintentionally using unnormalized sector frequency data. Lower the frequency to exceed or, if the intent is to use normalized joint frequency data as is done in the GENII code, set inorm=T.

ERROR #9 - Invalid mode specified

GXQ has three modes of operation. Mode should only be assigned integer values of 1, 2 or 3.

ERROR #10 - Invalid plume depletion model selected

GXQ has one plume depletion model. Set idep to 1 or 0.

ERROR #11 - Invalid building wake model selected

GXQ has one building wake model. Set iwake to 1 or 0.

ERROR #12 - Invalid plume meander model selected

GXQ has three plume meander models. Set ipm to 1, 2, 3 or 0.

ERROR #13 - Invalid plume rise model selected

GXQ has one plume rise model. Set irise to 1 or 0.

ERROR #14 - Invalid gravitational settling model selected

GXQ has one gravitational settling model. Set igrav to 1 or 0.

ERROR #15 - Invalid down wash model selected

GXQ has two stack downwash models that are selected internally. Set iwash to 1 or 0.

ERROR #16 - Invalid flow rate adjustment model selected

GXQ has one flow rate adjustment model. Set iflow to 1 or 0.

ERROR #17 - Invalid wind adjustment model selected

GXQ has one wind adjustment model. Set iwind to 1 or 0.

ERROR #18 - Momentum rise requires non-zero initial vertical plume flow rate (V_0)

As seen in equation 4.3-24, an initial plume flow rate of zero will cause a vertical plume velocity of zero and a divide by zero error in the entrainment coefficient. Select a positive value for V_0 .

ERROR #19 - Plume rise requires non-zero release diameter (d)

As seen in equation 4.3-2, a zero stack diameter will cause a divide by zero error when calculating an initial plume vertical velocity. Select a positive value for d.

ERROR #20 - Stack down wash requires non-zero release diameter (d)

As seen in equation 4.3-2, a zero stack diameter will cause a divide by zero error when calculating an initial plume vertical velocity. Select a positive value for d.

ERROR #21 - Flow adjustment requires non-zero release diameter (d)

As seen in equation 4.2-18, a zero stack diameter will cause a divide by zero error when calculating an initial vertical diffusion coefficient. Select a positive value for d.

ERROR #22 - Sector must be an integer from 0 to 16

The sectors 1 through 16 correspond to the 16 compass sectors with 1 meaning south, 2 meaning south-south-west, etc. A zero value is a short cut meaning all 16 sectors. For mode 1 operation, ensure that *isec* is set to an integer value between 0 to 16.

ERROR #23 - Puff model requires non-zero release duration

Selection of the Gaussian puff model requires a non-zero release duration since the X/Q' is also calculated using the continuous plume equation divided by the release duration (t_{rd}).

ERROR #24 - GXQ encountered an error reading the receptor location data.
Most likely this is caused by a carriage return after the last line.

The code checks for the end-of-file to signal the end of receptor input data. However, when editing the GXQ.IN file it is easy to enter a carriage return at the end of the file or to leave some portion of the receptor input data out and not take notice. In this event the code attempts to read additional receptor data and encounters an end-of-file instead. Check the receptor input data to ensure that it is complete and does not include additional blank lines.

ERROR #25 - Invalid source adjustment model selected.

An invalid source adjustment option has been selected. Set *isrc* to 0, 1 or 2.

ERROR #26 - Evaporation model inconsistent with puff source.

Use of the evaporation model implies a continuous release due to evaporation. The Gaussian continuous plume model should be used for this purpose by setting *ipuff* to 0.

ERROR #27 - Invalid ground effect model selected.

Setting *igrnd* to 1 turns on Mills' modification to the Briggs' plume rise equations. No other non-zero integer value is valid.

ERROR #28 - Invalid plume rise air entrainment model selected.

Setting *ientr* to 1 turns implements the method of Pasquill for modeling entrainment in a rising plume. No other non-zero integer value is valid.

ERROR #29 - Code does not handle releases above mixing layer.

The code detects that stack height h_s is greater than mixing layer height h_m . The code does not have the capability to model this release scenario.

WARNING #1 - Selected frequency is below minimum available.

Selected frequency is C_x
Minimum cumulative frequency is $cd(1)$
 X/Q below set equal to value corresponding
to minimum cumulative frequency.

For *mode=1* operation with *ifox=T*, the selected frequency to exceed is too small. Thus, an interpolation can not be performed. This is caused by selecting a frequency that is below the frequency corresponding to the worst-case combination of wind speed and stability class. Increase the frequency to exceed or use the calculated X/Q' with the understanding that the corresponding frequency is $cd(1)$ and not C_x .

WARNING #2 - Release duration outside validity of One-fifth Power Law.
Release duration must be between 10 min. and 100 h.

As seen in Equation 4.2-13, the One-fifth Power Law formula has a limited range of applicability. The user should remain within this range unless otherwise justified.

WARNING #3 - Scaled X/Q units are not adjusted for user specified scaling factor.

The scaling factor *c* is provided as a convenience to the user. However the units of the scaler will cause the units of the reported X/Q' to be other than what is reported. The user should always be aware of this.

WARNING #4 - Annual average X/Q is normally sector averaged.

An annual average X/Q' assumes a uniform distribution of wind direction within a sector this is accomplished by setting *ipm=3*. Results may be overly conservative otherwise.

WARNING #5 - NRC RG 1.145 building wake model may not be compatible with plume flow adjustment.

The NRC RG 1.145 building wake model does not adjust the lateral dispersion coefficient. Therefore, it is difficult to justify its use with another model that does. The user should not combine these options unless otherwise justified.

WARNING #6 - Population weighted X/Q is normally sector averaged to simulate uniform distribution.

Population weighting normally assumes uniform population distribution within a sector. This can be simulated by setting $ipm=3$. Results may be overly conservative otherwise.

WARNING #7 - Maximum normalized air concentration may be underestimated if plume meander on.

Instantaneous air concentration is independent of wind direction. If a plume meander adjustment is used, then the air concentration is time averaged laterally which may be non-conservative.

WARNING #8

Deleted.

WARNING #9

Deleted.

WARNING #10 - X/Q may be underestimated for plume rise scenario without accounting for entrainment.

The code detects a plume rise scenario without consideration of entrainment. There is additional mixing of the plume as it is rising due to entrainment. This effect could be modeled using the method of Pasquill by setting $ientr=1$. Neglecting the increase in the rising plume dimensions due to entrainment could result in non-conservative X/Q' estimates for receptors close to the release point.

WARNING #11 - Effective plume rise from ground level may be overestimated using Briggs plume rise model for stacks. Consider Mills modification.

The code detects a plume rise scenario from ground level. This could cause an overestimate in the calculated plume rise since Briggs' equations were developed for stack releases and do not consider ground effects. The reduced rise could be modeled using Mills' modification to the Briggs' plume rise equations by setting $igrnd=1$.

7.0 EXAMPLE USAGE

In the examples listed below, all logical flags are set to false and all integer (model) flags are set to zero unless otherwise specified.

GENII Approach

If a 95% sector normalized X/Q' for evaluating an acute release is desired as calculated by the GENII code; then, set $ifox=t$, $inorm=t$, and specify $C_x=5.0$.

If an annual average X/Q' for evaluating a chronic release is intended; then, it also should be sector averaged. To calculate annual average X/Q' for each sector as in GENII, set $ipm=3$.

NRC RG 1.145 Approach

If a 99.5% sector X/Q' for evaluating an acute release with building wake and plume meander is desired as described in NRC (1982); then, set $ifox=t$, $iwake=1$, $ipm=1$, and specify $C_x=0.5$.

If a 95% overall site X/Q' for evaluating an acute release with building wake and plume meander is desired as described in NRC (1982); then, set $ifox=t$, $isite=t$, $iwake=1$, $ipm=1$, and specify $C_x=5.0$.

If an annual average X/Q' for evaluating a chronic release is intended; then, it also should be sector averaged. To calculate annual average X/Q' for each sector set $ipm=3$.

Population Weighting

If a 99.5% population weighted X/Q' for evaluating an acute release on a surrounding population is desired; then, set $ifox=t$, $ipop=t$, $ipm=3$, and specify $C_x=0.5$.

If an overall site annual average, population weighted X/Q' for evaluating a chronic release on a surrounding population is desired; then, set $isite=t$, $ipop=t$, and $ipm=3$.

If a 50%, population weighted X/Q' is desired; then, set $ifox=t$, $ipop=t$, $ipm=3$, and specify $C_x=50.0$.

Further example calculations can be found in the GXQ Verification and Validation report (Hey 1994).

8.0 REFERENCES

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APPENDIX A
INDEPENDENT REVIEW CHECKLIST

PEER REVIEW CHECKLIST

Document Reviewed: Hey, B. E., 1994, *GXQ Program Users' Guide*, WHC-SD-GN-SWD-30002, Rev. 1, Westinghouse Hanford Company, Richland, Washington.

Scope of Review: Entire Document

Yes No NA

☒ ☐ ☐

Previous reviews complete and cover analysis, up to scope of this review, with no gaps.

☒ ☐ ☐

Problem completely defined.

☐ ☐ ☒

Accident scenarios developed in a clear and logical manner.

☒ ☐ ☐

Necessary assumptions explicitly stated and supported.

☒ ☐ ☐

Computer codes and data files documented.

☒ ☐ ☐

Data used in calculations explicitly stated in document.

☒ ☐ ☐

Data checked for consistency with original source information as applicable.

☒ ☐ ☐

Mathematical derivations checked including dimensional consistency of results.

☒ ☐ ☐

Models appropriate and used within range of validity or use outside range of established validity justified.

☒ ☐ ☐

Hand calculations checked for errors. Spreadsheet results should be treated exactly the same as hand calculations.

☒ ☐ ☐

Software input correct and consistent with document reviewed.

☒ ☐ ☐

Software output consistent with input and with results reported in document reviewed.

☐ ☐ ☒

Limits/criteria/guidelines applied to analysis results are appropriate and referenced. Limits/criteria/guidelines checked against references.

☐ ☐ ☒

Safety margins consistent with good engineering practices.

☒ ☐ ☐

Conclusions consistent with analytical results and applicable limits.

☒ ☐ ☐

Results and conclusions address all points required in the problem statement.

☐ ☐ ☒

Format consistent with appropriate NRC Regulatory Guide or other standards

☐ ☐ ☒

Review calculations, comments, and/or notes are attached.

☒ ☐ ☐

Document approved.

Paul Rittmann
Reviewer (Printed Name and Signature)

3-28-95

Date

☐ ☐ ☐ Analysis entered into analysis database

NA
(Printed Name and Signature)

Date