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Consequence Assessment For Airborne Releases of SO_2 from the Y-12 Pilot Dechlorination Facility

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Abstract

The Atmospheric Turbulence and Diffusion Division was requested by the Department of Energy's Oak Ridge Operations Office to conduct a consequence assessment for potential atmospheric releases of SO_2 from the Y-12 Pilot Dechlorination Facility. The focus of the assessment was to identify "worst" case meteorology which posed the highest concentration exposure potential for both on-site as well as off-site populations. A series of plausible SO_2 release scenarios were provided by Y-12 for the consequence assessment. Each scenario was evaluated for predictions of downwind concentration, estimates of a five-minute time weighted average, and estimate of the dimension of the puff. The highest hazard potential was associated with Scenario I, in which a total of eight SO_2 cylinders are released internally to the Pilot Facility and exhausted through the emergency venting system. A companion effort was also conducted to evaluate the potential for impact of releases of SO_2 from the Pilot Facility on the population of Oak Ridge. While specific transport trajectory data is not available for the Pilot Facility, extrapolations based on the Oak Ridge Site Survey and climatological records from the Y-12 meteorological program does not indicate the potential for impact on the city of Oak Ridge. Steering by the local topographical features severely limits the potential impact ares. Due to the lack of specific observational data, both tracer and meteorological, only inferences can be made concerning impact zones. It is recommended tat the Department of Energy Oak Ridge Operations examine the potential for off-site impact and develop the background data to prepare impact zones for releases of hazardous materials from the Y-12 facility.

DISCLAIMER

Introduction

The Atmospheric Turbulence and Diffusion Division (ATDD) of the National Oceanic and Atmospheric Administration (NOAA) was requested by the Department of Energy (DOE) Oak Ridge Operations Office (ORO) to conduct a consequence assessment for potential airborne releases of SO_2 from the Y-12 Pilot Dechlorination Facility. A set of plausible atmospheric release scenarios were developed by Y-12 and provided to ATDD as the basis of the consequence assessment. A focus of the consequence assessment was to define the "worst" case meteorological conditions. By "worst" case, this implies atmospheric conditions under which the highest exposures would be anticipated. An earlier screening assessment (Bloom, 1992) had indicated the potential for on/off-site impacts above acceptable levels. The ATDD was requested to review the earlier screening assessment and conduct a consequence assessment to further define the potential problems identified in the screening process. After the initial assessment had been completed, ATDD was also requested to evaluate the potential for impact of releases from the Y-12 Pilot Dechlorination Facility on the city of Oak Ridge(Littleton, 1992). This request was predicated on discussions of release trajectories and wind fields within the complex terrain structure of the Oak Ridge Reservation

Facility

A Pilot Dechlorination Plant has been installed along East Fork Popular Creek within the Y-12 Facility. The treatment process uses SO_2 gas supplied from commercially available SO_2 cylinders. This study focused on System I which provides treatment of the

North-South pipe and stream flow at Station F in the proximity of East Fork Popular Creek near Buildings 9204-1 and 9204-3. Figure 1 provides a map of the central section of the Y-12 facility; the pilot treatment facility is indicated on the map.

System I (Figure 2) is housed in a 12ftx12ftx8ft (3.65mx3.65mx2.43m) building located along East Fork Popular Creek. Exhaust vents provide emergency ventilation of the building; the exhaust system is activated when the internal concentration level of SO_2 exceeds 5 ppm. The two 9 inch (0.23m) exhaust fans are located 2 feet (0.61m) and 3.5 feet (1.07m) above the ground. Emergency exhaust venting rates are 358 cfm (0.0226 m^3/s)and 914 cfm (0.0575 m^3/s), respectively. Of the four supplied release scenarios, Scenarios 1-3 involve an internal (Pilot Plant) release of SO_2 gas with subsequent release to the ambient environment through the exhaust vents; the fourth release scenario is a release to the ambient environment through a process vent.

Release Scenarios

Four scenarios involving airborne releases of SO_2 (characteristics identified in Table I) were provided by Y-12 as source terms for the consequence assessment. The release scenarios are summarized in Table II; the transmittal letter is included in the appendices. Each of the release scenarios is considered below to determine an input value for dispersion modeling in the hazard assessment.

Release Scenarios 1-3 involve the discharge of SO_2 within the confines of the Pilot Facility with subsequent exhaust through the emergency venting system. In order to evaluate potential release rates for numerical model input, a simple box model approach was used. A schematic of the model is given in Figure 3. Further assumptions included assuming a composite exit vent equal to the two vents in total flow rates, sequential flushing of the building as the release ends, steady release of material from the cylinders with the supplied leak rates and duration, and complete mixing within the enclosure.

Making the above assumptions allows consideration of the mixing within the enclosure and determination of a discharge emission rate for SO_2 through the exhaust vents. As material is discharged into the enclosure, the internal concentration of SO_2 increases; however there is also a continuous discharge of SO_2 from the enclosure through the emergency venting system. A equilibrium is approached over the duration of the release between the discharge of SO_2 from the cylinders, internal mixing, and discharge of SO_2 through the vents. From the exhaust venting system, a source term is developed as a function of time. After the cylinders empty, the room is sequentially evacuated over the building exchange rate with a constant emission rate. The discharge rates for Scenarios 1-3 are given in Table III.

The fourth release scenario is a gas release to the ambient environment through the process vent. In this case, the source emission rate can be directly extracted from the supplied leak rates. Scenario 4 emission rate is include in Table III.

Figure 4 is a plot of release rate (grams/sec) for the four Scenarios. The release rates for scenario 3 and 4 are truncated at 500 seconds for this plot; actual release durations for Scenarios 3 and 4 are 19.3 minutes and 115.6 minutes, respectively.

Meteorology

For this consequence assessment, three key meteorological parameters are important. Wind speed, wind direction, and temperature determine the release characteristics and dispersion of the hazardous materials release. Wind direction provides a trajectory for the released material, wind speed gives a transport time, and the temperature coupled to both speed and direction defines the local stability which in turn determines dispersion of the contaminant.

For the Oak Ridge Reservation, the "worst" case meteorology is considered light winds, stable conditions. It is during these events that releases of hazardous materials pose the highest exposure potential. The stable case is characterized by limited mixing (both horizontal and vertical), providing little dilution of the released material; light or calm winds provide for a maximum in exposure times. For the Oak Ridge Reservation, "worst" case meteorology is also a function of the topography of the region. The ridge/valley orientation of the topography channels the local winds in a preferred southwest-northeast direction. Combined with the large building complex of the Y-12 Facility, the terrain forcing limits potential dispersion of released materials to trajectories along the valley floor. The following will extend this discussion of "worst" case for each meteorological parameter as related to releases of SO_2 from the pilot dechlorination facility.

As shown in Figure 5, the 30-year climatological record for Oak Ridge does not indicate the potential for ambient temperatures below -10 deg C, the boiling point for SO_2. This limits the possible release scenarios to a gas or gas/aerosol mixture. For the provided release scenarios, the three internal releases will only be considered in the gas phase; for the ambient release, the release quantity is small enough that the material can be considered as a gas for the duration of the release.

Temperature is also important in defining the potential for a "heavy" gas release. In the defined scenarios, simplifying assumptions were made concerning the release of material from the pressurized SO_2 cylinders. There will be some cooling associated with the sudden release of material from the storage cylinders but difficult to accurately determine. In the case of Scenarios 1-3, the material is released into a enclosure at ambient temperature (defined as 80 deg. F) with subsequent release of material through the exhaust vents. Assuming a low value for the initial dilution of the exhaust vent plume from the ambient environment, release density ratios should not exceed 1.2 - 1.4. At these ratios, "heavy" gas effects will not be important. A caveat is necessary; the above discussion applies only to the scenarios under review. Releases of the quantities identified in Scenarios 1-3 directly to the ambient environment, under "worst" case meteorology, may allow the material to exhibit "heavy gas" characteristics; in this evaluation, the material is released in a heated enclosure. This dominates the initial state of the release.

As indicated above, the local topography of the Oak Ridge Reservation is a dominating influence of the wind regime of the Y-12 facility. Numerous studies of the wind fields over the Oak Ridge Reservation (ORO-99, 1952, Eckman, et al, 1991) have documented steering of the local meteorological wind field by the East Tennessee ridge/valley structure. Terrain forcing is clearly evident in the wind rose data, Figure 6, for the meteorological towers located at the Y-12 facility. Clearly, the highest probability is associated with winds along the valley southwest-northeast orientation. The probabilities are actually higher for the prevailing wind directions when it is recognized that the small frequencies associated with south through east winds are associated either with light and variable winds, limited cold air drainage flow from the surrounding ridges, or increased fluctuations in wind direction due to the mechanical turbulence generated by the Y-12 building complex. The increased variability from the west to southwest of the East-End tower shows the fluctuations generated by the building complex of Y-12. Removing the light and variable winds (< =2 m/s) from non-prevailing directions increases the frequency of southwest-northeast winds above 98%. It is important to note that the directions presented in the wind rose plots represent point measurements of the frequency of occurrence of the wind direction **NOT** transport trajectories. Transport trajectories within the Oak Ridge Reservation are dominated by the local topographical features and cannot be obtained strictly from wind direction frequency distributions.

Figure 7 presents several wind rose plots from the Oak Ridge Site Survey (Eckman, et al, 1992) illustrating the preferred along-valley direction of the wind flow and distinct differences between above and within valley flow. Results of this study coupled with the analysis of probable impact regions for emergency management (Eckman, 1992) indicated that for releases of material below ridge top height there was little potential for airborne material to cross the local ridge line (Chestnut Ridge).

Non-prevailing wind directions were observed during the Oak Ridge Site Survey to be very localized with channeling along the valley floor to represent the local trajectory. Combined with the local building configuration near the pilot Dechlorination Facility(refer to Figure 1), trajectories of material released from the facility should propagate in a northeast or southwest direction.

While specific data does not exists to confirm release trajectories from the location of the pilot facility, evidence from both the Oak Ridge Site Survey and local on-site meteorological measurements show little or no potential for impact of release from the pilot facility on the population centers of Oak Ridge. It would be difficult with the limited site specific data to make a blanket statement of the potential impact; one could always contrive a release scenario which had the appearance of potential impact however improbable. Assigning a probability to such an event would be incompetent. It is recommended the DOE/ORO undertake the program to obtain the data needed to perform the trajectory analysis. Without the confirming data sets, potential impact must be based on scientific judgement.

The above discussion focused on situations under which there was a direction steering component to the local wind field. However, as identified, the "worst" case meteorology refers to light and variable winds under stable conditions as having the highest potential for exposure. It is during this period that limited mixing of potential releases of SO_2 would occur. Currently there is very little guidance in the literature on techniques to predict dispersion during light winds or calm conditions. To develop a consequence assessment for the given Scenarios the material is allowed a 1.0 m/s transport wind in the preferred wind directions identified in the previous discussion. The 1.0 m/s wind speed is used since the theoretical basic for most atmospheric dispersion models is not valid below 1.0 m/s

Consequence Assessment

As previously mentioned, there is little guidance in the literature regarding numerical modeling in light winds, stable conditions. Due to the rather large uncertainties in both development of the source terms and dispersion characteristics in this situation, a simplistic Gaussian puff model approach was utilized. Also, for the given source terms, there are no indicated circumstances in which the released material would not be considered passive. With the source term defined, the initial source dimensions must be considered.

For the puff simulation, the release was divided into 10 second time steps. A puff of material (SO_2) was generated and modeled with a composite mass equivalent to a 10 second period. For Scenarios 1-3 the source varied with time as the material was released, ingested in the enclosure , and emitted through the exhaust vents. For Scenario 4 the release was considered constant over the release duration. The initial puff dimensions were developed from the exhaust rate, enclosure dimensions, and initial exit dilution.

Scenario 1 represents the largest release of SO_2 from the Pilot Facility. The contents of eight cylinders (544 kg) are release from the simultaneous melting of the safety plugs due to the temperature within the building reaching 157 deg F.
Total contents of the SO_2 cylinders would be released into the building over 210 seconds

with another 55 seconds allowed for the evacuation of the Pilot Plant enclosure. It is expected that the material would fill the enclosure with internal concentrations building to the point at which the emergency exhaust system would be initiated. A balance would be approached between the release of SO_2, buildup of the internal concentration, and exhaust of material through the ventilation system. Figure 4 illustrated the time history of emissions from the enclosure. To simulate the time history of potential exposure to the released material the total release duration was divided into five periods with an average release rate obtained for each period. Table 4 is a summary of source terms and initial conditions for Scenario I. For each period the exposure estimate was obtained and a time-weighted five-minute average concentration. Figure 8 present a series of plots of SO_2 concentrations as a function of downwind distance. Also given is the five-minute average concentration developed from the time history exposure. For Scenario 1 the IDLH is not reached until almost 2 kilometers downwind. At this point the full width of the plume is approximately 250 m.

Scenario 2 is a liquid release of the contents of 1 cylinder over a 4.6 second period. The material is released into the enclosure at an ambient temperature of 80 deg. F. The sudden release of material from the cylinder will fill the enclosure; the source term developed is the subsequent evacuation of the enclosure through the emergency exhaust system. Table 5 is a summary of initial conditions for this scenario. Figure 9 is a plot of downwind concentration as a function of distance for the release; also included is the five-minute average. This scenario represents a short duration (55 seconds) release of material. Downwind populations will be exposed to a short duration high concentration. However the five-minute average will be considerably lower. Using the five minute average concentrations, IDLH values are reached at roughly 600 meters downwind.

Scenario 3 is the release of SO_2 from three cylinders at ambient temperature (80 deg F) through a pig-tail leak. The leak duration is 19.3 minutes. The same scenario regarding an internal release applies to this scenario. The material is allowed to leak into the enclosure and exhausted through the emergency venting system. Table 6 provides a summary of initial conditions for this scenario. IDLH values (Figure 10) are reached roughly 550 meters downwind of the source. The release rate of 174 g/sec was simulated over a five-minute period; concentrations reflect an anticipated five-minute average. These values reflect the maximum concentration exposure anticipated in this scenario.

Scenario 4 is a slow leak of SO_2 through a process-vent. the leak occurs over a 115.6 minute duration. Table 7 gives a summary of initial conditions for this simulation. This release is emitted directly to the ambient environment; except for an additional initial source size, the release is treated directly as a point source. Figure 11 provides a plot of concentration prediction for this scenario. IDLH values are reached near the source (approximately 200 meters downwind). The concentration values presented are predicted maximums as well as five-minute averages anticipated for the long duration release.

Summary/Conclusions

Four airborne release scenarios provided by the Y-12 Facility were evaluated for this consequence assessment under assumed "worst" case meteorology. "Worst" case was identified as light winds, stable conditions which provide for limited dilution of the release plume and long exposure times. In order to provide a credible numerical simulation, a 1.0 m/s wind speed was used in the dispersion model. For each release scenario, the downwind distance to the IDLH value was defined from five-minute time-weighted average concentrations.

Scenario 1 represented the highest potential for exposure above acceptable levels.

The combination of relatively large source term (large release and short release period) and long residence times produce high hazard levels. Since the concentration estimates in this analysis are linear with respect to the source term, as estimate of an acceptable SO_2 cylinder storage level can be extrapolated (ie., release of two cylinders represents 2/8 of the Scenario 1 concentration estimates.

A short discussion was also presented to illustrate the low probability of impact from the SO_2 on the City of Oak Ridge. It was shown that wind rose frequency data should not be confused with transport trajectories. Frequency data relates to point measurements of direction frequency; this can only be used for "flat" terrain as trajectory frequencies. Within the Oak Ridge Reservation, trajectories are dominated by the ridge/valley topographical orientation. The small frequency of non-prevailing wind directions are associated with local perturbations; these fluctuations can also be attributed to the increased turbulence levels generated by the Y-12 building complex. While no specific probabilities were given for an Oak Ridge trajectory, it can be inferred from the observational and meteorological research data to be quite minimal - beyond the need for consideration. It was recommended that the DOE/ORO undertake a program to define potential impact regions for each facility under its jurisdiction.

References

Bloom, S.G., 1992. SO_2 Release Scenarios. Personal Communication.

Eckman, R. M., R. J. Dobosy, W. R. Pendergrass, 1992. Preliminary Analysis of Wind Data from the Oak Ridge Site Survey. NOAA Tech. Memo. ERL ARL - 193, NOAA Air Resources Laboratory, Silver Spring, Md, 45p.

Eckman, R. M., 1992. Recommended Meteorological Measurement Network for the Oak Ridge Y-12 Plant. ATDD Contribution No. 92/10, NOAA Atmospheric Turbulence and Diffusion Division, Oak Ridge, TN, 8p.

Attachments

1. Authorizing letter from DOE/ORO.
2. Bloom, 1992 Report.
3. Source term letter.
4. Preliminary Analysis of Wind Data from the Oak Ridge Site Survey.
5. Recommended meteorological Measurement network for the Oak Ridge Y-12 Plant.
6. Flow Visualization Experiments on Stably Stratified Flow Over Ridges and Valleys.
7. Wind Tunnel Studies of Flow Channeling in Valleys.

Table 1

SO_2 Characteristics

Formula	SO_2
Molecular Weight	64.06
Latent Heat	397 Kj/Kg
Boiling Point	- 10 deg C
Specific Gravity	1.45 (-10)
Vapor Pressure	2538 mm Hg
Vapor Density	2.3
IDLH	266 mg/m^3
TLV	5 mg/m^3
STEL	13 mg/m^3

Table 2

Release Scenarios

1) Simultaneous melting of the safety plugs on eight cylinders releasing 544 kg SO_2 into the Pilot Plant enclosure over 3.49 minutes.

2) Liquid release of SO_2 at ambient temperature with vaporization of 68 Kg over 4.6 seconds into the Pilot Plant.

3) Pigtail release of 3 cylinders of SO_2 at ambient temperature into the Pilot Plant - 204 Kg over 19.3 minutes.

4) Release of three cylinders (204 Kg) of SO_2 through a process vent leak for a duration of 115.6 minutes.

Table 3

Emission Rates
(g/s)

Scenario	t(1)	t(10)	t(30)	t(max)
1	47.6	438	1106	2580
2	1236	1236	1236	1236
3	3	29	74	176
4	29.4	29.4	29.4	29.4

Table 4

Initial Conditions
Scenario 1

u = 1.0 m/s
S = F (Pasquil-Gifford)
T = 5.0 C
Rh = 30%

SO_2 Release Rates

Period	Duration (sec)	Release Rate (g/s)
1	30	40
2	30	955
3	40	2000
4	100	2350
5	60	2550

Table 5

Initial Conditions
Scenario 2

u = 1.0 m/s
S = F (Pasquil-Gifford)
T = 5.0 C
Rh = 30%

SO_2 Release Rates

Period	Duration (sec)	Release Rate (g/s)
1	55	1236

Table 6

Initial Conditions
Scenario 3

u = 1.0 m/s
S = F (Pasquil-Gifford)
T = 5.0 C
Rh = 30%

SO_2 Release Rates

Period	Duration (sec)	Release Rate (g/s)
1	300	174

Table 7

Initial Conditions
Scenario 4

u = 1.0 m/s
S = F (Pasquil-Gifford)
T = 5.0 C
Rh = 30%

SO_2 Release Rates

Period	Duration (sec)	Release Rate (g/s)
1	115 (min)	29.4


9201-1
9201-2
9201-3
9202
9203
9207
9208
9210
9211
9220
9224
9720-1
9786
9737
9401-1
9104-1
9104-2
9104-3
9102-1
9710-3
9711-1
9704-1
9706-2
9116
9106
9723-24
9723-28
9123-4
9728
9723-33
9733-1
9733-2
9733-3
9733-4
9734
9739
9735
9736
9764
FIRST STREET
BENZENE DR
POPLAR CREEK
CWSA
CWSA
CWSA
CWSA

Figure 1

Figure 2

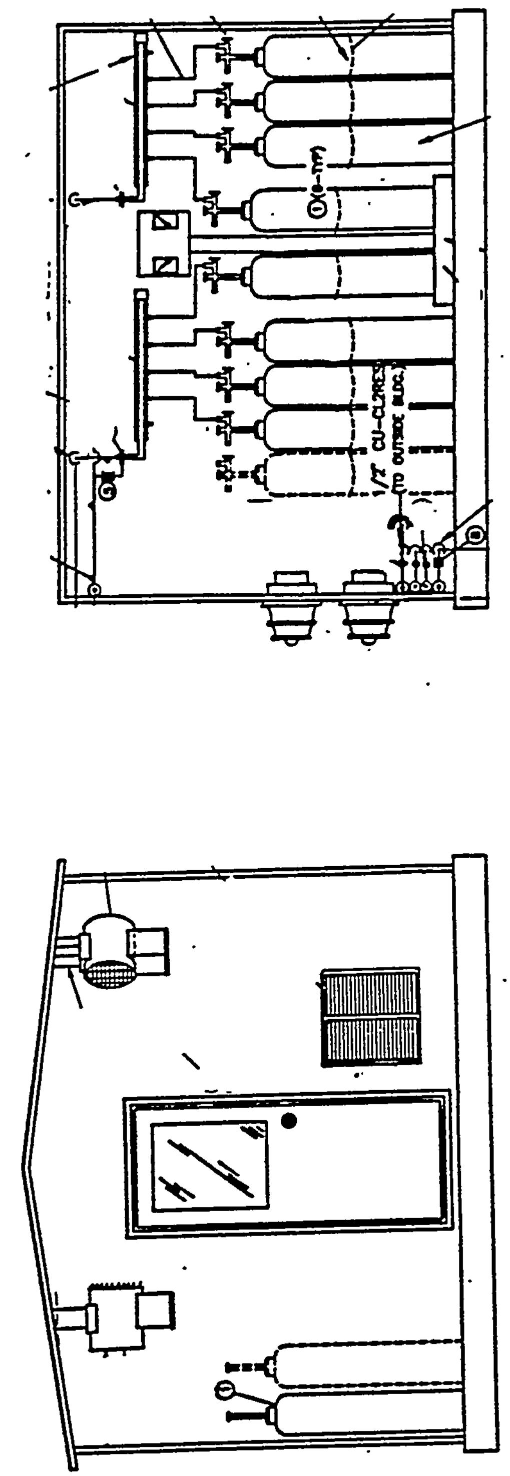
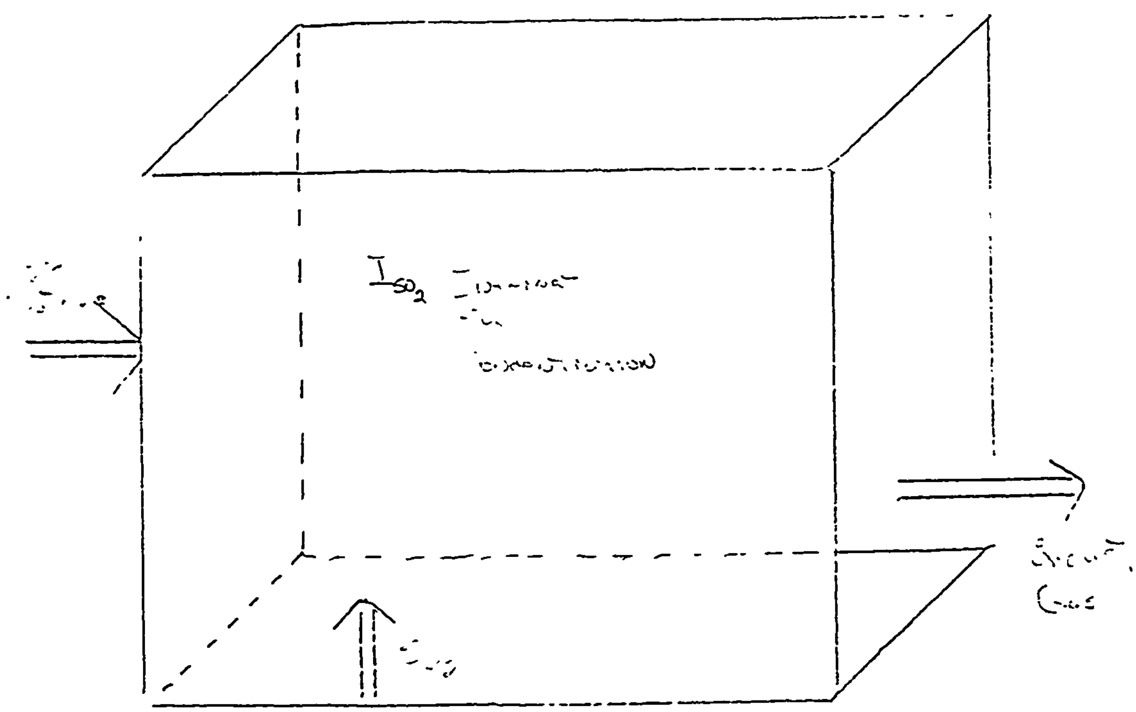
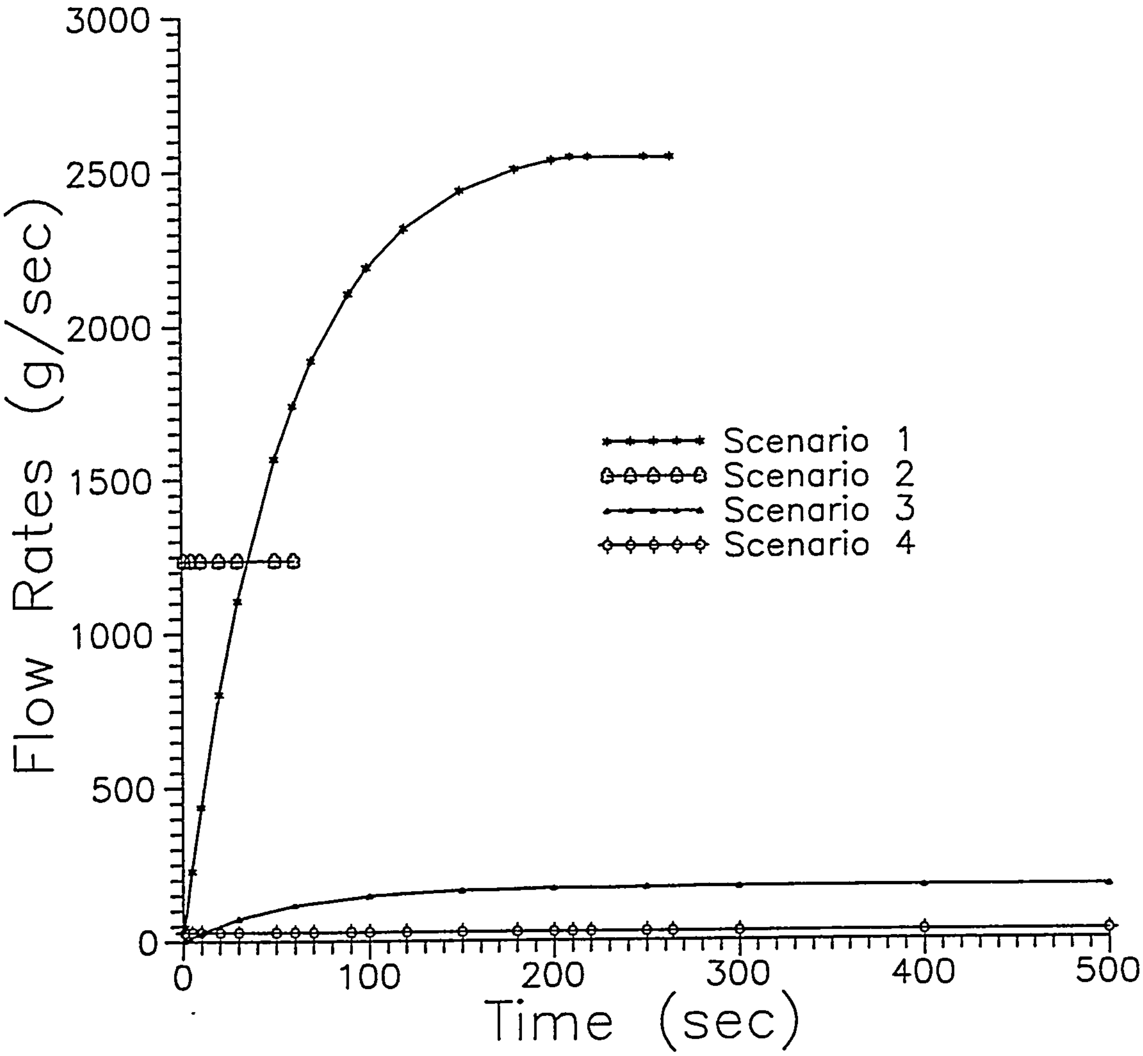


Figure 3



Enclosure Volume   8ftx12ftx12ft   => 32.40 m^3
Exhaust Rates   358 cfm + 914 cfm => 0.08 m^3/sec

Figure 4



3000
2500
2000
1500
1000
500
0
Flow Rates (g/sec)
Scenario 1
Scenario 2
Scenario 3
Scenario 4
0
100
200
300
400
500
Time (sec)

LOCAL CLIMATOLOGICAL DATA

ANNUAL SUMMARY WITH COMPARATIVE DATA

OAK RIDGE,

TENNESSEE

Daily Data

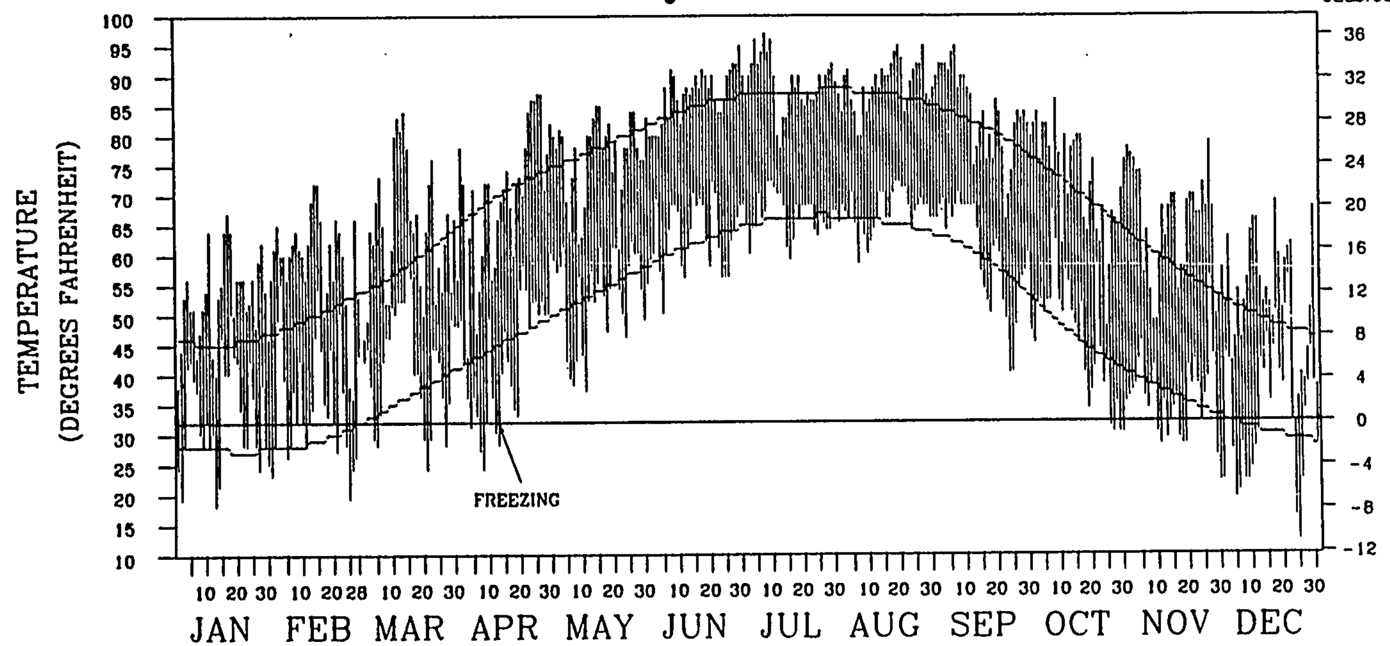
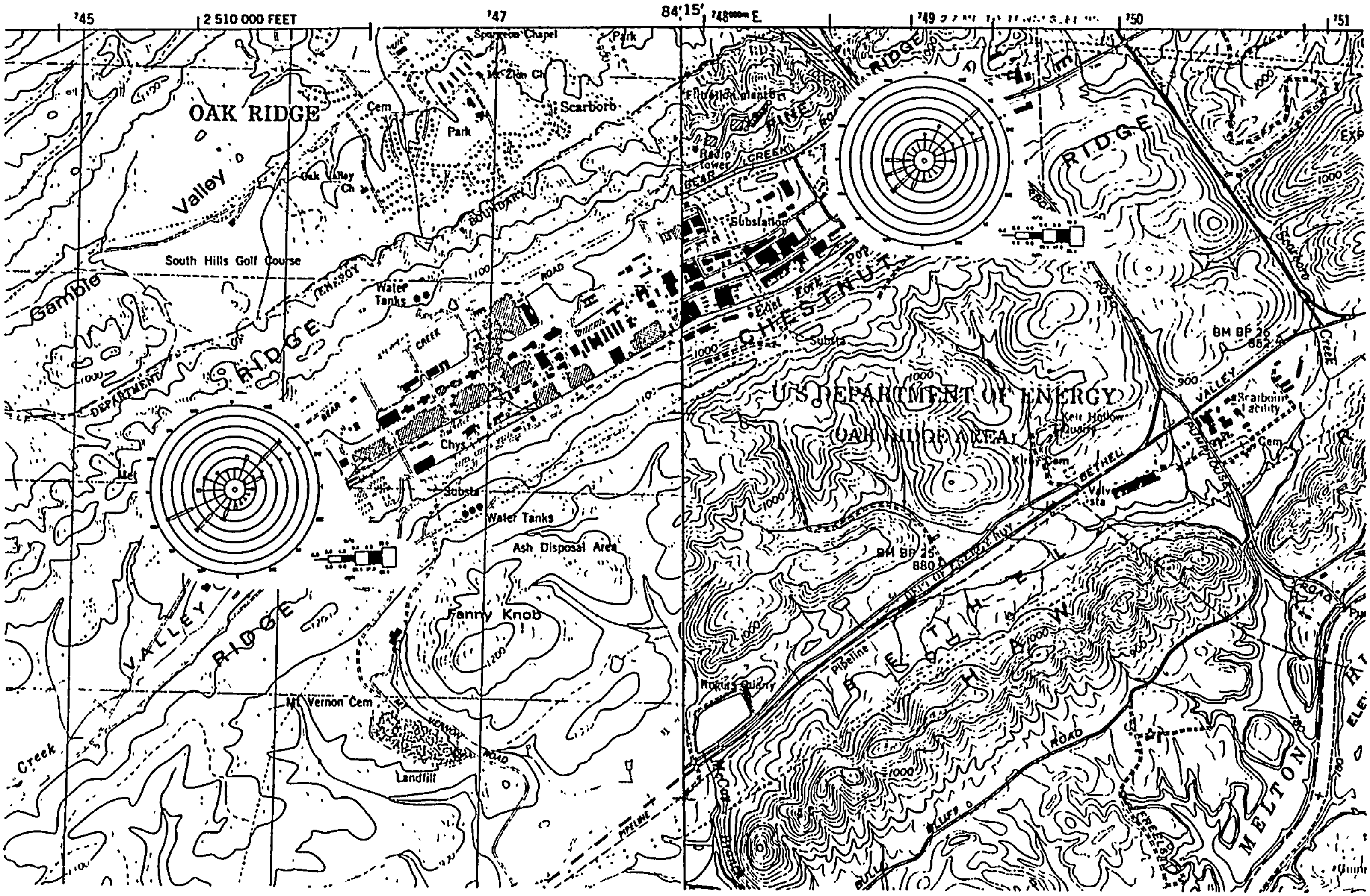
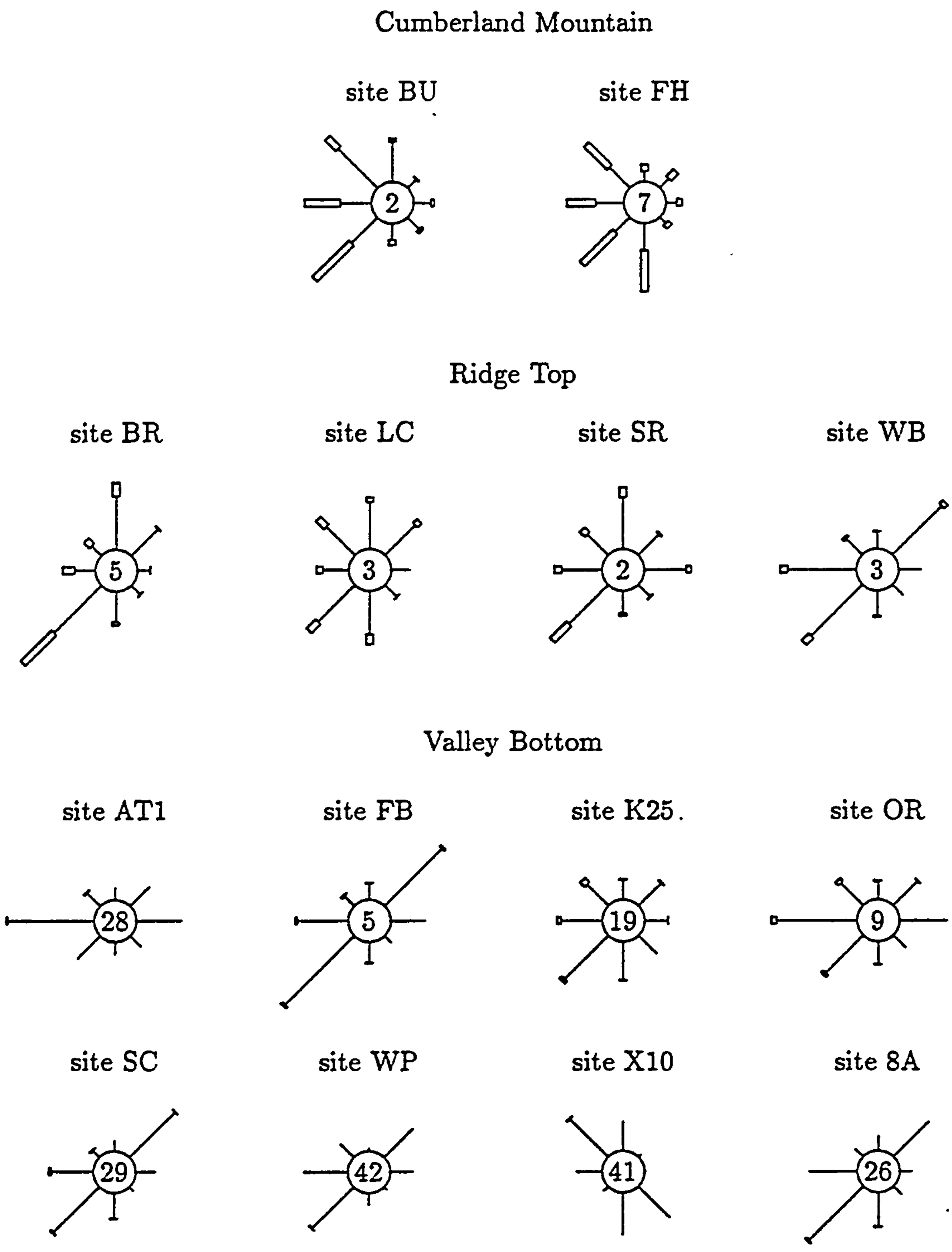


Figure 5

Figure 6



745
2 510 000 FEET
747
84°15'
748000m E.
749
750
751
OAK RIDGE
Valley
South Hills Golf Course
Gamble
RIDGE
DEPARTMENT
ENERGY
BOUNDARY
Water Tanks
Spurgeon Chapel
Mt Zion Ch
Scarboro
Park
Cem
Oak Valley Ch
CREEK
BEAR
ROAD
Chys
Substa
Water Tanks
Ash Disposal Area
Fanny Knob
VALLEY
RIDGE
Mt Vernon Cem
VERNON
ROAD
Landfill
Creek
PIPELINE
Filtration plant
Radio Tower
BEAR CREEK
PINE
RIDGE
Substation
East Fork
CHESTNUT
Substa
U S DEPARTMENT OF ENERGY
OAK RIDGE AREA
Kerr Hollow Quarry
Kerr Cem
BM BF 25 880
BM BF 26 862.4
Scarboro Facility
Cem
VALLEY
BETHEL
Valve Sta
PUMPHOUSE
Pipeline
Rogers Quarry
BETHEL
HAW
ROAD
McCoy Branch
BULL BLUFF
FREELS
MELTON
HILL
Scarboro
Creek



Cumberland Mountain
site BU
site FH
2
7
Ridge Top
site BR
site LC
site SR
site WB
5
3
2
3
Valley Bottom
site AT1
site FB
site K25
site OR
28
5
19
9
site SC
site WP
site X10
site 8A
29
42
41
26

Figure 1

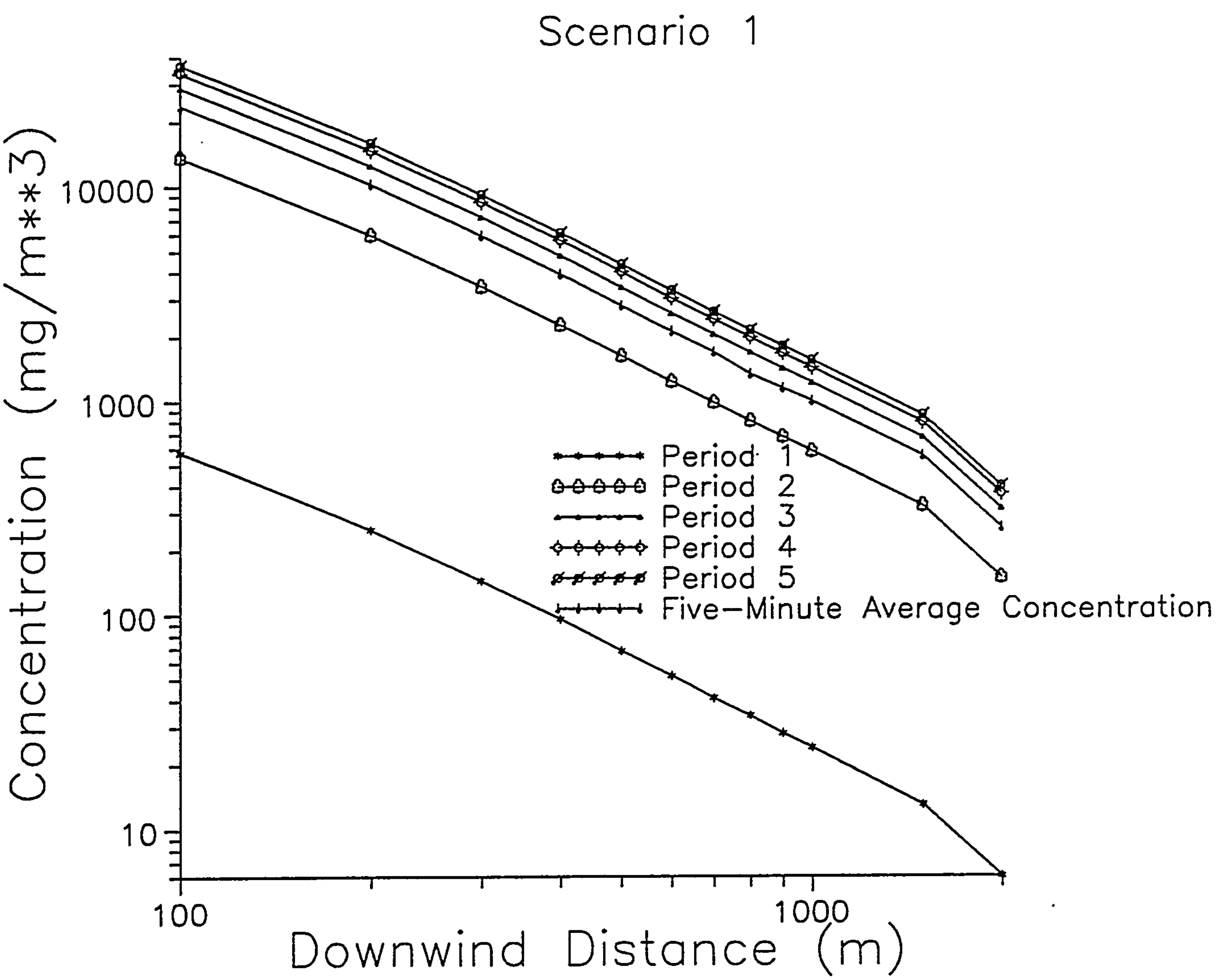

Scenario 1
Concentration (mg/m**3)
10000
1000
100
10
100
1000
Downwind Distance (m)
Period 1
Period 2
Period 3
Period 4
Period 5
Five-Minute Average Concentration

Figure 9

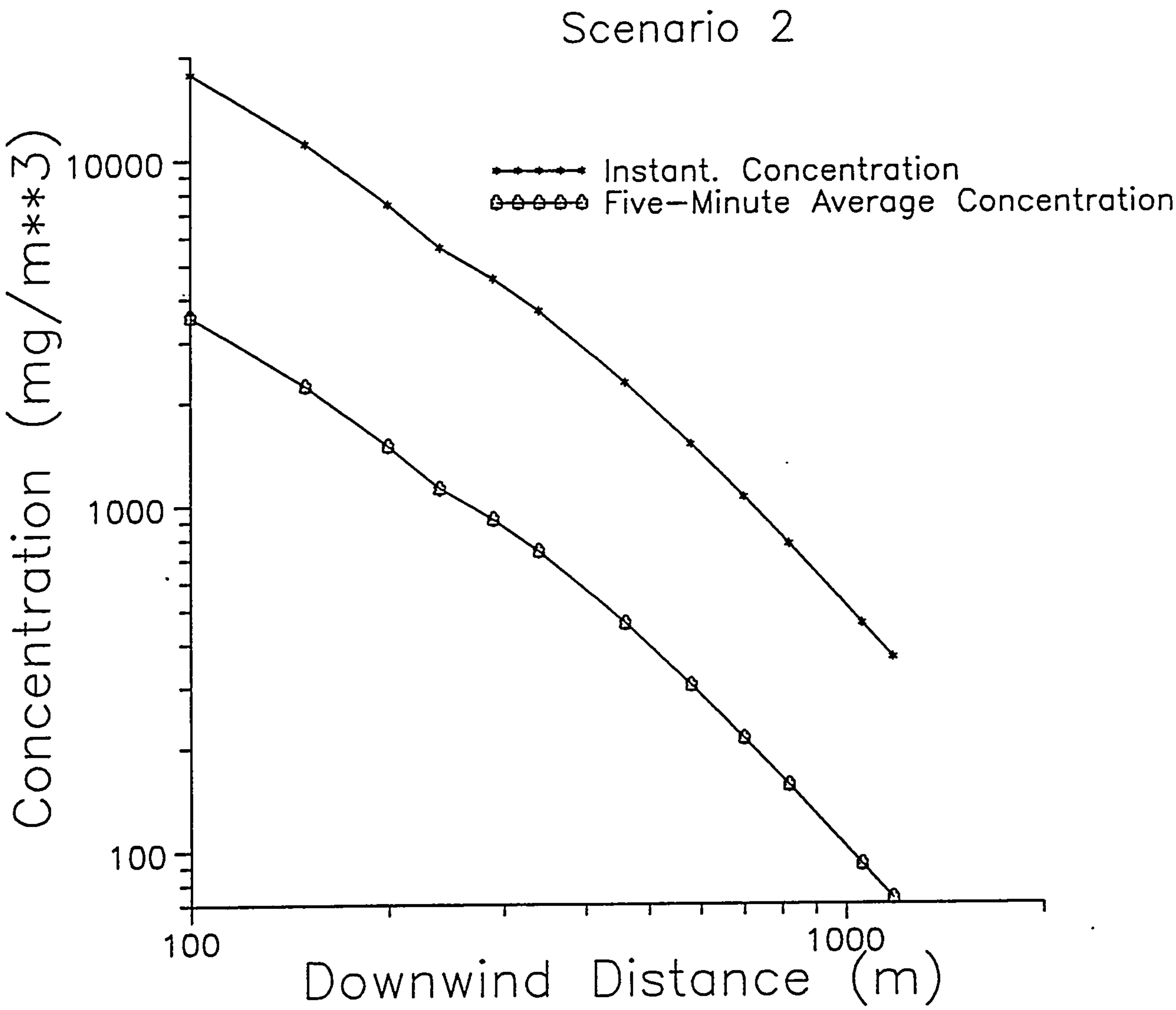
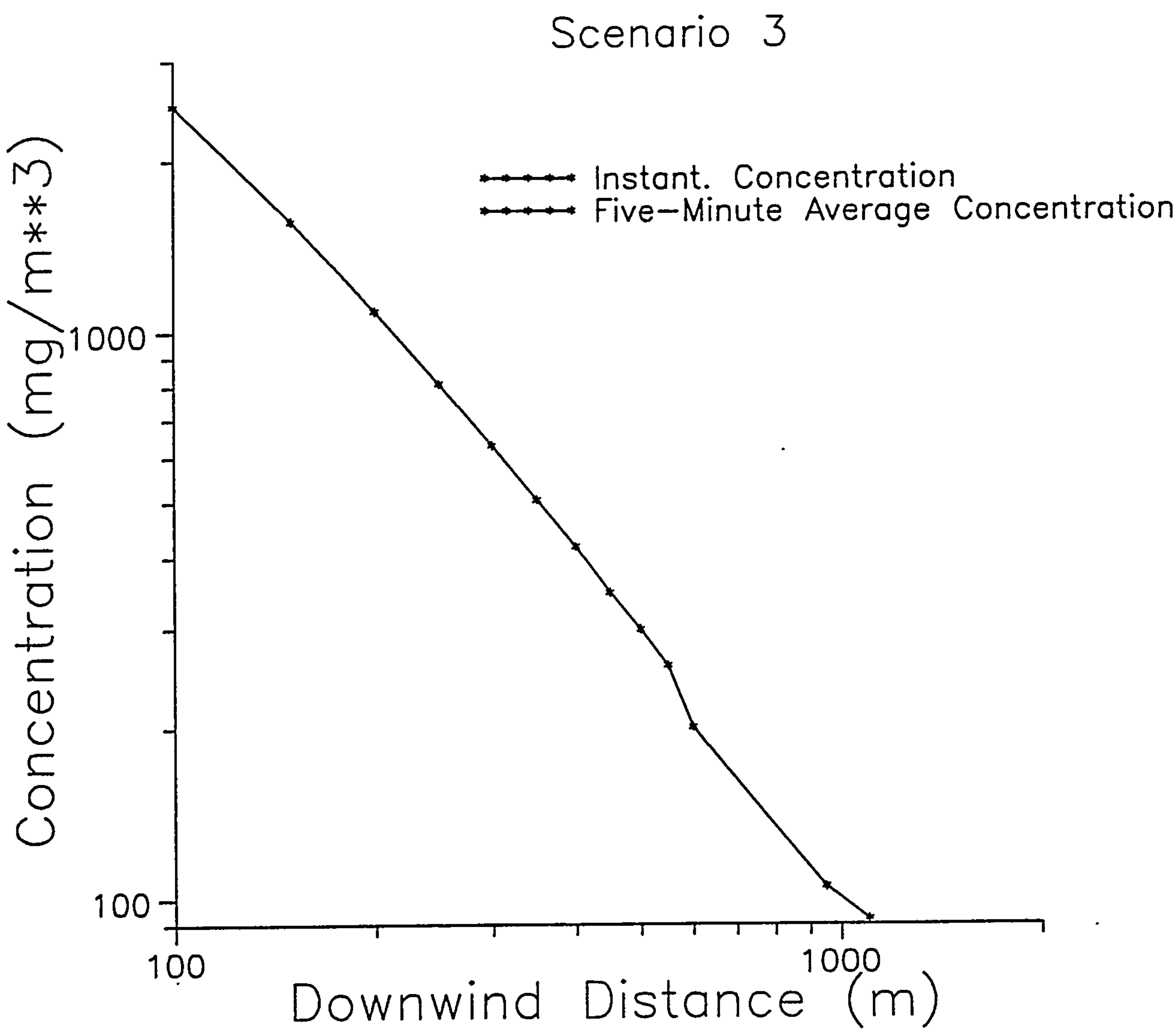
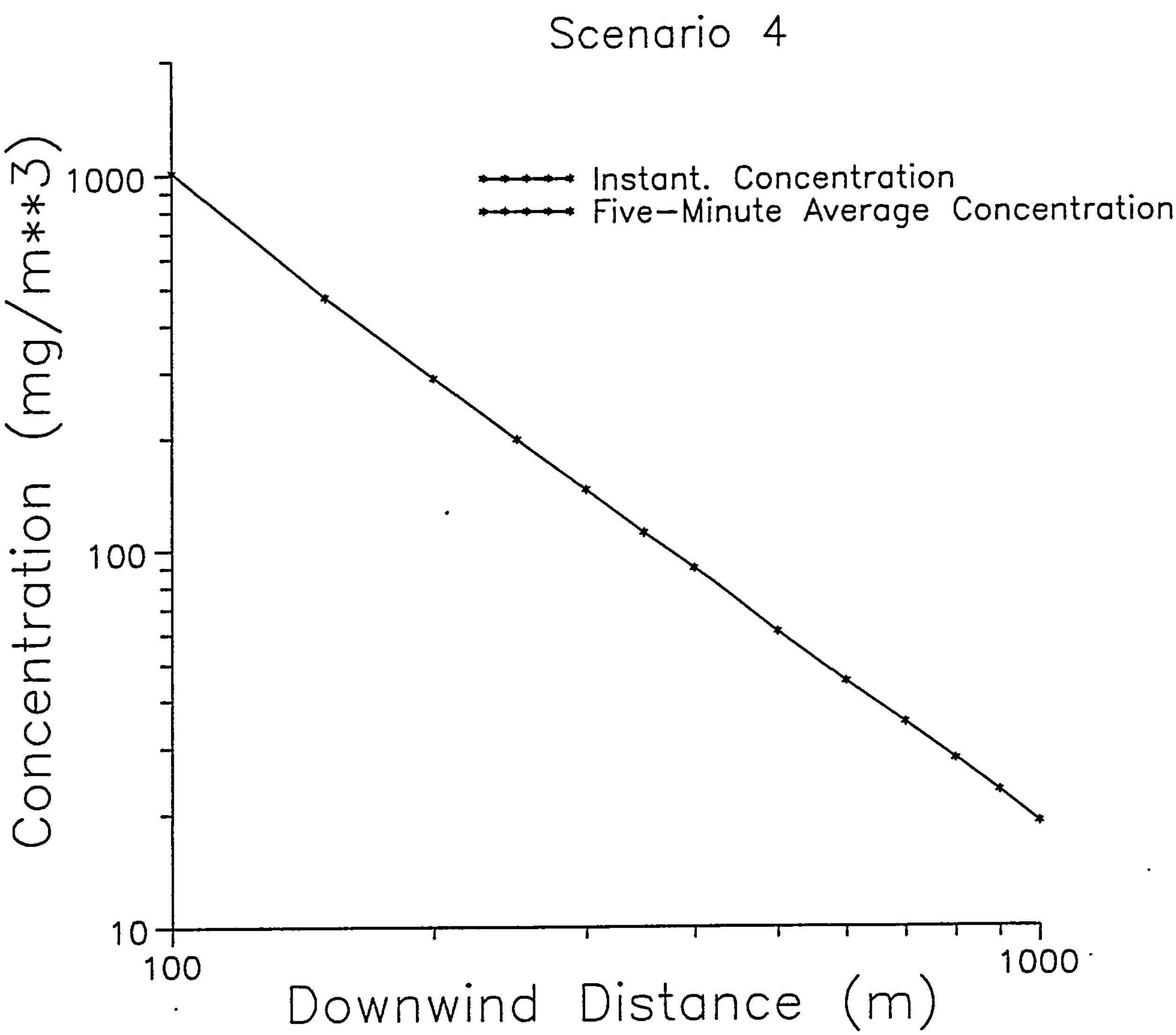

Scenario 2
Concentration (mg/m**3)
10000
1000
100
Instant. Concentration
Five-Minute Average Concentration
100
1000
Downwind Distance (m)

Figure 10



Scenario 3
Instant. Concentration
Five-Minute Average Concentration
Concentration (mg/m**3)
1000
100
100
1000
Downwind Distance (m)

Figure 11


Scenario 4
Instant. Concentration
Five-Minute Average Concentration
Concentration (mg/m**3)
1000
100
10
100
1000
Downwind Distance (m)