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## Packaging Performance Evaluation and Performance Oriented Packaging Standards for Large Packages for Poison Inhalation Hazard Materials

Nancy R. Griego, G. Scott Mills, James D. McClure, Ruth F. Weiner, Nancy C. Finley

Prepared by  
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## **Packaging Performance Evaluation and Performance Oriented Packaging Standards for Large Packages for Poison Inhalation Hazard Materials**

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### **Abstract**

The U. S. Department of Transportation Research & Special Programs Administration (DOT-RSPA) has sponsored a project at Sandia National Laboratories to evaluate the protection provided by current packagings used for truck and rail transport of materials that have been classified as Poison Inhalation Hazards (PIH) and to recommend performance standards for these PIH packagings.

Hazardous materials span a wide range of toxicity and there are many parameters used to characterize toxicity; for any given hazardous material, data are not available for all of the possible toxicity parameters. Therefore, it was necessary to select a toxicity criterion to characterize all of the PIH compounds (a value of the criterion was derived from other parameters in many cases) and to calculate their dispersion in the event of a release resulting from a transportation accident. Methodologies which account for material toxicity and dispersal characteristics were developed as a major portion of this project and applied to 72 PIH materials.

This report presents details of the PIH material toxicity comparisons, calculation of their dispersion, and their classification into five severity categories.

## ACKNOWLEDGMENTS

The authors acknowledge the U.S. Department of Transportation Research & Special Programs Administration for their support of this effort. We specifically acknowledge Charles Hochman and James O'Steen for their contributions as project monitors during this effort. The authors also wish to acknowledge Robert E. Glass and Douglas Ammerman for participating in numerous conversations about packaging performance and regulations, K. Sieglinde Neuhauser for participating in conversations on radioactive material transport regulations and risk analysis, and John Ludwigsen for his finite-element calculations of packaging performance. Finally, we wish to thank Daniel Maloney and Anthony Policastro of Argonne National Laboratory and William Dunn of the University of Illinois for their assistance in selecting toxic exposure guidelines.

## NOMENCLATURE

AAR	Association of American Railroads
CAB	Civil Aeronautics Board
CFR	Code of Federal Regulations
DOT	U.S. Department of Transportation
DOT-RSPA	U.S. Department of Transportation Research & Special Programs Administration
EODA	Explosives & Other Dangerous Articles Act
ERPG-1	Emergency Response Planning Guideline 1
ERPG-2	Emergency Response Planning Guideline 2
ERPG-3	Emergency Response Planning Guideline 3
FAA	Federal Aviation Administration
ft	foot/feet
g/s	grams per second
Hazmat	Hazardous Materials
HMRB	Hazardous Materials Regulations Board
HMTA	Hazardous Materials Transportation Act
HPPE	Hazardous Materials Packaging Performance Evaluation
IAEA	International Atomic Energy Agency
IATA	International Air Transport Association
ICAO	International Civil Aviation Organization
ICC	Interstate Commerce Commission
IDLH	Immediate Danger to Live and Health
IMCO	International Maritime & Consultative Organization
kg/s	kilograms per second
km	kilometer
LCF	Latent Cancer Fatality
LC <sub>10</sub>	Lowest observed lethal concentration by inhalation
LC <sub>50</sub>	Lethal Concentration by Inhalation to 50% of exposed population
LD <sub>10</sub>	Lowest observed lethal concentration by ingestion
LD <sub>50</sub>	Lethal Dose by Ingestion to 50% of exposed population
LEL	Lowest Effect Level
LOAEL	Lowest Observed Adverse Effect Level
LSE	Level of Significant Exposure
m	meter(s)
min	minute(s)
mph	miles per hour
NOAEL	No Observed Adverse Effect Level
NPRM	Notice of Proposed Rulemaking
NRC	U.S. Nuclear Regulatory Commission
NTSB	National Transportation Safety Board
OED	Occupational Effective Dose
PIH	Poison Inhalation Hazard

ppm	parts per million
RAM	Radioactive Materials
s	second(s)
STEL	Short Term Exposure Limit
TLV	Threshold Limit Value
UN	United Nations
US	United States of America

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## 1.0 INTRODUCTION

Approximately 1.5 billion tons of hazardous material are transported in the U.S. annually [OTA86]. This material reaches its destination safely because conformity with regulations ensure that this transportation occurs in a safe manner. Infrequently, there are transport accidents in which releases of hazardous material that potentially can cause health effects to the general population and do damage to the environment. These events, though infrequent, cause genuine public concerns. Hazardous material transport accidents may involve fatalities and injuries. During the nine-year period from 1971 and 1979, hazardous materials transportation accidents claimed 229 deaths (average of 25 per year) and caused more than 6,000 injuries (average of more than 667 per year) [SMI84]. During this period, the accident-related property damage alone was more than \$100 million dollars (average of more than \$11 million dollars per year; not including legal costs and settlements).

When such accidents occur, concerns regarding potential hazards are raised and passed on to the Congress or other government officials. Expressed concerns often are rooted in fear of harm coupled with a relatively low level of understanding about hazardous materials in general and the need for hazardous materials transportation. Technical experts and regulators from industry and government are not trusted by the public to provide complete information about the level of risk associated with hazardous materials transportation [OTA86].

A simple comparison of the risks associated with hazardous material transportation can be made by comparing the 229 deaths cited above in a nine-year period with the annual fatalities associated with automobile transportation. The 229 deaths would, on an annual basis, represent approximately 25 fatalities per year, as noted above. Each year in the U. S., there are approximately 50,000 fatalities due to automobile accidents. In this comparison, hazardous-material transportation fatalities represent about 0.05 percent of the fatalities associated with the annual automobile-accident fatalities. Since we are comparing the safety of two transportation components of modern society, both of which are considered to be necessary rather than optional in modern life, this is a compelling contrast. The automobile is no longer a luxury but is rather a necessary part of modern life. Similarly, the U. S. population is highly dependent on hazardous materials, gasoline being one obvious dependency.

Since hazardous-material transportation is a relatively low-risk operation, the United States Department of Transportation Research & Special Programs Administration (DOT-RSPA) sponsored this project to evaluate the protection provided by the current packagings used to transport materials that have been classified as Poison Inhalation Hazards (PIH) and possibly to recommend additional performance standards for PIH packagings.

## 2.0 BACKGROUND OF US HAZMAT REGULATIONS (OTA86, Chapter 4)

In 1866, the first Federal law was passed regulating the transportation of hazardous materials (hereinafter frequently referred to as hazmat). Rail shipments of explosives during and after the Civil War were addressed by uncodified statutes and other contractual obligations between shippers and carriers based on English common-law principles. The establishment of the Interstate Commerce Commission (ICC) in 1887 marked the real beginning of a Federal effort to impose a degree of regulatory uniformity on all modes of transportation. While the ICC requirements were first developed for rail transportation, they were eventually expanded to include other transport modes.

In 1908, Congress passed a law that would govern hazardous materials transportation for more than six decades. The Explosives and Combustibles Act (which was later called the Explosives and Other Dangerous Articles Act, or EODA) authorized ICC to issue regulations covering the packing, marking, loading, and handling of explosives and other dangerous substances in transit. The act provided criminal penalties for shippers or carriers who violated the regulations. EODA codified many of the informal arrangements that had developed between shippers and rail carriers.

Regulations adopted by the ICC in 1911 to implement EODA were based on rail safety standards developed by the Bureau of Explosives, a division of the Association of American Railroads (AAR). The Bureau of Explosives was founded in 1905 and developed standards for the handling of explosives and other dangerous materials transported by the railroads. Amendments to EODA in 1921 authorized the ICC to utilize groups with technical expertise such as the Bureau of Explosives in the conduct of the ICC hazardous materials safety program. ICC delegated extensive rulemaking and enforcement responsibility to the Bureau of Explosives.

Under EODA, all hazardous materials transportation activity was barred unless specifically authorized by the ICC. As a consequence, ICC regulations were developed on a case-by-case basis in response to specific industry initiatives. Each time a new hazardous material container was developed, a special permit for its use was issued by the ICC. This pattern has continued so that today's packaging authorizations are individual in character.

Over the next forty years, the roles of the ICC and the Bureau of Explosives continued to expand as different transport modes became available for large scale transport of dangerous goods. In 1929, the U.S. Coast Guard adopted ICC rules for maritime transport of hazmat. In the 1930's, the ICC was given authority over highway transport. In the 1940's, the Civil Aeronautics Board (CAB) along with safety officials from the Department of Commerce developed regulations for the air transport of hazmat. During this period, ICC continued to rely on the expertise of non-governmental organizations by authorizing the use of carrier and shipper associations in addition to the Bureau of Explosives. As a result, the Tank Car Committee of the AAR was given authority to approve applications submitted to the ICC for designs, materials, construction, conversions, or alterations of tank cars.

In 1966, the Department of Transportation (DOT) was formed. The authority to regulate hazardous materials transport was transferred from the ICC to the DOT. Within the DOT, separate modal administrations were retained for the sake of continuity; the Federal Highway and Railroad Administrations for land transport, the Federal Aviation Administration (FAA) for air transport, and the Coast Guard for water transport. Regulations for each mode were published in separate parts of the Code of Federal Regulations (CFR). The National Transportation Safety Board (NTSB) was established to investigate the cause of transportation accidents and to conduct special studies related to safety and accident prevention. A Hazardous Materials Regulations Board (HMRB) was created by the Secretary of Transportation.

The Hazardous Materials Transportation Act (HMTA) was passed in 1975 which broadened the authority of the DOT to improve its regulatory and enforcement activities. Within the DOT, the Research and Special Programs Administration (RSPA) has been designated as the lead DOT agency for hazardous materials regulation. Within RSPA, the Office of Hazardous Materials Transportation was formed and was delegated the authority for issuing all hazmat transportation regulations except those for bulk transport by water. These regulations remained with the Coast Guard. The various modal administrations continued to be responsible for the development of regulations applicable to each mode. Thus, the responsibility for modal regulations and inspection and enforcement is divided between MTB and the modal administrations.

Members of RSPA staff represent the U. S. to the international regulatory bodies. These international organizations act through the United Nations in some cases. For example, the International Atomic Energy Agency (IAEA) is an agency of the UN. Other groups include the UN Committee of Experts on the Transport of Dangerous Goods, the International Civil Aviation Organization (ICAO), International Air Transport Association (IATA), and the International Maritime and Consultative Organization (IMCO). The principal objectives of most of these organizations are (1) to promote the safe transport of dangerous goods and (2) to ensure some degree of consistency in the regulations of each of the organization member states.

### 3.0 COMPARISON OF SPECIFICATION PACKAGINGS AND PERFORMANCE STANDARDS FOR HAZMAT PACKAGINGS

In the transport of hazmat, there are two regimes which describe methodology used to obtain an approved packaging for transport. These regimes are (1) design specification and (2) performance specification. Design-specification packagings (also called specification or spec packagings), which are described in 49 CFR, are built according to a set of rules or specifications that describe package properties such as rated capacity, construction details of rolling hoops and heads (if applicable), closures, material composition, seam construction and details, chine reinforcement, parts and dimensions, disposition of defective containers, marking instructions, type-tests, and leakage tests.

Whether the package is a metal drum or a fabricated wooden box, the specifications outline the details of construction of the package. The type-tests may detail the provisions for drop tests or

hydrostatic pressure tests on the packaging. In addition, there is usually some provision for acceptable behavior of the package following the performance of the type-tests, i.e., no leakage, or some other statement. The main thrust of the details in a specification is usually the description of the materials and processes that are to be used to fabricate the "specification container." The test-performance details, while present in many cases, are not the prominent features of the specifications for the package. These spec packagings have their origin in the historic development of the hazmat regulations.

In contrast, performance specification packagings meet performance tests usually described in some detail, to which a package must be subjected in order to provide some certainty that the package can be transported and will survive normal and some abnormal conditions. Performance standards usually do not state or require any specific features of construction or fabrication. Such details of construction are left to the development engineer but the finished package design must be able to pass the performance standards. Impact (drop), puncture, and fire (thermal) typify performance tests that could be specified for hazmat packagings.

Most hazmat transportation packages were placed into service through the specification packaging process under 49 CFR prior to 1995. An exception to the specification process is represented by the packages used to transport radioactive materials. Radioactive-material packagings have a development history which dates to 1946. These packagings have always been subjected to performance standards for certification. The regulations for radioactive-material packagings found in 49 CFR are derived from the IAEA regulations. References are made in 49 CFR to the regulations of the U. S. Nuclear Regulatory Commission (NRC), 10 CFR 71, for accident-resistant Type B packagings for transporting radioactive materials.

Most regulatory requirements, such as these, which govern the transport of hazmat, are under continuous scrutiny. In 1969, a few years after the formation of the DOT, the National Research Council of the National Academy of Sciences was requested to assemble a review panel of experts to study the transportation of hazardous materials. A workshop was convened in which panels of experts were invited to discuss the subject. These panels studied the transportation environment, hazard classification, hazardous material containment, hazardous cargo identification, and the reporting of statistical information related to hazmat transportation [NAS69].

One of the conclusions of the National Academy review [NAS69] was that, while hazardous material transportation control is a complex process, it was possible to develop a unified standards-based system. Such a system would include containment performance standards for hazardous material packaging systems.

Recommendations of a similar nature were published in 1984 [UN86] by the UN Committee of Experts On The Transport of Dangerous Goods. The committee felt that there was a trend toward replacement of detailed specifications of packagings, which may vary from one country to another, by performance-oriented packagings.

On May 5, 1987, the DOT issued a notice of proposed rulemaking (NPRM), that addressed the inclusion of performance-oriented packagings in 49 CFR. On November 6, 1987, corrections to the NPRM were published in the Federal Register. The NPRM proposed the inclusion of the performance standards which were recommended by the UN committee of experts [UN86]. The performance standards in UN86 were designated for hazmat packages not exceeding 400 kg mass (880 lb.) and a volume capacity of 450 liters (119 gal). The Final Rule was published on December 21, 1990. The performance standards, with the restrictions mentioned, are intended for non-bulk packagings. An additional restriction excludes radioactive-material packages and cylinders and other vessels for gas from the performance standard provisions. As mentioned above, most radioactive-materials packagings already were designed to performance-oriented standards.

The performance standards in the Final Rule involve a series of tests for each of three different packing groups. Packaging Group I represents the most hazardous materials; Group II represents materials less hazardous than those in Group I, and Group III represents materials less hazardous than those in Group II. The performance tests involve a drop test, a leak test, a hydrostatic-pressure test, a stacking test, and a cooperage test for wooden barrels. Currently, materials that are transported as compressed gases are not covered in the Final Rule.

One of the fundamental issues of this study is an assessment of the merit of incorporating the concept of performance standards into the regulatory framework for hazardous-material packagings larger than 2000 gallons.

#### 4.0 RELEASE SCENARIOS

The commercial transportation of hazardous materials occurs routinely in the U.S., mainly through truck and rail modes. Thus, hazmat transportation is wide-spread and occurs in normal commercial transportation. Both surface transport-modes (truck and rail) offer two regimes to the hazmat package. First, and primarily, is the normal transport mode which includes exposure to handling, vibration, temperature variations, stacking loads, drops, and lateral or longitudinal compression of the package due to acceleration and deceleration of the transport vehicle. All of the environmental loadings placed upon packagings containing hazardous materials in this regime are those that can occur routinely during the course of normal (accident-free) transportation. The second regime is one in which the vehicle is involved in a transportation accident. A transportation accident may range from minor (of low severity) to one in which the hazmat packaging is severely damaged. In severe accidents, a major concern is the condition of the containment boundary of the package. Does the package survive the accident with its containment intact or does the boundary fail and release the hazardous material to the environment? The primary issue addressed in this report is what levels of performance are required in order to provide adequate protection for the public.

#### 4.1 Performance Standards - Normal Conditions of Transport

The normal conditions of transport can be evaluated by performing a systems analysis of the conditions that are likely to be imposed on a hazmat package during normal transportation. For example, a package might be dropped some distance during rough handling. Small packagings can be accidentally dropped off a truck bed or fall from a rail car. Bulk packagings are usually handled by crane for fork lift and drop heights may be on the order of 4 to 6 feet or more.

Temperature variations occur during transportation. Seasonal variations can be significant. Even daily variations can be significant if one considers long hauls by truck or rail. Nighttime temperatures may be significantly below daytime temperatures. Enclosed and confined spaces in truck trailer spaces or in rail cars may produce an insulating effect in the winter or elevate temperatures above ambient in summer. These temperatures may cause changes in the internal pressure of a package with hazardous contents. Judgments or calculations can be used to specify the magnitude of an internal pressure test to simulate such conditions normally incident to commercial transportation. Internal pressures within the containment boundary can simulate these types of pressure loadings.

During transportation, lateral and longitudinal loadings occur because of the acceleration/deceleration of transport vehicles. Such loadings can be simulated by applying hydrostatic pressure to a package. Such a pressure test demonstrates the integrity of the package in all directions to specified levels of pressure.

Small packages may be stacked upon each other in transit or in warehouse storage. Stacking places a crush load on the lower packages. This loading can be simulated by a specified lateral loading or in a hydrostatic pressure test. Crush loads from stacking are only likely for small packages; large hazmat packages would not normally experience such loads. It should also be noted that the lateral crush resistance of a package to loads caused by either acceleration/deceleration or stacking, is an intrinsic property of the package design.

#### 4.2 Performance Standards - Accident Conditions of Transport

To develop performance standards in the accident regime, an estimate of the severity range of transportation accidents is needed. Severities can be presented as cumulative distributions of the parameters that describe accident severity. One estimate has been performed specifically for large packages [DEN77]. In this work, severity estimates were produced for the impact velocity of large packages and the durations of fires (assumed 1000 C) that might occur in transportation accidents. A fire temperature of 1000 C was determined to be the most probable fire temperature based on typical hydrocarbon fuels [CLA76]. Figures 1 through 5 present cumulative distributions for impact velocity and fire duration for truck and rail accidents involving large packages such as bulk hazardous-material packagings. Investigating accident severity means determining measures of parameters such as accident impact velocities (since truck and rail accidents involve collisions, rollovers, etc.) where deceleration from the pre-accident velocity occurs. Fire may or may not



occur as a consequence of an accident and is always treated as an independent event that may accompany accident-related mechanical forces.

For protection against impact and fire, the regulations for radioactive material Type-B packagings require that the packaging be able to withstand a 30 mph (44 ft/s) impact onto an unyielding surface and a subsequent 30 minute all-engulfing fire. The Type-B packaging must withstand these events, in addition to other specified events for protection against additional insults (for example, puncture and crush), without losing radioactive shielding or leaking more than an A2 amount per week [see 10CFR71 for further details]. These regulations may provide guidance for possible regulations that could be developed for hazardous materials. Notice in Figure 1 that a 30-mph instantaneous velocity change is more severe than at least 97 percent of all truck collisions. Figures 2 and 3 show that a 30-mph velocity change is more severe than about 99.5 percent of train derailment and collision accidents. Figure 4 shows that a 30-minute fire is more severe than approximately 96 percent of all truck accidents, and Figure 5 shows that a 30-minute fire is more severe than at least half of all train accidents.

Notice from Figures 1 through 5 that different accident-resistance requirements for velocity change and fire duration would provide protection against varying percentages of accidents. A common characteristic of Figures 1 through 5 is that they have relatively steep slopes at the lower values of the abscissa and are basically asymptotic at larger values of the abscissa. This means that significant changes in protection levels can be achieved by increasing the performance standard for either impact velocity or fire duration, when the abscissa is below the level where the curve becomes asymptotic. Once past this point, further increases in protection levels cannot be readily achieved due to the small positive slope of the curve. For example, in Figure 1, a 10-mph instantaneous velocity change during a truck collision involving a 10-gross-ton truck is more severe than about 76 percent of truck accidents for that size truck, whereas a 20-mph instantaneous velocity change for the same size truck is more severe than about 92 percent of all accidents for that size truck. Thus, raising the velocity-change requirement from 10 mph to 20 mph would raise the protection level significantly from 76 to 92 percent and decrease the likely failure percentage from 24% to 8%. In contrast, from Figure 1, a 40-mph velocity change is more severe than about 98 percent of all 10-gross-ton truck collisions. In this case, raising the velocity change requirement from 30 mph to 40 mph would only increase the protection level by about 1 percent. Information like that presented in Figures 1 through 5 are useful in determining when increases in performance requirement actually result in sufficiently increased accident resistance to merit the increased difficulty and/or cost in designing the packaging. The final selection of performance standards must be achieved by consensus of a standard-setting regulatory body. Arbitrary increases in performance standards may cause significant impacts on development costs with only a small increase in actual protection level.

In application of packaging performance standards, the impact-velocity criterion can be demonstrated by a drop from an equivalent drop height. In satisfying this "drop test", the packaging must be able to withstand a drop from a specified height, with an initial velocity of zero, onto an essentially unyielding surface without leaking more than a specified amount. This drop test

is intended to simulate the impact velocity associated with an accident more severe than over 98% of all accidents. Impact velocity can be converted to an equivalent drop-height by ensuring that all of the potential energy the packaging has while suspended at the drop height is converted to kinetic energy at the point of impact, which is achieved by dropping packagings onto unyielding surfaces (all energy is absorbed by the packaging rather than being distributed between the packaging and the surface). Therefore, impact velocity is related to equivalent drop height by  $V^2 = 2gh$  where "g" is the acceleration due to gravity. The equivalent drop-height corresponding to several impact velocities are tabulated in Table 1. From Figures 1 through 3, the cumulative probability of an accident occurring with a severity less than or equal to a drop from that equivalent drop-height are also tabulated in Table 1.

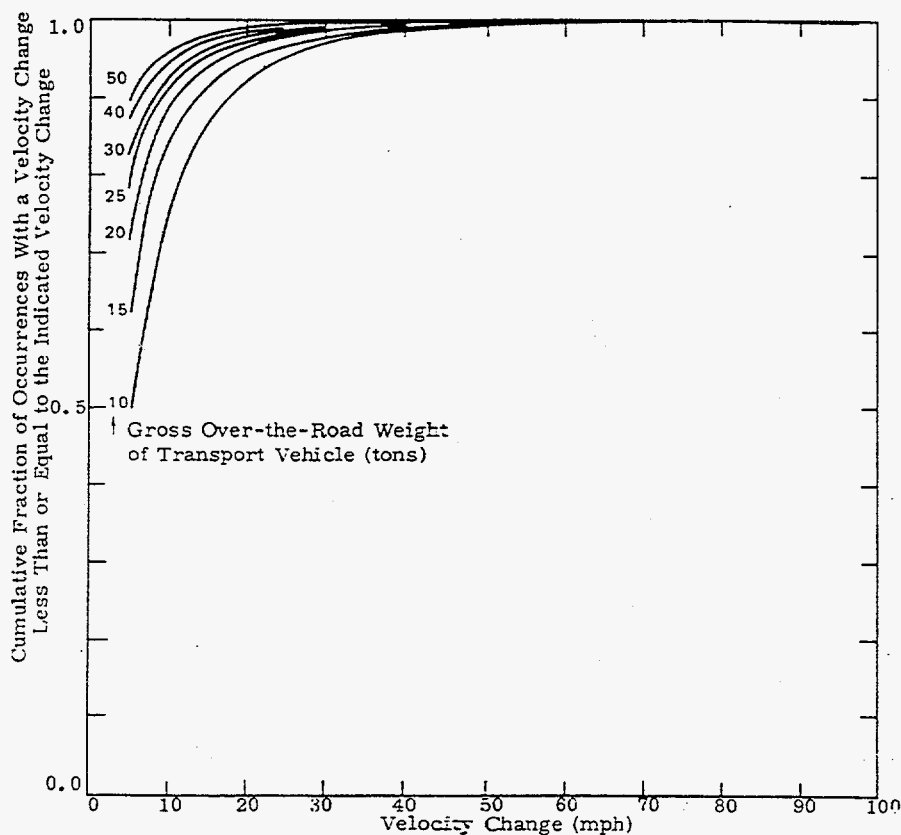


Figure 1. Cumulative Probability of a Highway Transportation Collision Occurring with Velocity Change (Due to Impact) Less than or Equal to the Indicated Amount [DEN77]

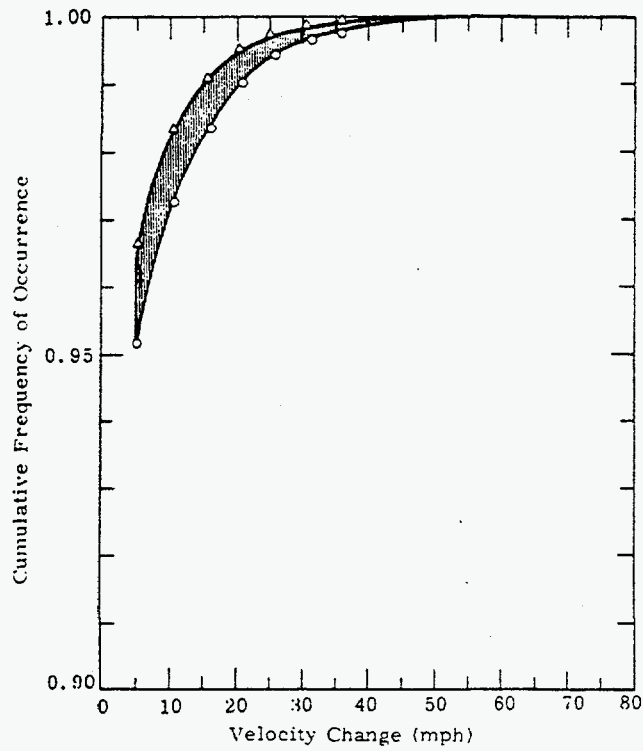


Figure 2. Cumulative Probability of a Train Derailment Accident Occurring with Velocity Change (Due to Impact) Less than or Equal to the Indicated Amount [DEN77]

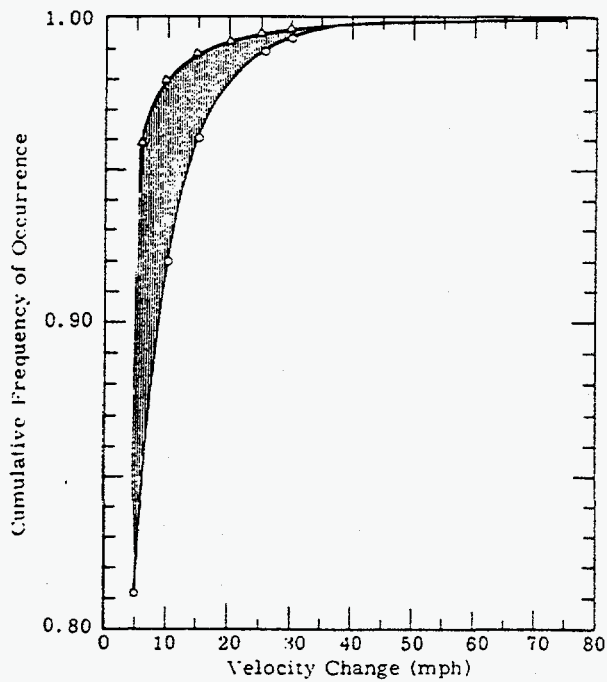
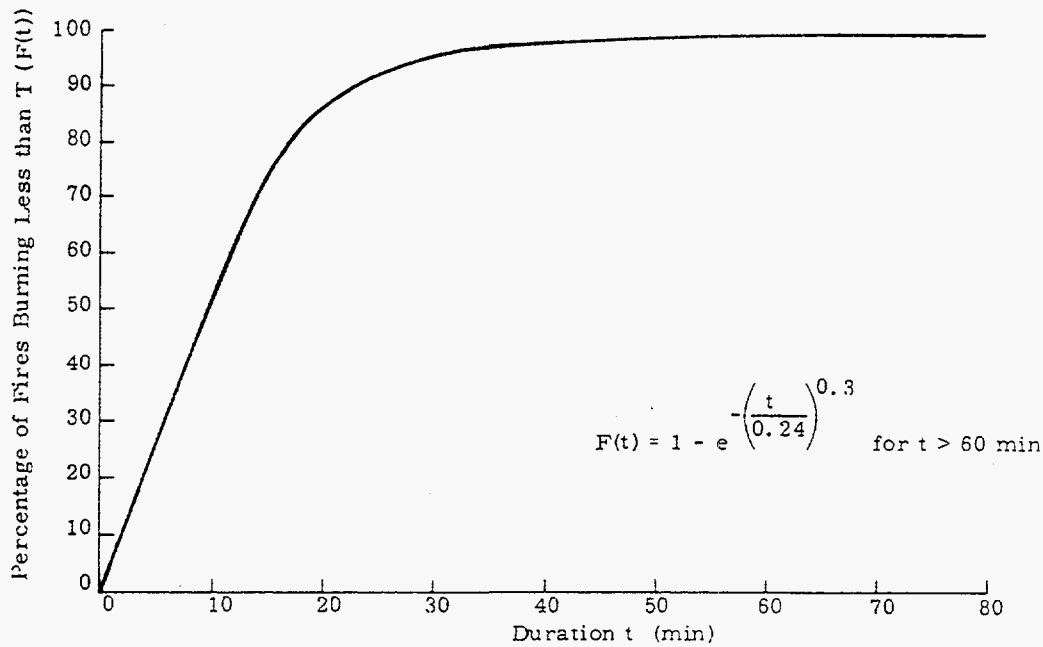
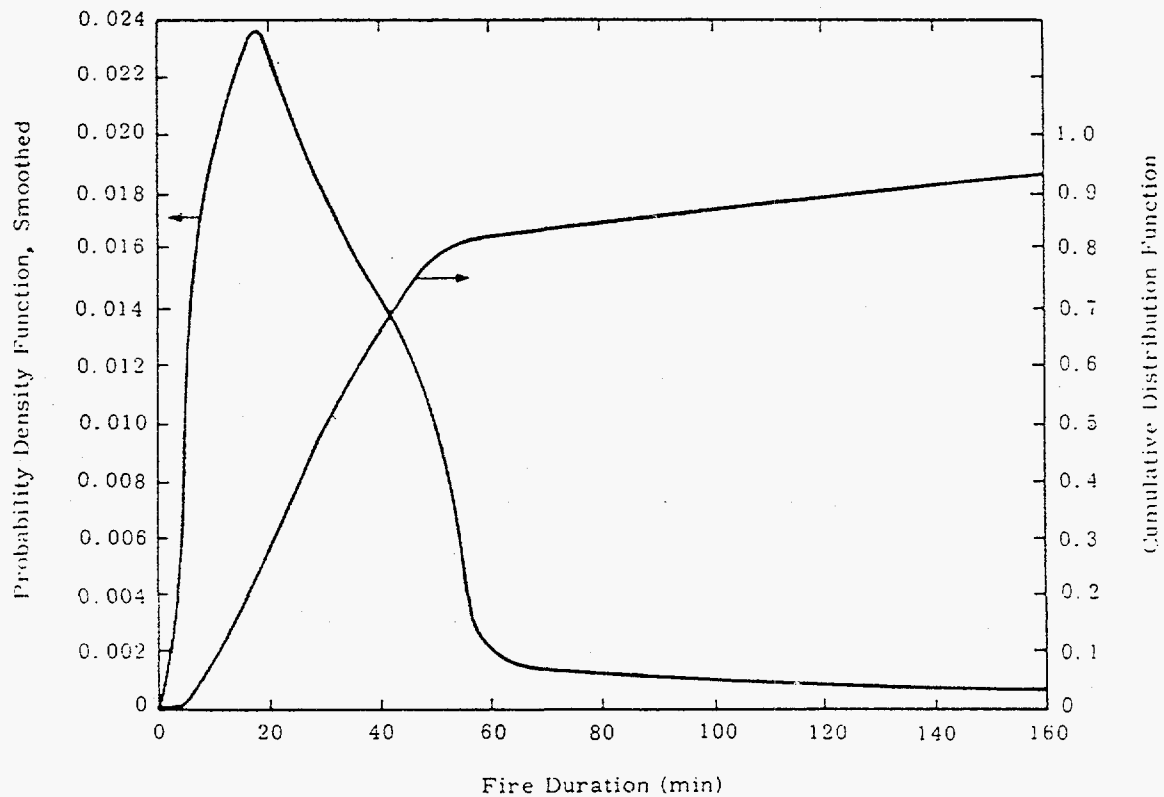


Figure 3. Cumulative Probability of a Train Collision Accident Occurring with Velocity Change (Due to Impact) Less than or Equal to the Indicated Amount [DEN77]



**Figure 4. Cumulative Probability of a Truck Collision Accident Occurring with a Resulting Fire of Duration Less than or Equal to the Indicated Amount [DEN77]**



**Figure 5. Cumulative Probability of a Train Collision Accident Occurring with a Resulting Fire of Duration Less than or Equal to the Indicated Amount [DEN77]**

Table 1. Impact Velocity and Equivalent Drop-Height versus Cumulative Probability of Occurrence (as determined from data in [DEN77], see Figures 1 through 3)

Impact Velocity (mph)/(kph)	Equivalent Drop Height (ft)/(meters)	Cumulative Probability of Occurrence (%)				
		Highway Collision Gross Over-the-Road Weight of Vehicle (tons)			Train Derailment	Train Collision
		15	25	50		
5.5/8.8	1.0/0.3	63	78	90	95.2-96.7	81.0-96.0
8.8/14.2	2.6/0.8	79	88	94	96.8-98.0	90.0-97.5
10.8/17.4	3.9/1.2	86	92	96	97.5-98.5	92.0-98.0
13.4/21.6	6.0/1.8	90	94	97	98.0-98.8	95.0-98.5
15/24	7.5/2.3	92	95	98	98.3-99.1	96.0-98.9
20/32	13/4.0	95	97	99	99.0-99.5	98.0-99.2
30/48	30/9.1	98	99	100	99.6-99.8	99.2-99.6

Several additional comments should be made about the accident-severity data displayed in Figures 1 through 5. First, these figures do not include the effects of impact target hardness, which is an extremely important consideration. For example, in the "Modal Study" [NRC87] it was determined that a spent nuclear fuel cask may experience 0.2% strain in end-on collisions at 38, 84 and 38 mph with rock, tillable soil and water, respectively. Secondly, the fire durations given do not include information about whether a packaging was in a fully engulfing fire. Some long-duration fires tend to migrate and may not fully engulf a hazmat packaging for the full duration of the fire or may not even involve the packaging at all. The latter consideration applies most particularly to rail-mode transportation, in which only one or a few railcars may experience a fire environment during an accident leaving other cars untouched.

Regulatory test procedures for packaging certification tend to be severe for several reasons. First, impact testing is performed on an unyielding target because it maximizes the damage to a candidate packaging design for a given drop-height and simplifies calculations. The specification of an unyielding target also imposes a target condition that is highly repeatable. In the case of fire (thermal) testing, the fully-engulfed condition is imposed to maximize thermal loading. Finally, the imposed sequence is impact followed by fire, which is the logical sequence that comes closest to replicating actual transportation accidents.

The forensic analysis of real transport accidents provides estimates of accident severities, although such information is never as complete as desired. An important caution is that performance standards are not "definitions" of transportation-accident severity. Performance standards are set such that compliance with them will protect against a suitably large percentage of accidents without making the packaging prohibitively expensive to build. No packaging can be expected to protect against 100 percent of all conceivable accidents. Therefore, a sensitive decision must be made as to how much protection is enough.

The discussion of accident scenarios provided in this section is derived from experience with radioactive material packagings and their performance standards. The level of performance standards for hazmat bulk packagings can be suggested in studies such as those described in this report, but in the final analysis, such studies are used as input to regulatory panels convened by the Department of Transportation. Such panels consider the various performance standards that might be invoked and any public comments received in response to notices of proposed rulemakings.

## 5.0 MEASURES OF HARM

There are a number of pathways via which exposure to hazardous materials might occur and cause environmental and/or health effects. These pathways include: toxic effects from inhalation and skin contact, etc.; irritability from skin and lung contact, etc.; thermal effects (burns); mechanical damage from explosions; and carcinogenicity, mutagenicity, teratogenicity, and tumorigenicity.

The environmental and physiological effects on humans of exposure to radioactive materials, which are a subset of hazardous materials, have been studied extensively. The harm from radioactive materials stems primarily from their carcinogenic/mutagenic characteristics. As a result of extensive study of the effects of exposure to radioactive materials, dose-response relationships for radiation exposure are well understood, with the possible exception of the threshold for minimum dose response. In contrast, for non-radioactive hazardous materials, the spectrum of potential exposure pathways is broader than for RAM and the mechanisms by which harm is produced are more numerous. For many materials, the dose-response curves are poorly known. As a result, the capability for predicting the effects of exposure to non-radioactive hazardous materials is not nearly as well developed as it is for radioactive materials.

The measures-of-harm used to characterize exposure to radioactive material are highly standardized. These measures are listed below. The first two apply *only* to persons who are exposed to very high levels of radiation.

- early fatalities, which represents individuals who die early (e.g., in less than one year) following exposure (involves comparison of exposure to a dose that is lethal to 50% of an exposed population (LD50));

- early morbidities, which represents individuals who become ill promptly (within perhaps 2 weeks) after exposure;
- latent cancer fatalities (LCFs), which represents individuals who are expected to develop cancer within 30 or more years after exposure; and
- genetic effects, which represents genetic abnormalities in succeeding generations, resulting from exposure of a progenitor.

Effects of exposure to non-radioactive hazardous materials can often be more difficult to characterize than that for radioactive materials. One difficulty is that, for many hazardous materials, human exposure data necessary to quantify measures of harm are limited and sometimes non-existent. There are a variety of methods for extrapolating from animal-exposure data to assess the results of human exposure, but there is considerable uncertainty as to how well these extrapolations actually represent the human effects. Another difficulty in quantifying harm from exposure to hazardous materials is that there may be multiple exposure pathways that result in distinct potential population effects. For example, a material that is explosive either on contact with air or on contact with other chemicals, may kill or injure persons should it explode. The damage that might occur as a result of such an explosion is not different from the damage that might occur following an explosion of any other explosive materials. The original material also may be toxic or corrosive, which presents an additional, material-specific exposure pathway. However, this report is concerned with materials that primarily produce harm as a result of inhalation.

Measures of harm that have been used to characterize population and individual exposures to hazardous materials have included [In82]: immediate fatalities, loss of income earning potential, loss of productivity (person-days lost, occupational or public), decrease in lifespan, increased cancer risk, increase in disease potential, injuries, disabilities (occupational or public), and dollar cost of human life. These measures of harm are often subdivided further into the categories of voluntary (occupational) and involuntary (public) risk acceptance. In both cases, it is desirable to have lower-bound human-exposure levels that correspond to a specified loss of income-earning potential, decreased lifespan, etc.

Measures that have been used to establish a lower-bound level for the onset of adverse physiological effects from inhalation of non-radioactive hazardous materials include:

- ERPG-1, Emergency Response Planning Guideline 1, which is the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing other than mild discomfort or objectionable odor;
- ERPG-2, Emergency Response Planning Guideline 2 (used by the DOT in preparation of the evacuation tables for the Emergency Response Guidebook) which is the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other

serious health effects or symptoms that could impair their abilities to take protective action;

- ERPG-3, Emergency Response Planning Guideline 3, which is the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects;
- FEL, Franks Effect Level;
- IDLH, ImmEDIATE Danger to Life and Health (a time-weighted concentration relating to inhalation of materials);
- LC50, Lethal Concentration by inhalation for fatality of 50% of an exposed test group (usually associated with an exposure duration);
- LClo, lowest observed lethal concentration, by inhalation, for an individual;
- LEL, Lowest Effect Level at which any effects are noted;
- LOAEL, Lowest Observed Adverse Effect Level;
- LSE, Level of Significant Exposure;
- NOAEL, No Observed Adverse Effect Level;
- OED, Occupational Effective Dose;
- STEL, Short Term Exposure Limit (a level of exposure permitted for brief periods of time, perhaps to permit life-saving activities, etc.); and
- TLV, Threshold Limit Value for occupational exposure (customarily a time-weighted average value for 40 hours of exposure), that was developed by the Occupational Safety and Health Administration.

For any given hazardous material, data are not available for all of these metrics. Thus, regardless of the measure of harm that is chosen for evaluating potential exposures to hazardous materials, provisions must be made to allow for interim use of whichever measures of harm are actually available for the given material. When different measures of harm are used for different materials, a scaling factor can be used to provide consistency among analyses. In addition to the measures of harm listed above, collateral effects from explosive blasts, thermal pulses, etc. must also be factored into an evaluation of the adverse physiological effects from exposure to hazardous materials, but for simplicity they are not considered here.



If measures of harm used for evaluating the adverse effects of exposure to radioactive materials are to be extended to non-radioactive hazardous materials, then definitions need to be established to relate the two. For example, the measure of harm for hazardous material that is equivalent to the radioactive "early fatality" measure of harm could be defined as the fatalities resulting from exposure to doses or concentrations of airborne hazardous material (LC50, for example) plus fatalities resulting from explosions and other "non-toxic" exposures where the latter are inevitable or likely features of any dispersion of the material. This allows an "early fatality" measure of harm to be used that is approximately equivalent for both hazardous materials and radioactive materials.

An additional difficulty in evaluating the consequences of exposure to hazardous material stems from the overlapping effects of hazardous materials. For example, someone exposed to a toxic cloud may also be injured by an explosion or fire. This can result in multiple counting of individuals impacted by a hazardous material release event. It is necessary to rank the potential impacts from hazardous material release events to avoid this. There are several methods for accomplishing this. Because adverse effects from explosions and fires typically occur more quickly than those from exposure to toxic clouds, etc., potential fatalities and incapacitations from explosions and fires should be considered before impacts of exposure to airborne toxic material, etc. That is, estimates of prompt fatalities from explosions ideally should be subtracted from overall estimates of health effects from inhalation of airborne material. This avoids multiple counting for consequence and risk calculations. However, this report only addresses the hazards associated with the exposure to the airborne concentrations of the released PIH. The hazards associated with explosion, fire, etc., have not been analyzed in this report.

The selection of exposure guidelines for assessing consequences resulting from releases of the PIH materials is based on the DOT report "Support Documentation for the Development of Initial Isolation and Protective Action Distances Table in the DOT Publication *1990 Emergency Response Guidebook*" [MAL90]. As described in this report, the ERPG-2 (the maximum airborne concentration below which nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action) is considered the most appropriate. As is also described in this report, the DOT sought advice from expert toxicologists concerning exposure guidelines that could be used when ERPG-2 values were not available. The recommendations from this committee of toxicological experts are that toxicological guidelines be chosen in the following order:

- 1) ERPG-2
- 2) SPEGL
- 3) STEL
- 4) Ceiling TLV
- 5) EEGL
- 6) TLV/TWA
- 7) Estimates of short-term limits based on LC<sub>50</sub>s and LCLOs.

The methods for adjusting the toxicological parameters to exposure times different from those reported for the parameter are based on the DOT report [MAL90]. They are:

1. When the predicted exposure time is on the order of the time period of the guideline, then the guideline limit is to be treated as an "average concentration" over the time of exposure rather than a peak concentration never to be exceeded. The exception is the ceiling TLVs, which are maximum not-to-be-exceeded values.
2. When the predicted exposure time is less than 1/4 the time period of the guideline (e.g., 15 minutes for a 1-hour guideline), then the time-weighted concentration allowed for the short exposure time is equal to  $2 \cdot C_o \cdot t$ , where " $C_o$ " is the guideline exposure concentration and " $t$ " is the time of exposure.
3. When the predicted exposure is greater than the time period of the guideline (e.g., 25 minutes for a 15-minute guideline), then the predicted dosage (i.e., integrated concentration over 25 minutes) cannot exceed the integrated exposure-guideline concentration over the guideline time-period.
4. For TLV/TWAs, an exposure of 30 minutes or less is allowed an average concentration of 3 times the associated TLV/TWA values.

## 6.0 DISPERSION CALCULATIONS FOR PIH GASES

Dispersion calculations were performed for PIH substances to support the selection of performance standards for the containers used to transport them. The calculations reveal the relationship between leak rates for these various compounds and the distances downwind from the leak beyond which the ground-level concentrations of the hazardous substance are at or below the exposure guideline for a period of half an hour.

### 6.1 Dispersion Modeling

Dispersion modeling was performed to quantify the relationship between leak rates for PIH materials and the distance downwind from the release-site within which the 30-minute average ground-level concentration of the PIH is at or above the chosen exposure guideline. These results support classifying the various PIHs into groups of comparable relative-severity so that each severity-group may have a different performance oriented packaging standard.

Exposure guideline data are available for 72 of the 169 PIH compounds listed in Table A-1. The physical form that each of these materials would take in the event of a leak was identified as either an ideal gas, dense gas, liquid, or fine powder. Ideal gases were modeled using a Gaussian dispersion model with a continuous leak rate; dense gases were modeled as a horizontal release using the dense-gas dispersion code SLAB [ERM88]. Liquids and powders were not modeled since

their dispersal into accident surroundings is much more complicated, i.e., beyond the scope of this study.

The release classification and exposure guideline data for the PIH compounds that have packaging performance specifications (i.e., Packaging Groups I, II, or III) for non-bulk packagings (defined as less than 118 gallons) per 49 CFR are listed in Table 2. The same information is listed in Table 3 for the PIH compounds that are not in Packaging Groups I, II, or III in 49 CFR. For example, materials that are typically transported as compressed gases do not have Packaging Groups assigned to them in 49 CFR. Also listed in Tables 2 and 3 are the hazard classes and the Packaging Group specified for each material per 49 CFR. When more than one hazard class is listed for a material, the first one listed is the primary hazard class, the second one listed is the secondary hazard class, etc.

Some PIH compounds react with a chemical typically available in the environment and then disperse as a different chemical. For example, Fluorine and Carbonyl Fluorine react with water vapor in the air and actually disperse as hydrogen fluoride (HF). For these compounds, the actual chemical expected to disperse in the event of a release is noted in brackets "[]" after the name of the compound in Tables 2 and 3. For compounds that are expected to react in this manner, the dispersion modeling was performed and the toxicity data was selected for the actual material expected to be dispersing (i.e., the reaction product).

For each PIH, ground-level concentrations corresponding to applicable exposure guidelines (specific to each PIH) were calculated. For the ideal gases, the leak-rate (release rate) resulting in a ground level concentration corresponding to the exposure guideline for each PIH at a range of downwind distances was calculated with a Gaussian dispersion equation. This type of calculation was not possible with the SLAB model, so the SLAB model was run for a range of leak rates, and the leak rate was plotted versus the distance at which the ground-level concentration was equal to the exposure guideline.

The parameters used with each dispersion model are given in Tables 4 and 5. To produce conservative results (i.e., the lowest leak rate that produces ground-level concentrations that exceed guidelines at a given distance) with the Gaussian dispersion model, F atmospheric stability with an appropriate wind speed was selected. The parameters used with the Gaussian dispersion model are shown in Table 4.

The SLAB model was most reliable with a wind speed of 4.6 m/s, so the appropriate conservative atmospheric stability class corresponding to this wind speed (Class 3 or C) was selected. The parameters used with the SLAB model are shown in Table 5. Because Hydrogen Sulfide has a vapor density that is only 1.2 times the vapor density of air, Hydrogen Sulfide could behave as either an ideal gas or as a dense gas in the event of a release. Therefore, it was modeled both as an ideal gas and as a dense gas, and the results of both calculations are shown in Table 3.

Table 2. PIH Compounds with Available Exposure Guideline Data that have Packaging Performance Standards (per 49 CFR) for Packages Smaller than 118 gallons

Compound	Hazard Class	1km safe release rate (g/s)	Packaging Group	Type of Exposure Limit	Exposure Limit (ppm by volume)	Nature of Release L=Liquid D=Dense Gas I=Ideal Gas	Mol. Wt.
Hydrazine	Flammable Liquid, Poison, Corrosive	0.15	I	TWA/TLV	.13mg/m <sup>3</sup>	I	32.05
Bromine pentafluoride [Br(F)3]	Oxidizer, Poison, Corrosive	0.80	I	TWA/TLV	.72mg/m <sup>3</sup>	I	174.91
Nickel carbonyl	Poison, Flammable Liquid	50	I	TWA/TLV	.12mg/m <sup>3</sup>	D	170.70
Hydrogen Fluoride	Corrosive, Poison	54	I	ERPG2	20ppm	I	20.01
Nitric acid, nitrating acid	Corrosive, Oxidizer, Poison	89	I	STEL	10mg/m <sup>3</sup>	I	63.02
Ethylene oxide/propylene	Flammable Liquid, Poison	300	I	EEGL	50ppm	I	44.06
Acrylonitrile	Flammable Liquid, Poison	820	I	TLV/TWA	4.3mg/m <sup>3</sup>	D	53.07
Cyanogen bromide	Poison, Corrosive	1500	I	TWA	0.5ppm	D	105.93
Sulfuric acid, fuming	Corrosive		I	EPRG2	10mg/m <sup>3</sup>	L	98.08
Allyl alcohol	Poison, Flammable Liquid		I	STEL	9.5mg/m <sup>3</sup>	L	58.09
Bromine	Corrosive, Poison		I	STEL	2mg/m <sup>3</sup>	L	159.82
Pentaborane	Spontaneously Combustible, Poison		I	STEL	.03mg/m <sup>3</sup>	D	63.14
Iron pentacarbonyl	Poison, Flammable Liquid		I	STEL	.45mg/m <sup>3</sup>	L	195.90
Bromine trifluoride	Oxidizer, Poison, Corrosive		I	TLV	1ppm	L	136.91
Ethyleneimine	Poison, Flammable Liquid		I	TLV/TWA	.88mg/m <sup>3</sup>	L	43.08
Methyl isocyanate	Poison, Flammable Liquid		I	TWA/TLV	.047mg/m <sup>3</sup>	L	57.06
Methylhydrazine	Poison, Flammable Liquid, Corrosive		I	TWA/TLV	.38mg/m <sup>3</sup>	L	46.09
Hexachlorocyclopentadiene	Poison		I	TWA/TLV	.11mg/m <sup>3</sup>	L	272.77
Sulfur chloride [HCl,(H)2S]	Corrosive		I	TWA/TLV	1ppm	L	135.03
Tetranitromethane	Oxidizer, Poison		I	TWA/TLV	8mg/m <sup>3</sup>	L	196.05

Compound	Hazard Class	1km safe release rate (g/s)	Packaging Group	Type of Exposure Limit	Exposure Limit (ppm by volume)	Nature of Release L=Liquid D=Dense Gas I=Ideal Gas	Mol. Wt.
Perchloromethyl mercaptan	Poison		I	TWA/TLV	.76mg/m <sup>3</sup>	L	185.87
Crotonaldehyde	Flammable Liquid, Poison	94	II	EPRG2	10 ppm	I	70.10
Chlorine dioxide	Oxidizer, Poison	200	II	STEL	.83mg/m <sup>3</sup>	D	67.45
Thiophosgene	Poison	300	II	ERPG2	.2ppm	D	114.97
2,2-Dichlorodiethyl ether	Poison, Flammable Liquid	3000	II	STEL	58mg/m <sup>3</sup>	D	143.02
Phosphorus trichloride [PO(Cl)3]	Corrosive, Poison		II	STEL	2.8mg/m <sup>3</sup>	L	137.32
Phosphorus oxychloride	Corrosive, Poison		II	STEL	3.1mg/m <sup>3</sup>	L	153.32
Ethylene dibromide	Poison		II	TWA	20 ppm	L	187.88
Ethylene chlorohydrin	Poison		II	TWA/TLV	1ppm	L	80.52
Phenyl mercaptan [PhS-SPh]	Poison, Flammable Liquid		II	TWA/TLV	2.3mg/m <sup>3</sup>	L	110.18
Phosphorus pentachloride	Corrosive		II	TWA/TLV	.85mg/m <sup>3</sup>	D	208.22

**Table 3. PIH Compounds with Available Exposure Guideline Data that do not have Packaging Performance Standards (per 49 CFR) for Packages Smaller than 118 gallons (ordered by 1 km safe Release Rate)**

Compound	Hazard Class	1km safe Release Rate (g/s)	Type of Exposure Limit	Exposure Limit (ppm by volume)	Release Type L=Liquid D=Dense Gas I=Ideal Gas	Mol. Wt.
Oxygen difluoride [HF]	Poison Gas, Oxider	0.13	TWA/TLV	.11mg/m <sup>3</sup>	I	54.00
Diborane	Poison Gas, Flammable Gas	0.13	TWA/TLV	.11mg/m <sup>3</sup>	I	27.68
Hydrogen Selenide	Poison Gas, Flammable Gas	0.18	TWA/TLV	.16mg/m <sup>3</sup>	I	80.98
Germane	Poison Gas, Flammable Gas	0.70	TWA/TLV	.63mg/m <sup>3</sup>	I	76.63
Cyanogen chloride	Poison Gas, Flammable Gas	0.83	TWA/TLV	.75mg/m <sup>3</sup>	I	61.47
Arsine	Poison Gas, Flammable Gas	12	EEGL	1.0ppm	I	77.95
Carbonyl sulfide	Poison Gas, Flammable Gas	12	TLV	10ppm	I	60.07
Hydrogen Bromide	Poison Gas, Corrosive	12	TWA	10mg/m <sup>3</sup>	I	80.92
Nitrogen fluoride oxide		12	TWA/TLV	10ppm	I	87.01
Phosphine	Poison Gas, Flammable Gas	15	STEL	1.4mg/m <sup>3</sup>	I	34.00
Chlorine trifluoride	Poison Gas, Oxidizer, Corrosive	15	EEGL	1ppm	I	92.45
Methyl bromide	Poison Gas	22	TWA/TLV	19mg/m <sup>3</sup>	I	94.95
Cyanogen	Poison Gas, Corrosive	24	TWA/TLV	21mg/m <sup>3</sup>	I	52.00
Fluorine [HF]	Poison Gas, Oxidizer	28	STEL	3.1mg/m <sup>3</sup>	I	38.00
Nitrogen trifluoride	Non-Flammable Gas, Oxidizer	33	TWA/TLV	29mg/m <sup>3</sup>	I	71.01
Nitric oxide	Poison Gas	34	TWA/TLV	31mg/m <sup>3</sup>	I	30.01
Sulfur dioxide	Poison Gas	44	EPRG2	3ppm	I	64.07
Selenium hexafluoride (as Selenium tetrafluoride)	Poison Gas	50	TWA/TLV	.16mg/m <sup>3</sup>	D	192.96
Nitrogen dioxide; dinitrogen tetroxide	Poison Gas, Oxidizer	83	STEL	9.4mg/m <sup>3</sup>	I	30.01
Hydrogen chloride	Poison Gas, Corrosive	99	ERPG2	20ppm	I	36.46
Sulfur tetrafluoride	Poison Gas	100	TWA/TLV	.44mg/m <sup>3</sup>	D	108.06
Carbonyl fluoride [HF]	Poison Gas	120	STEL	13mg/m <sup>3</sup>	I	66.01
Ethylene oxide	Poison Gas, Flammable Gas	130	EEGL	20ppm	I	44.06
Methylmercaptan	Poison Gas, Flammable Gas	170	EPRG2	25ppm	I	48.11

Compound	Hazard Class	1km safe Release Rate (g/s)	Type of Exposure Limit	Exposure Limit (ppm by volume)	Release Type L=Liquid D=Dense Gas I=Ideal Gas	Mol. Wt.
Hydrogen sulfide	Poison Gas, Flammable Gas	180	STEL	21mg/m <sup>3</sup>	I	34.08
		4000	STEL	21mg/m <sup>3</sup>	D	34.08
Bromine chloride [chlorine]	Poison Gas, Corrosive, Oxidizer	220	TLV	.1ppmBr	D	115.36
Perchloryl fluoride	Poison Gas, Oxidizer	220	STEL	25mg/m <sup>3</sup>	I	102.45
Phosgene	Poison Gas, Corrosive	300	ERPG2	.2ppm	D	98.91
Dichlorodifluoro methane	Non-Flammable Gas	320	EEGL	20ppm	I	120.91
Sulfuryl Fluoride	Poison Gas	370	STEL	40mg/m <sup>3</sup>	I	102.26
Ammonia; ammonium hydroxide	Poison Gas	450	ERPG2	200ppm	I	17.04
Silicon tetrafluoride	Poison Gas, Corrosive	500	TWA/TLV	2.5mg/m <sup>3</sup> fluorine	D	104.09
Chlorine [Hcl]	Poison Gas	1900	ERPG2	3ppm	D	70.90
Dichlorosilane	Poison Gas, Flammable Gas	4000	TLV	6.0mg/m <sup>3</sup> silane	D	101.01
Carbon monoxide	Poison Gas, Flammable Gas		STEL	458mg/m <sup>3</sup>	I	28.00
Carbon monoxide/hydrogen	Flammable Gas		STEL	458mg/m <sup>3</sup>	I	28.00
Phosphorus pentafluoride	Poison Gas		TWA	2.5mg/m <sup>3</sup>	I	125.95
Boron trichloride	Poison Gas, Corrosive		TWA	1ppm	L	117.16
Chlorine pentafluoride	Poison Gas, Oxidizer, Corrosive		TWA	2.5mg/m <sup>3</sup> -F	D	92.50
Hydrochloric acid	Poison Gas, Corrosive		TWA/TLV	20ppm		36.46

Table 4. Parameters used in the Gaussian dispersion model.

GAUSSIAN DISPERSION MODEL PARAMETER	PARAMETER VALUE
Atmospheric stability class	F
Wind speed	1 m/s
Ambient temperature	298°K
Atmospheric pressure	1.0 atmosphere
Allowable dosage calculated from exposure guideline	See Table 3.1 of [MAL90]

Table 5. Parameters used in the SLAB model.

PARAMETER IN THE SLAB MODEL	PARAMETER VALUE
Liquid fraction	0
Source temperature	boiling point
Source emission rate (leak rate)	0 to 10 kg/s
Source area	1 m <sup>2</sup>
Duration of leak	36,000 seconds
Instantaneous source mass	0
Source height above ground	2 meters
Averaging time	1800 seconds
Measurement heights	0, 1m., 1m., 1m.
Surface roughness	0.001
Wind speed measurement height	10 meters
Wind speed	4.6 m/s
Ambient temperature	298°K
Relative humidity	50%
Atmospheric stability class	3
Inverse Monin-Obukhov length	0
Source (leak) type	horizontal jet



To assess the relative severity of the PIHs, the maximum allowable leak rate for each PIH resulting in a ground-level concentration at 1 km from the leak equal to the exposure guideline for that PIH was calculated. This parameter is referred to as the 1-km safe release rate. The selection of 1 km is not intended to imply that the safety of people within 1 km is being neglected. This distance was used solely as a metric for comparing the relative-dispersibility of each PIH with respect to the other PIH materials. The calculated 1-km safe release rates for each compound are listed in Tables 2 and 3. Additional dispersion modeling results are in Appendix B.

## 6.2 Dispersion Modeling Results

For the 72 PIH analyzed in this report, the values for the 1-km safe release rate ranged from less than 1 g/s (Hydrazine, Bromine Pentafluoride, Oxygen difluoride, Diborane, Hydrogen Selenide, Germane, and Cyanogen Chloride) to greater than 1000 g/s (Cyanogen Bromide, 2,2-Dichlorodiethyl ether, and Dichlorosilane).

Figures 1-8 in Appendix B show the relationship between downwind distance and leak rate for compounds which behave like ideal gases when the exposure guideline is based on ERPG-2, EEGl or STEL. Figures 9-16 in Appendix B show the same relationship for ideal gases for which the exposure guideline is based on a TLV. Figures 17-20 in Appendix B show the relationship for compounds which behave like dense gases. Figures 21-24 in Appendix B are plots of concentration vs. downwind distance for the dense gases, and are shown to illustrate the application of the SLAB model. In all cases, compounds that yielded comparable scales were grouped together.

Figures 25-32 in Appendix B compare leak rates which result in the half-hour concentration equal to the EPA exposure guideline at three different distances: 50 meters, 1 km, and 8.33 km (5 miles). Three different sets of figures are given. Figures 25, 26 and 27 in Appendix B show the leak rates when the exposure guideline is based on a TLV, and the compounds are treated like ideal gases. Figures 28, 29 and 30 in Appendix B show the leak rates when the exposure guideline is based on the ERPG2, EEGl or STEL value, and the compounds are treated like ideal gases. Figures 31 and 32 in Appendix B show the leak rates when the ground-level concentration is equal to the exposure guideline at 1 km and 8 km, respectively, for gases treated like dense gases and modeled with SLAB.

For the ideal gases, a ground-level concentration equal to the exposure guideline at five miles (8.33 km) from the source yields a range of allowed leak rates from a low of 2.75 g/s for oxygen difluoride to a high of 10.7 kg/s for ammonia. Fewer dense gases were modeled, but even for these the range of allowed leak rates, when the ground-level concentration is equal to the exposure guideline at 8 km, is from 180 g/s for diborane to 6.7 kg/s for chlorine dioxide. These ranges are given to show the wide variation from compound to compound.

### 6.3 Classification of the PIH Materials into Bulk Hazard Zones

It is extremely impractical to have a separate performance standard, and consequently a separate packaging, for each PIH compound. Therefore, the PIH compounds have been grouped according to their relative severity and placed in Hazard Zones analogous in concept to those in 49 CFR.

The first step in classifying the PIH materials into Hazard Zones involved comparing the various PIH to determine "relative severity" with respect to each other. This was accomplished by calculating the effect of release rate and/or release amount on the distance from the release within which the concentration of the released material exceeds the threshold value for that material. From these calculations, then, the relative severity of the various PIH compounds was determined by comparing the release rates required to produce the threshold value at a given distance (i.e., the lower the maximum allowable leak rate, the more relatively severe the compound). This methodology takes into account not only the toxicity of the material but also the ease with which it disperses. This will be referred to as the TD method. The results of these comparisons indicate that the maximum allowable leak rates span five orders of magnitude for the various PIHs. In addition to using these TD-based criteria, 49CFR173 was used to provide information with respect to additional hazard classes (i.e., corrosive, explosive, flammable, etc.) as an additional, and perhaps more limiting, consideration to categorization of PIHs into Hazard Zones (49CFR173, 1991).

As a general criterion for defining the PIHs into Hazard Zones, the materials with maximum allowable leak rates (per the TD method) less than 10 g/s were placed in Hazard Zone BA, those with maximum allowable leak rates between 10 and 100 g/s in Hazard Zone BB, those with maximum allowable leak rates between 100 and 1000 g/s in Hazard Zone BC, and those with maximum allowable leak rates larger than 1000 g/s in Hazard Zone BD.

The consideration of 49CFR173 affects the PIH materials that are categorized in more stringent hazard zones for non-bulk shipments in 49CFR173 than those indicated by the TD criteria discussed above. For example, even though the maximum leak rates calculated by the TD method for the PIH listed in Packaging Group I (per 49CFR173) range from 0.15 g/s (Hazard Zone BA) to 1500 g/s (Hazard Zone BD), they were not placed in Hazard Zones BC or BD because that is less stringent than the 49CFR173 classification, which placed these materials in Packaging Group I (which is the most stringent group). Similarly, even though the maximum leak rates calculated for the Packaging Group II materials range from 12 g/s (Hazard Zone BB) to 3000 g/s (Hazard Zone BD), they were not placed in Hazard Zone BD.

For example, ethylene oxide/propylene (maximum leak rate of 300 g/s) and acrylonitrile (maximum leak rate of 820 g/s) are in Packaging Group I yet have higher maximum leak rates than crotonaldehyde (maximum leak rate of 94 g/s) and chlorine dioxide (maximum leak rate of 200 g/s) which are in Packaging Group II. Although ethylene oxide/propylene and acrylonitrile are less relatively severe, according to the TD-based criterion, than crotonaldehyde and chlorine dioxide, they are required to satisfy more stringent packaging performance standards because of the severity

of their primary hazard (in this case, flammability). For all four of these PIH compounds, toxicity is only the secondary hazard.

Chlorine was an exception to our method of giving priority to 49CFR173. Chlorine, which is normally transported as a compressed gas, was placed in Hazard Zone BD. This is actually less stringent than recommended for non-bulk transport in 49CFR173, which classifies chlorine in Hazard Zone B. The TD calculations are based on the assumption that released chlorine would quickly react with moisture in the air to become hydrogen chloride. The calculations for chlorine, therefore, are based on the toxicity and dispersibility of hydrogen chloride. However, the authors recognize the potential, though less likely, for incidents where the relative humidity is low and the chlorine does not disperse as hydrogen chloride. The hazard zone used in 49CFR173 appears to assume that chlorine is always released as  $\text{Cl}_2$ , rather than as hydrogen chloride.

An additional PIH worthy of specific mention is hydrogen sulfide. As previously noted, since hydrogen sulfide has a vapor density that is only 1.2 times the vapor density of air, hydrogen sulfide might behave as either an ideal gas or as a dense gas in the event of a release. Therefore, it was modeled both as an ideal gas and as a dense gas. The model which produced the lower maximum allowable leak rate (ideal gas model) was used.

Dispersion calculations were not performed for the PIH materials that are classified to behave as liquids in the event of a release. Those materials that are in Packaging Group I, were placed in Hazard Zone BB, and those that are in Packaging Group II, were placed in Hazard Zone BC. Again, this is intended to be consistent with the treatment of the other Packaging Group I and II materials. In general, since a released liquid must evaporate before dispersing as a gas, liquids are less likely than gases to disperse in high concentrations at a given distance from the release point.

The analysis performed according to the classification methodology described above resulted in a scheme which classifies PIHs into four severity groups. The categorization of the PIH materials into Hazard Zones BA, BB, BC, and BD, is shown in Table 6. Thus, Hazard Zones A, B, C, and D pertain to shipments smaller than 118 gallons, and Hazard Zones BA, BB, BC, and BD pertain to shipments larger than 2000 gallons. Hazard Zone BA represents the relatively more severe materials (as does Hazard Zone A for non-bulk transport), and Hazard Zone BD represents the least relatively-severe materials (as does Hazard Zone D for non-bulk transport).

**Table 6. Hazard Zones for PIH Transport in Packages Larger than 2000 Gallons**

Name of Compound	Hazard Zone	Name of Compound	Hazard Zone
Acrylonitrile	BB	Hydrogen Fluoride	BB
Allyl Alcohol	BB	Hydrogen Selenide	BA
Ammonia; ammonium hydroxide	BC	Hydrogen Sulfide	BC
Arsine	BB	Iron Pentacarbonyl	BB
Bromine	BB	Methyl Bromide	BB
Bromine Chloride	BC	Methyl Isocyanate	BB
Bromine Pentafluoride	BA	Methyl Mercaptan	BC
Bromine Trifluoride	BB	Methylhydrazine	BB
Carbon Monoxide		Nickel Carbonyl	BB
Carbon Monoxide/Hydrogen		Nitric Acid, Nitrating Acid	BB
Carbonyl Fluoride	BC	Nitric Oxide	BB
Carbonyl Sulfide	BB	Nitrogen Dioxide	BB
Chlorine	BD	Nitrogen Fluoride Oxide	BB
Chlorine Dioxide	BC	Nitrogen Trifluoride	BB
Chlorine Trifluoride	BB	Oxygen Difluoride	BA
Crotonaldehyde	BC	Pentaborane	
Cyanogen	BB	Perchloromethyl Mercaptan	BB
Cyanogen Bromide	BB	Perchloryl Fluoride	BC
Cyanogen Chloride	BA	Phenyl Mercaptan	BC
Diborane	BA	Phosgene	BC
2,2-Dichlorodiethyl Ether	BC	Phosphine	BB
Dichlorodifluoromethane	BC	Phosphorus Oxychloride	BC
Dichlorosilane	BD	Phosphorus Pentafluoride	
Ethylene Chlorohydrin	BC	Phosphorus Pentachloride	
Ethylene Dibromide	BC	Phosphorus Trichloride	BC
Ethylene Oxide	BC	Selenium Hexafluoride	BB
Ethylene Oxide/Propylene	BB	Silicon Tetrafluoride	BC
Ethyleneimine	BB	Sulfur Chloride	BB
Fluorine	BB	Sulfur Dioxide	BB
Germane	BA	Sulfuric Acid, fuming	BB
Hexachlorocyclopentadiene	BB	Sulfuryl Fluoride	BC
Hydrazine	BA	Tetranitromethane	BB
Hydrogen Bromide	BB	Thiophosgene	BC
Hydrogen Chloride	BB		

## 7.0 DERIVED PACKAGING PERFORMANCE STANDARDS

The information discussed in Section 4 concerning accident conditions of transport can be combined with the PIH Hazard Zone classification discussed in Section 6 to guide the selection of packaging performance standards for PIH compounds. This is especially useful because it helps quantify the amount of increased safety provided by increasing the performance standards. It will also help to quantify at what point increasing the performance standard does not significantly increase safety, especially when costs associated with the increased performance are considered.

Once the PIH materials in Tables 2 and 3 were grouped into Hazard Zones, Packaging Groups and performance standards for these Hazard Zones could be defined. Each Hazard Zone corresponds to a Packaging Group or, as in 49CFR for non-bulk packagings, one Packaging Group may cover more than one Hazard Zone. A two-step process for selecting the performance requirements was developed. First, the cumulative percentage of accidents to be protected against (see section 4.2, Figures 1 through 5, and Table 1) must be determined by the appropriate authorities. Secondly, the protection radius must be determined by the appropriate authorities. In this context, the term "protection radius" refers to the distance from a release within which the ground-level concentration of the released material exceeds the exposure guideline. In this study, the protection radius is modeled as extending equally in all directions with the release point at the center of the zone, because it is impossible to have any prior knowledge of wind direction. The information and results discussed in this report are intended to provide quantitative guidance for the appropriate authorities to use in making these decisions.

By definition, a maximum allowable leak rate of .10 g/s for Hazard Zone BA would prevent the ground-level concentrations of any of the released materials in Hazard Zone BA from exceeding their threshold levels beyond a hazard zone with a radius of 1 km. Similarly, a maximum allowable leak rate of 10 g/s for Hazard Zone BB, 100 g/s for Hazard Zone BC, and 1000 g/s for Hazard Zone BD would prevent the ground-level concentrations of any of the materials in those Hazard Zones from exceeding their threshold levels at one kilometer in any direction from the release point. In reality, for Hazard Zone BA with a maximum allowable leak rate of 0.10 g/s, the packaging manufacturers may opt for a zero leak rate since 0.10 g/s is already small.

If the packaging performance standards for each Group required the packaging to withstand a 2.6 foot drop (current drop requirement for Packaging Group III) without leaking more than the maximum allowable leak rate for that Group, the packagings would be expected to protect people outside of the hazard zone from 79% of highway collisions for 15-ton vehicles, 88% of collisions for 25-ton vehicles, 94% of collisions for 50-ton vehicles, 96.8 - 98.0 % of train-derailment accidents, and 90.0-97.5 % of train collisions (see Table 1).

If the packaging performance standards for each Group required the packaging to withstand a 3.9 foot drop (current drop requirement for Packaging Group II) without leaking more than the maximum allowable leak rate for that Group, the packagings would be expected to protect people outside of the hazard zone from 86% of collisions for 15-ton vehicles, 92% of collisions for 25-ton

vehicles, 96% of highway collisions for 50-ton vehicles, 97.5 - 98.5% of train-derailment accidents, and 92.0-98.0% of train collisions (see Table 1).

If the packaging performance standards for each Group required the packaging to withstand a 6.0 foot drop (current drop requirement for Packaging Group I) without leaking more than the maximum allowable leak rate for that Group, the packagings would be expected to protect people outside of the hazard zone from 90% of collisions for 15-ton vehicles, 94% of highway collisions for 25-ton vehicles, 97% of highway collisions for 50-ton vehicles, 98.0 - 98.8% of train-derailment accidents, and 95.0-98.5% of train collisions (see Table 1).

The information presented in Figures 4 and 5 can be used to help quantify the increased level of protection provided by increasing the fire-duration requirements. For truck collisions with resulting fires, a 10-minute fire is more severe than approximately 50% of fires resulting from accidents, a 20-minute fire is more severe than approximately 85% of fires resulting from accidents, and a 30-minute fire is more severe than approximately 95% of fires resulting from accidents. For train collision accidents with resulting fires, a 10-minute fire is more severe than approximately 10% of fires resulting from train collisions, a 20-minute fire is more severe than approximately 30% of fires resulting from train collisions, and a 30-minute fire is more severe than approximately 50% of fires resulting from train collisions. These data are by themselves insufficient to set a guideline, however, because the likelihood of the package being engulfed or even involved must also be assessed.

## 8.0 SUMMARY

This report discusses the results of a Hazmat Packaging Performance Evaluation (HPPE) project conducted at Sandia National Laboratories for the U.S. Department of Transportation Research & Special Programs Administration (DOT-RSPA). The goal of this project was to recommend performance-oriented packaging standards for bulk packagings (larger than 2000 gallons) for transporting Poison Inhalation Hazard (PIH) materials.

In the course of doing this, a computer software system, HazCon, was developed which can calculate the dispersion of dense, neutral, and buoyant gases. HazCon also has a database of thermodynamic and toxicological data for the PIH materials, a user-friendly menu-driven format for creating input data sets for calculating dispersion of the PIH in the event of an accidental release, and a link between the PIH database and a dense-gas dispersion code (which requires thermodynamic properties).

The dispersion calculations performed for a number of PIH substances were intended to support the selection of performance standards for the containers used to transport them. The calculations revealed the relationship between leak rates for these various compounds and the distance downwind from the leak beyond which the ground-level concentrations of the hazardous substance

are at or below the exposure guideline for a period of half an hour. These leak rates may then serve as guidance for selection of performance standards.

Based on the results of the dispersion calculations, a severity-categorization scheme placing the compounds into Hazard Zones was developed that groups PIH materials according to their relative hazards. This scheme places many PIH materials by name into 4 Hazard Zones. A packaging performance standard was recommended in which each Packaging Group be required to not leak more than a maximum leak rate based on the most hazardous PIH material in that Hazard Zone or Zones included in that Packaging Group. The recommended leak rates are based on protecting everyone beyond one kilometer from the release-site from being exposed to ground-level concentration of the released material in excess of the threshold level for that material.

Finally, the report provides and discusses data for quantifying the percentage of accidents against which a proposed performance standard will protect. This information is meant to guide policy-makers in developing the final packaging-performance criteria for which this study was commissioned. Specifically, if a packaging can withstand a six-foot drop onto an essentially unyielding surface without leaking more than the maximum allowable leak rate, it follows that, for over 90% of all accidents, people beyond one kilometer from the accident will not be exposed to ground-level concentrations of the released PIH material that exceed threshold levels.

## 9.0 SUGGESTIONS FOR FUTURE WORK

The following are areas in which additional effort is recommended:

1. Selection and analysis of an internally consistent set of exposure guidelines. One possibility for consistency: if one type of guideline (e.g., threshold limit value) exists for all the PIH substances, an analysis of risk of exposure at that level and at various fractions of that level should be made, and an exposure guideline constructed based on such a risk.
2. The results reported in this study do not include analyses of PIH materials that leak as fine powders or as liquid aerosols. A dispersion model (or models) for these substances should be identified that yields reliable results for atmospheric conditions (stability, wind speed, etc.) roughly comparable to those used when modeling gases. It is expected that concentrations of powders and liquid aerosols will almost always be lower than those of ideal and dense gases at any given downwind distance from a release point, under otherwise comparable conditions of release. Thus, all PIH materials that leak as powders or as liquid aerosols will fall into the hazard groups established in this report.
3. The SLAB model should be validated and benchmarked over a wider range of source emission-rates and downwind distances than has been examined to date [ERM89]. The comparisons between modeled and measured values given by Ermak include only one

section of a typical SLAB output (see, for example, Figure 21). A sensitivity analysis of SLAB to various input parameters should also be performed, since all needed input parameters are not available for all PIH compounds. If SLAB is relatively insensitive to a given input parameter, acceptable representation of that material may be possible with an estimated value for that parameter. In contrast, if the SLAB results are sensitive to a given input parameter, then an accurate value would be necessary.

4. Further study of hypothetical and actual fire events that could compromise PIH highway and rail packagings is desirable. In particular, an attempt should be made to relate actual accident events to the probability data presented in Figures 1 through 5 (from [DEN77]).
5. Final decisions on the most desirable protection level can only be made by the appropriate authorities in government. The qualitative information and the hazard-group classification presented in this report represent performance-standards recommendations (including impact and fire conditions and maximum allowable leak rate guidelines) for various levels of protection of prototype bulk packagings for PIHs during rail and highway transportation..

## 10.0 REFERENCES

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## Appendix A

### Poison Inhalation Hazard Materials

Table A-1. Poison Inhalation Hazard Materials

PIH No.	Name	Formula
1	Iron Pentacarbonyl	C <sub>5</sub> FeO <sub>5</sub>
2	Arsenic Trichloride	AsCl <sub>3</sub>
3	Cyanogen Chloride	CClN
4	Carbonyl Sulfide	COS
5	Thiophosgene	CCl <sub>2</sub> S
6	Methyl Chloride	CH <sub>3</sub> Cl
7	Methylamine, Anhydrous	CH <sub>3</sub> N
8	Hydrazine	H <sub>4</sub> N <sub>2</sub>
9	Ethylene DiChloride	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>
10	Phosgene	CCl <sub>2</sub> O
11	Carbonyl Fluoride	CF <sub>2</sub> O
12	Pentaborane	B <sub>5</sub> H <sub>9</sub>
13	Ethylene DiBromide	C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>
14	Crotonaldehyde	C <sub>4</sub> H <sub>6</sub> O
15	Vanadium Oxytrichloride	Cl <sub>3</sub> OV
16	Tungsten Hexafluoride	WF <sub>6</sub>
17	Oxygen Difluoride	F <sub>2</sub> O
18	Arsine	AsH <sub>3</sub>
19	Selenium Hexafluoride	F <sub>6</sub> Se
20	Chlorine Trifluoride	ClF <sub>3</sub>
21	Phosphorus Pentoxide	O <sub>5</sub> P <sub>2</sub> or P <sub>2</sub> O <sub>5</sub>
22	Phosphorus Trichloride	Cl <sub>3</sub> P or PCl <sub>3</sub>
23	Phosphorous Oxychloride	Cl <sub>3</sub> OP
24	Boron Trifluoride	BF <sub>3</sub>
25	Phosphorous Pentachloride	Cl <sub>5</sub> P
26	Phosphine	H <sub>3</sub> P
27	Stibine	H <sub>3</sub> Sb
28	Hydrogen Selenide	H <sub>2</sub> Se
29	Thionyl Chloride	Cl <sub>2</sub> OS
30	Methylhydrazine	CH <sub>6</sub> N <sub>2</sub>
31	Cyanogen	C <sub>2</sub> N <sub>2</sub>
32	Cyanogen Bromide	CBrN
33	Ethylene Imine	C <sub>2</sub> H <sub>5</sub> N
34	Dichloroethyl Ether	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O
35	Methyl Orthosilicate	
36	Propyl Trichlorosilane	C <sub>3</sub> H <sub>7</sub> Cl <sub>3</sub> Si

PIH No.	Name	Formula
74	Carbon Tetrachloride	CCl <sub>4</sub>
75	Dimethyl Hydrazine, Unsymmetrical	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>
76	Dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>
77	Nitrogen Trioxide	N <sub>2</sub> O <sub>3</sub>
78	Chlorine	Cl <sub>2</sub>
79	Nitric Oxide	NO
80	Nitrogen Tetroxide	N <sub>2</sub> O <sub>4</sub>
81	Nitric Oxide/Nitrogen Tetroxide Mixture	
82	Propylene Oxide	C <sub>3</sub> H <sub>6</sub> O
83	Fluorine	F <sub>2</sub>
84	Dichlorodifluoromethane	CCl <sub>2</sub> F <sub>2</sub>
85	Sulfur Trioxide	SO <sub>3</sub>
86	Methyl Dichloroarsine	CH <sub>3</sub> AsCl <sub>2</sub>
87	Sulfur Chloride Pentafluoride	ClF <sub>5</sub> S
88	Dimethyl Phosphorochloridothioate	C <sub>2</sub> H <sub>6</sub> ClO <sub>2</sub> PS
89	Phosphorus Pentafluoride	F <sub>5</sub> P
90	Diborane	B <sub>2</sub> H <sub>6</sub>
91	Nitrogen Dioxide	NO <sub>2</sub>
92	Ethyl Chloroformate	C <sub>3</sub> H <sub>5</sub> ClO <sub>2</sub>
93	Methyl Chloroformate	C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub>
94	Propyl Chloroformate	C <sub>4</sub> H <sub>7</sub> ClO <sub>2</sub>
95	Chlorosulfonic Acid	ClHO <sub>2</sub> S
96	Isobutyl Chloroformate	C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub>
97	Butylchloroformate, sec-	C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub>
98	Butyl Chloroformate, N-	C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub>
99	Allylchloroformate	C <sub>4</sub> H <sub>5</sub> ClO <sub>2</sub>
100	Isopropyl Chloroformate	C <sub>4</sub> H <sub>7</sub> ClO <sub>2</sub>
101	Phenyl Mercaptan	C <sub>6</sub> H <sub>5</sub> S
102	Bromine Chloride	BrCl
103	Chloroacetic Acid	C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub>
104	Tellurium Hexafluoride	F <sub>6</sub> Te
105	Sulfuric Acid	H <sub>2</sub> O <sub>4</sub> S
106	Sulfuric Acid, Fuming	H <sub>2</sub> O <sub>4</sub> S.O <sub>3</sub> S
107	Cumyl Hydroperoxide	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>

PIH No.	Name	Formula
108	Bromine Trifluoride	BrF <sub>3</sub>
109	Methyl Bromide	CH <sub>3</sub> Br
110	Bromine Pentafluoride	BrF <sub>5</sub>
111	Trimethyl Acetyl Chloride	C <sub>3</sub> H <sub>9</sub> ClO
112	Hydrocyanic Acid, Liquified	CHN
113	Hydrocyanic Acid, <5%	CHN
114	Hydrocyanic Acid, > or = 5%	CHN
115	Ammonia	H <sub>3</sub> N
116	Ammonium Hydroxide	H <sub>4</sub> NHO
117	Ammonium Hydroxide	H <sub>4</sub> NHO
118	Hydrogen Fluoride	HF
119	Hydrofluoric Acid Solution	HFH <sub>2</sub> O
120	Carbon Monoxide	CO
121	Carbon Monoxide and Hydrogen, Mixture	
122	Hydrogen Chloride, Anhydrous	ClH
123	Hydrochloric Acid	ClH
124	Hydrochloric Acid	ClH
125	Hydrochloric Acid	ClH
126	Ethylene Oxide	C <sub>2</sub> H <sub>4</sub> O
127	Ethylene Oxide Mixed with Propylene	
128	Carbon Dioxide Ethylene Oxide Mixture	C <sub>2</sub> H <sub>4</sub> O.CO <sub>2</sub>
129	Carbon Dioxide Ethylene Oxide Mixture	C <sub>2</sub> H <sub>4</sub> O.CO <sub>2</sub>
130	Allyl Amine	C <sub>3</sub> H <sub>7</sub> N
131	Allyl Alcohol	C <sub>3</sub> H <sub>6</sub> O
132	Tetranitromethane	CN <sub>4</sub> O <sub>8</sub>
133	Bromine	Br <sub>2</sub>
134	Bromine Solution	Br <sub>2</sub>
135	Acrolein (2-Propenal)	C <sub>3</sub> H <sub>4</sub> O
136	Acrolein Dimer, Stabilized	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>
137	Diphenyl Chloroarsine	C <sub>12</sub> H <sub>10</sub> AsCl
138	Phenylcarbylamine Chloride	C <sub>7</sub> H <sub>5</sub> C <sub>12</sub> N
139	Ethylene Chlorohydrin	C <sub>2</sub> H <sub>5</sub> ClO
140	Perchloro Methylmercaptan	CCl <sub>4</sub> S

PIH No.	Name	Formula
141	Methyl Isothiocyanate	C <sub>2</sub> H <sub>3</sub> NS
142	Aldicarb	C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S
143	Tributylamine	C <sub>12</sub> H <sub>27</sub> N
144	Isophorone Diisocyanate	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
145	Phenyl Isocyanate	C <sub>7</sub> H <sub>5</sub> NO
146	Ethyl Chlorothio Formate	C <sub>3</sub> H <sub>5</sub> ClOS
147	Methoxymethyl Isocyanate	C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub>
148	Methylene Isocyanate	C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> O <sub>2</sub>
149	Methyl Isocyanate	C <sub>2</sub> H <sub>3</sub> NO
150	Tetraethyl Dithiopyrophosphate	C <sub>8</sub> H <sub>20</sub> O <sub>5</sub> P <sub>2</sub> S <sub>2</sub>
151	Tetraethyl Pyrophosphate	C <sub>8</sub> H <sub>20</sub> O - O <sub>7</sub> P <sub>2</sub>
152	Ethyl Isocyanate	C <sub>3</sub> H <sub>5</sub> NO
153	Hydrogen Bromide	BrH
154	Hydrobromic Acid, >49%	BrH
155	Hydrobromic Acid, < or = 49%	BrH
156	Nitric Acid, Fuming	HNO <sub>3</sub>
157	Nitrating Acid, Mixture >50% Nitric	
158	Nitric Acid	HNO <sub>3</sub>
159	Tert-Octyl Mercaptan	C <sub>8</sub> H <sub>18</sub> S
160	Dimethyl Thiophosphoryl Chloride	C <sub>2</sub> H <sub>6</sub> ClPS
161	Hexaethyltetraphosphate	C <sub>12</sub> H <sub>30</sub> O <sub>13</sub> P <sub>4</sub>
162	Chloropivaloyl Chloride	C <sub>5</sub> H <sub>8</sub> OCl <sub>2</sub>
163	N-Butyl Isocyanate	C <sub>5</sub> H <sub>9</sub> NO
164	Butyl Isocyanate, Tert	C <sub>5</sub> H <sub>9</sub> NO
165		C <sub>7</sub> H <sub>11</sub> NO
166		C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> NO
167	Nitrogen Fluoride Oxide	F <sub>3</sub> NO
168		C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>
169	1,1-Methylenebis[4-Isocyanato-	C <sub>15</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>

Appendix B

Dispersion Calculation Results

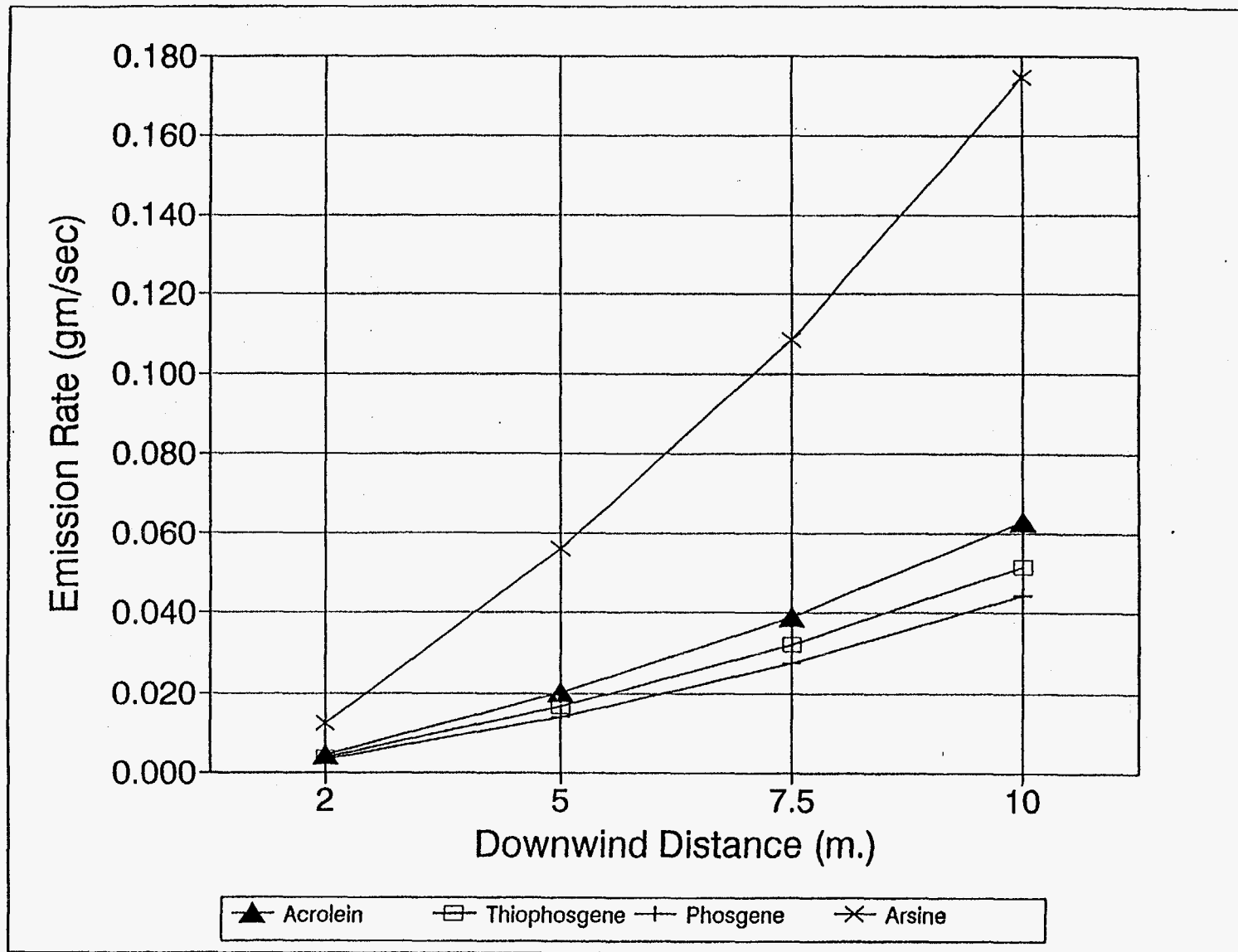


Figure 1

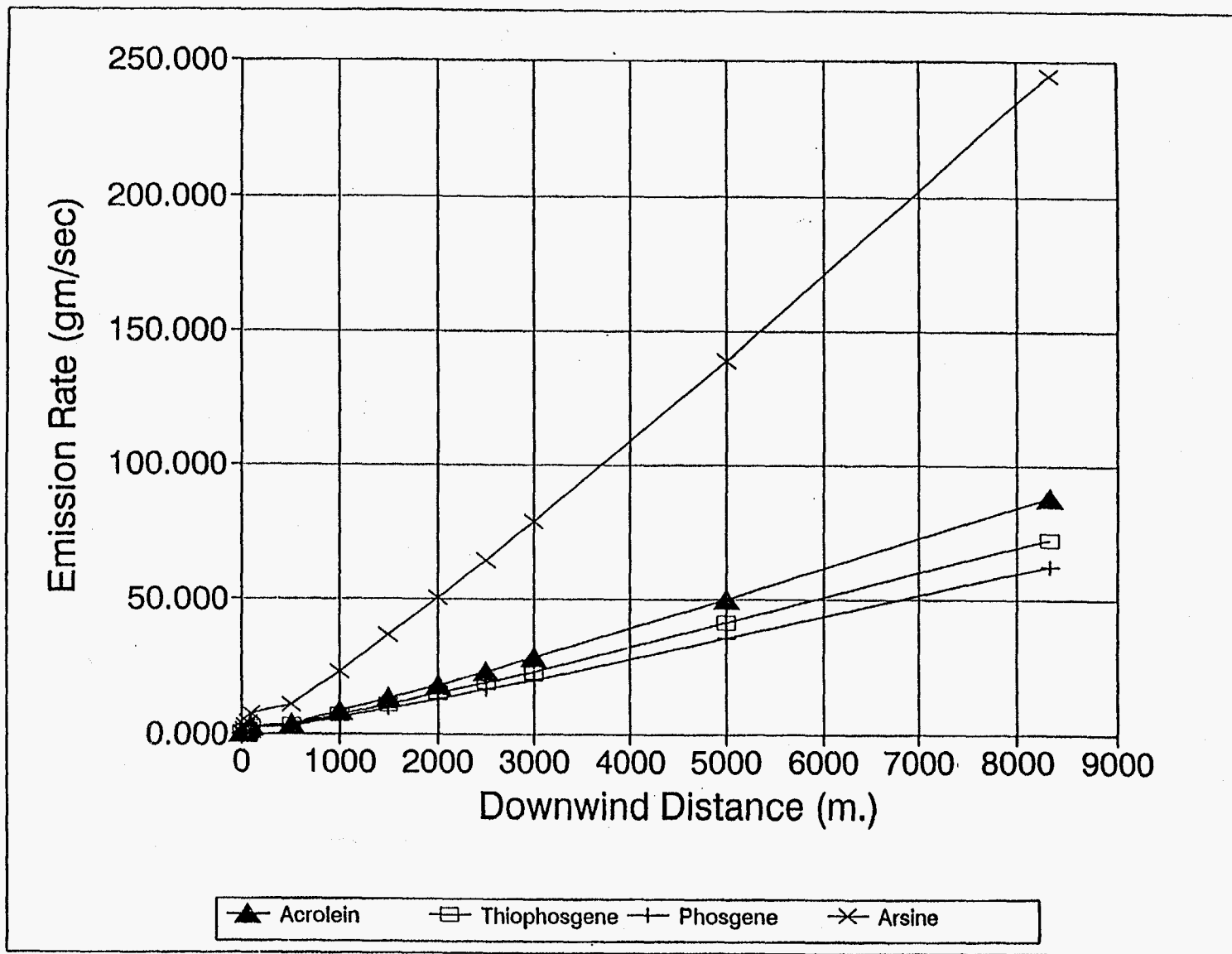


Figure 2

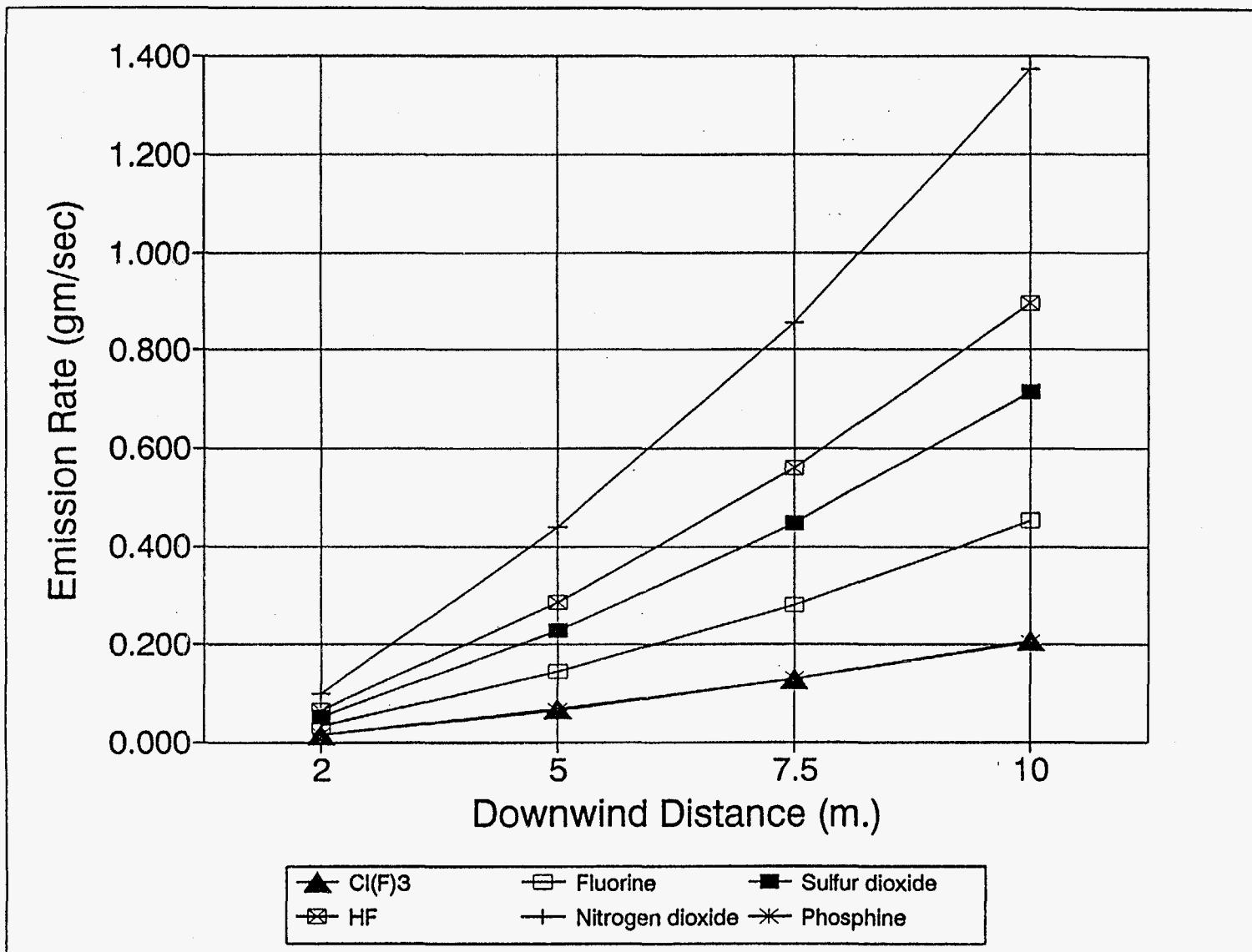


Figure 3



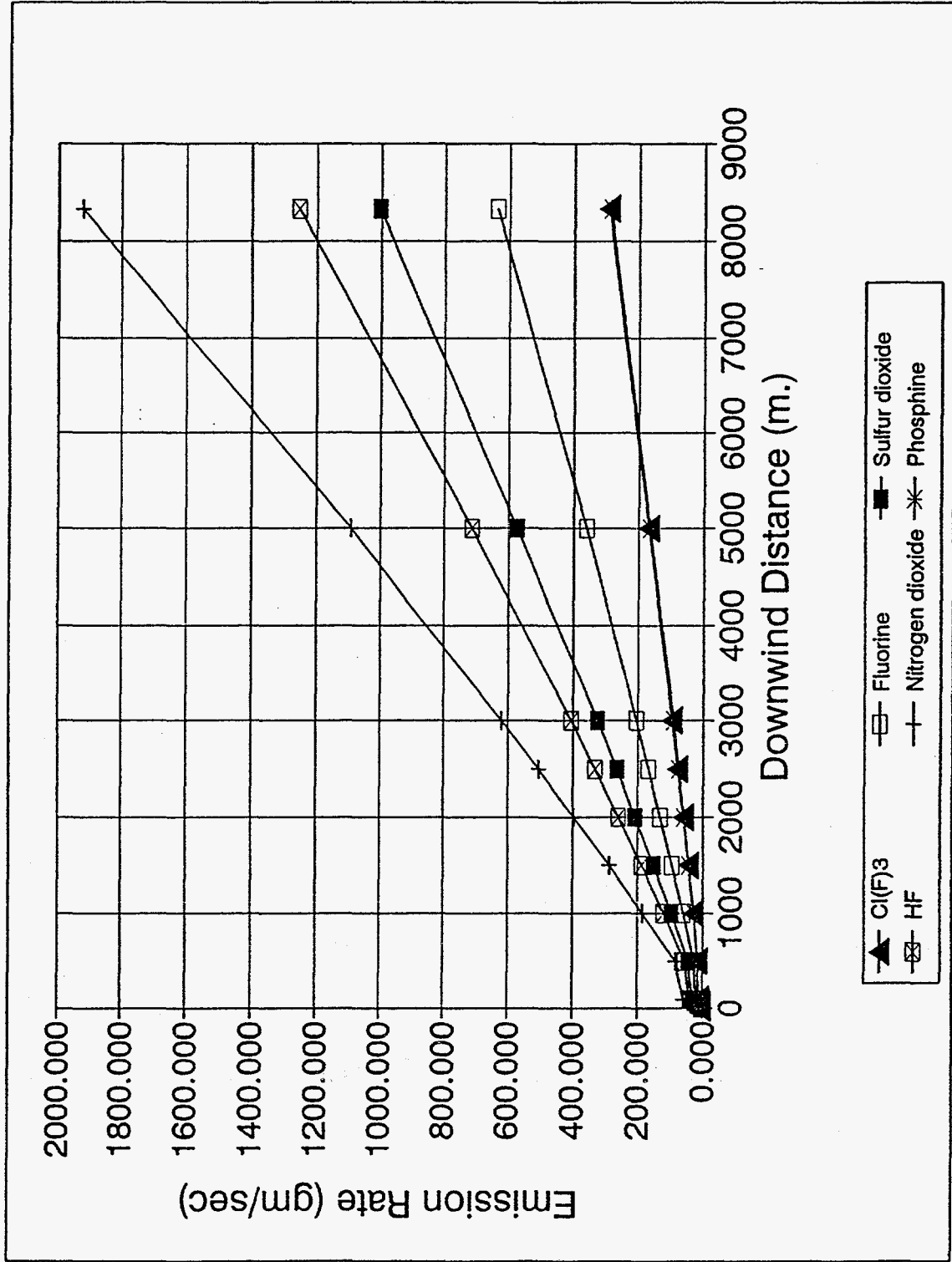


Figure 4

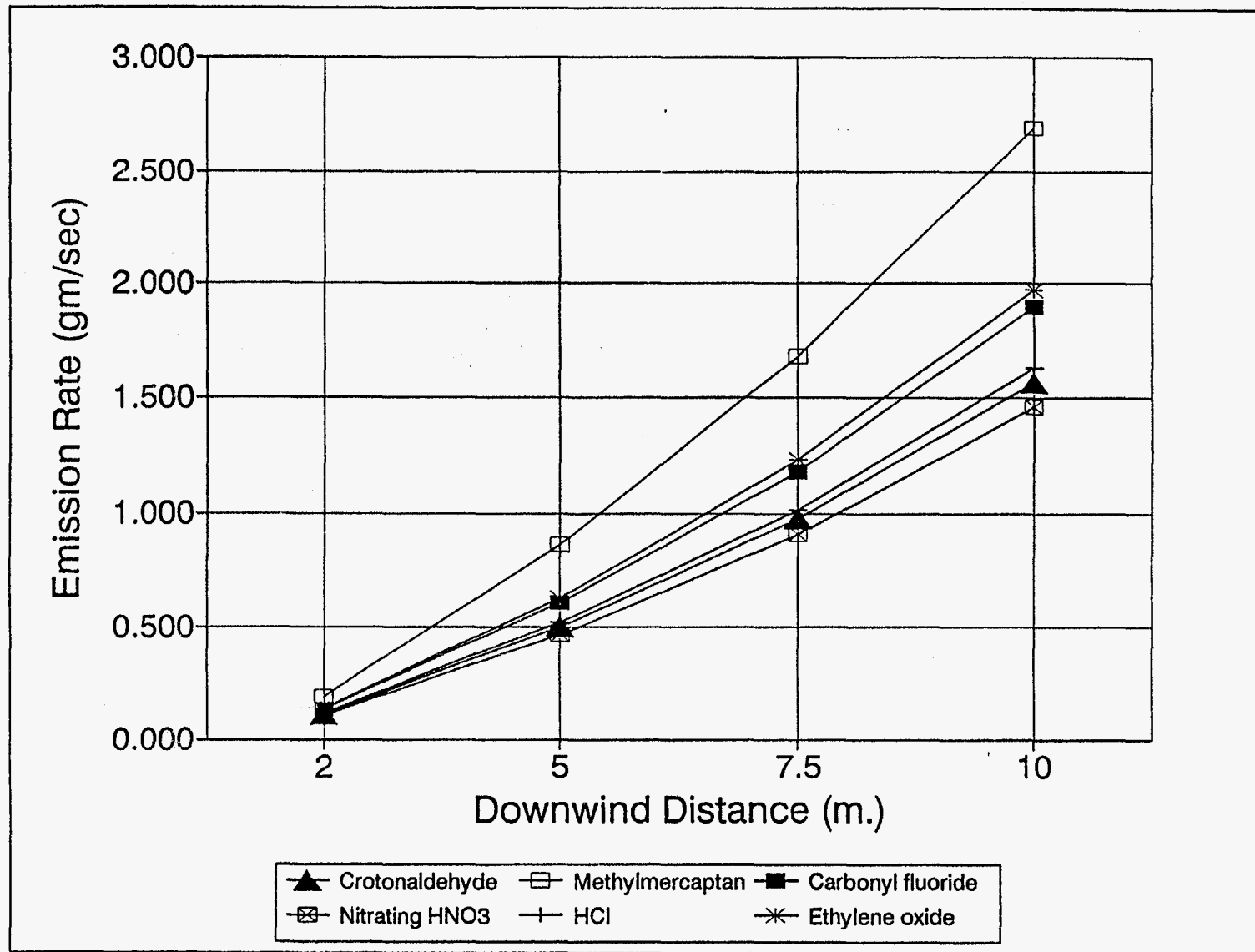


Figure 5

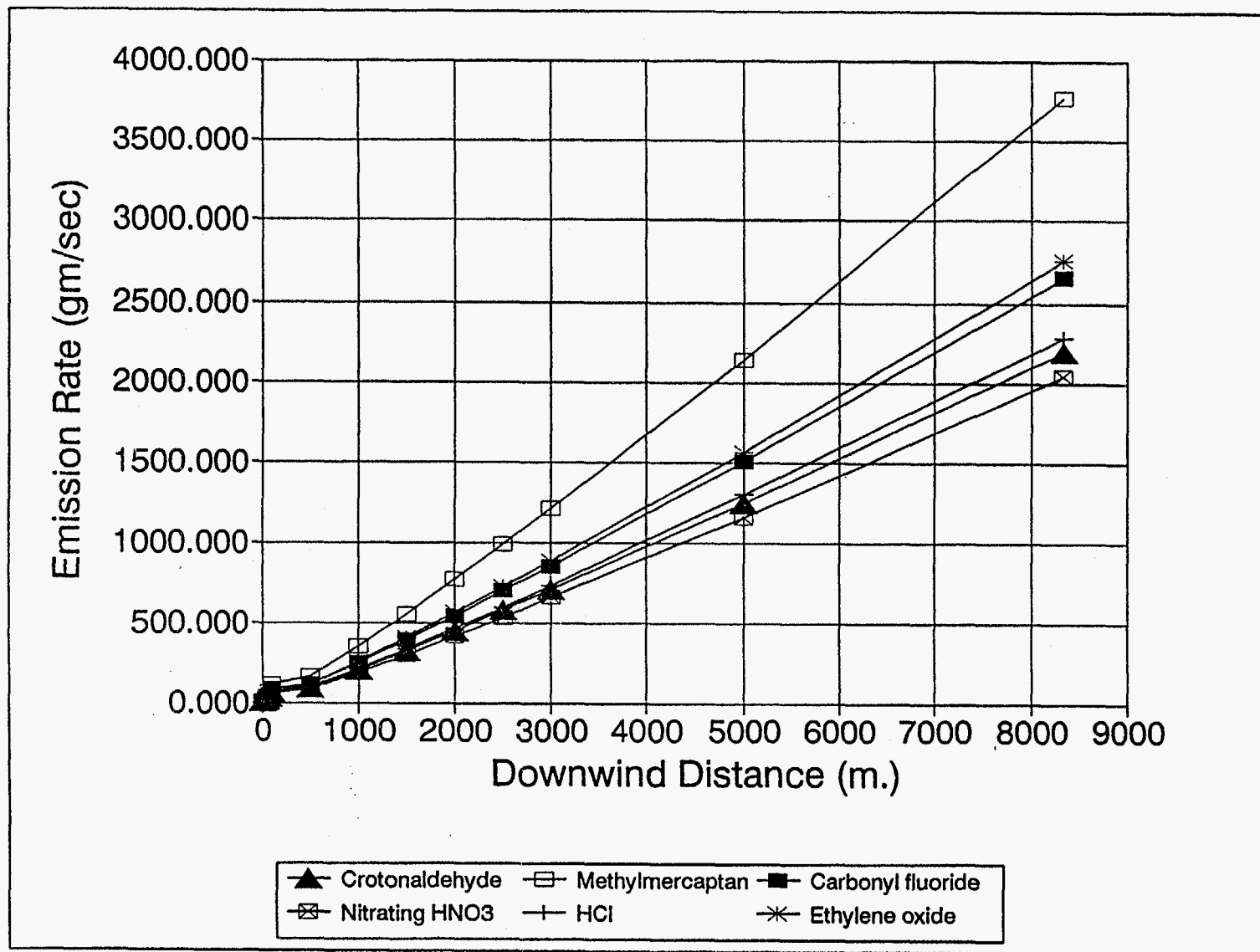


Figure 6

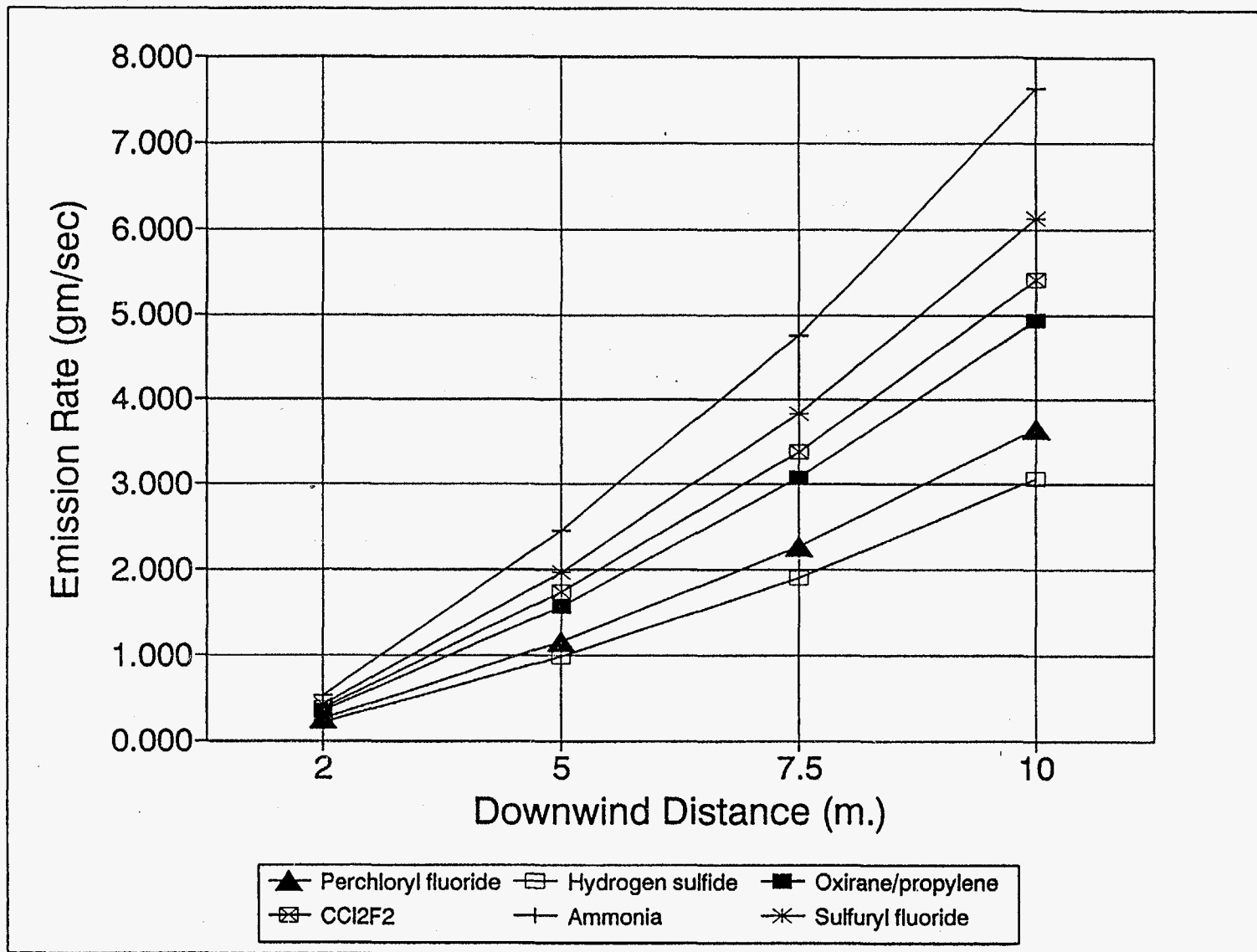


Figure 7

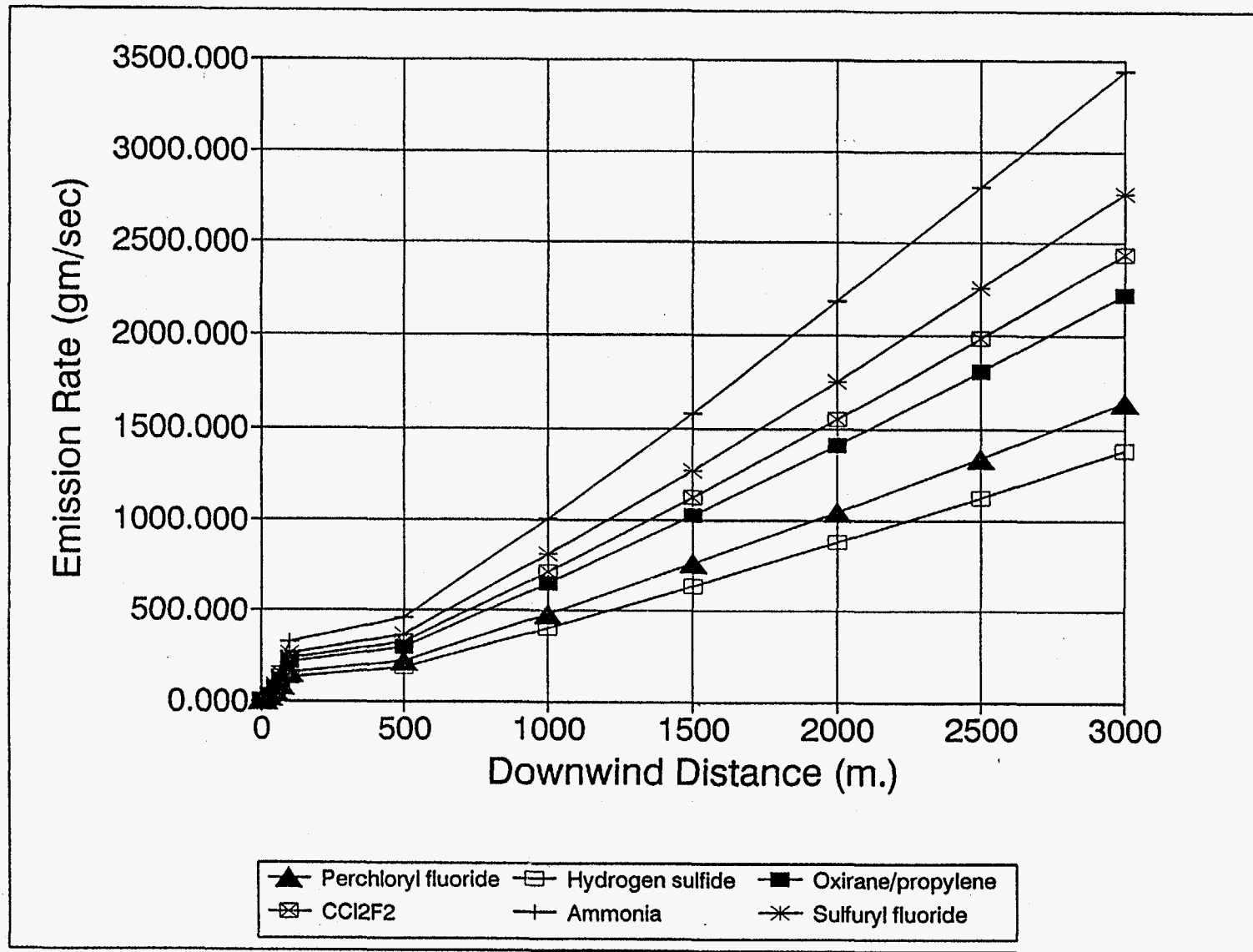


Figure 8

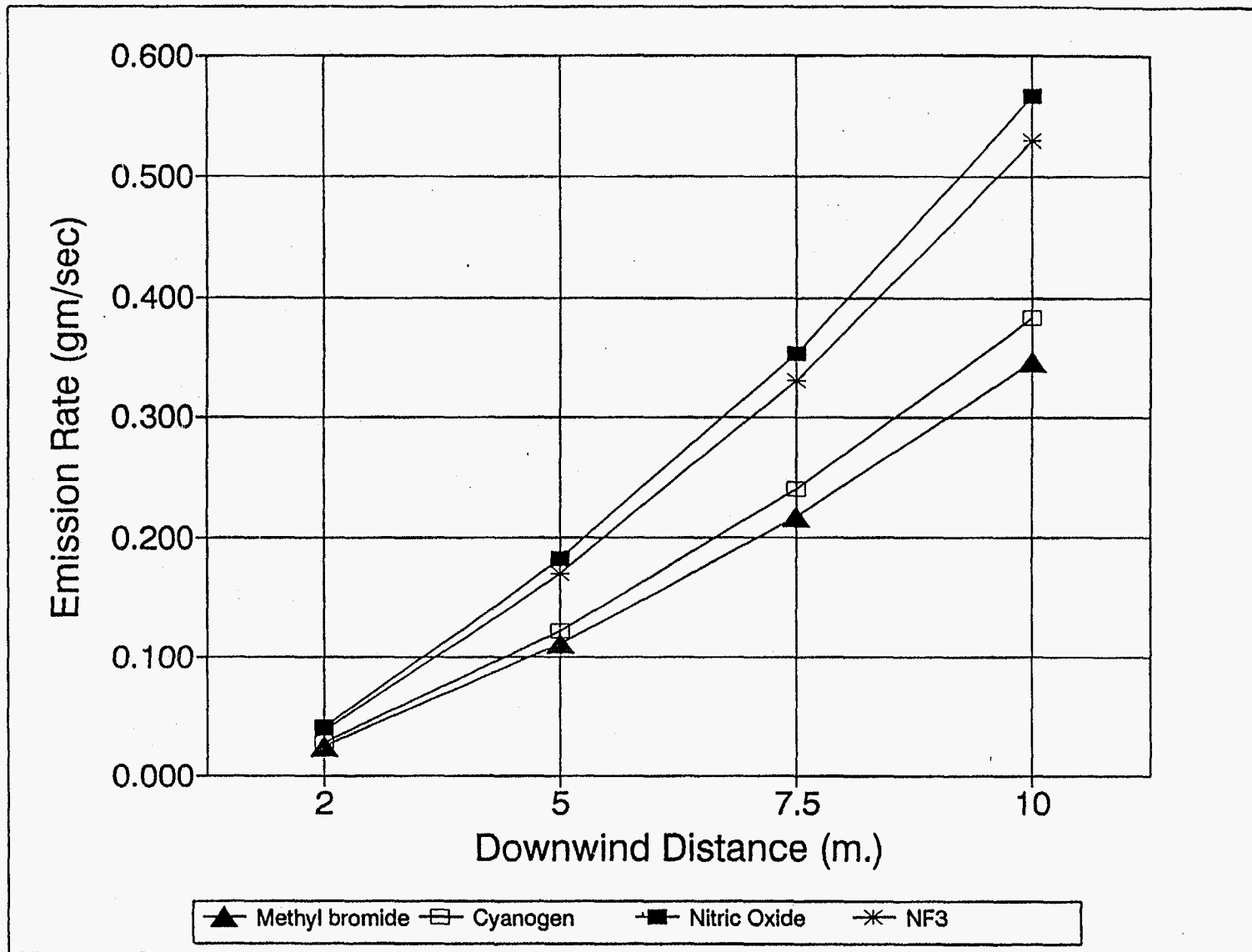


Figure 9

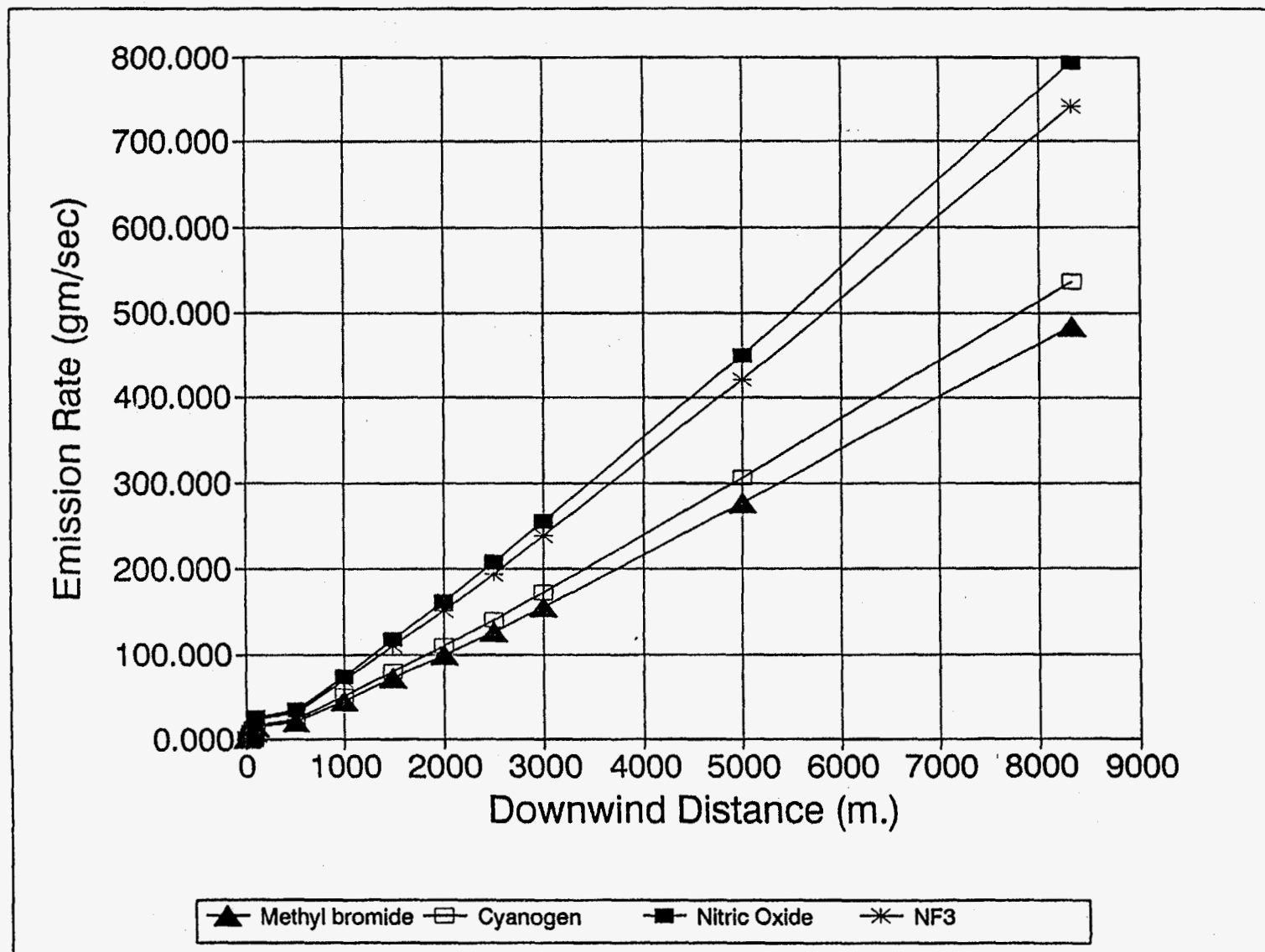


Figure 10

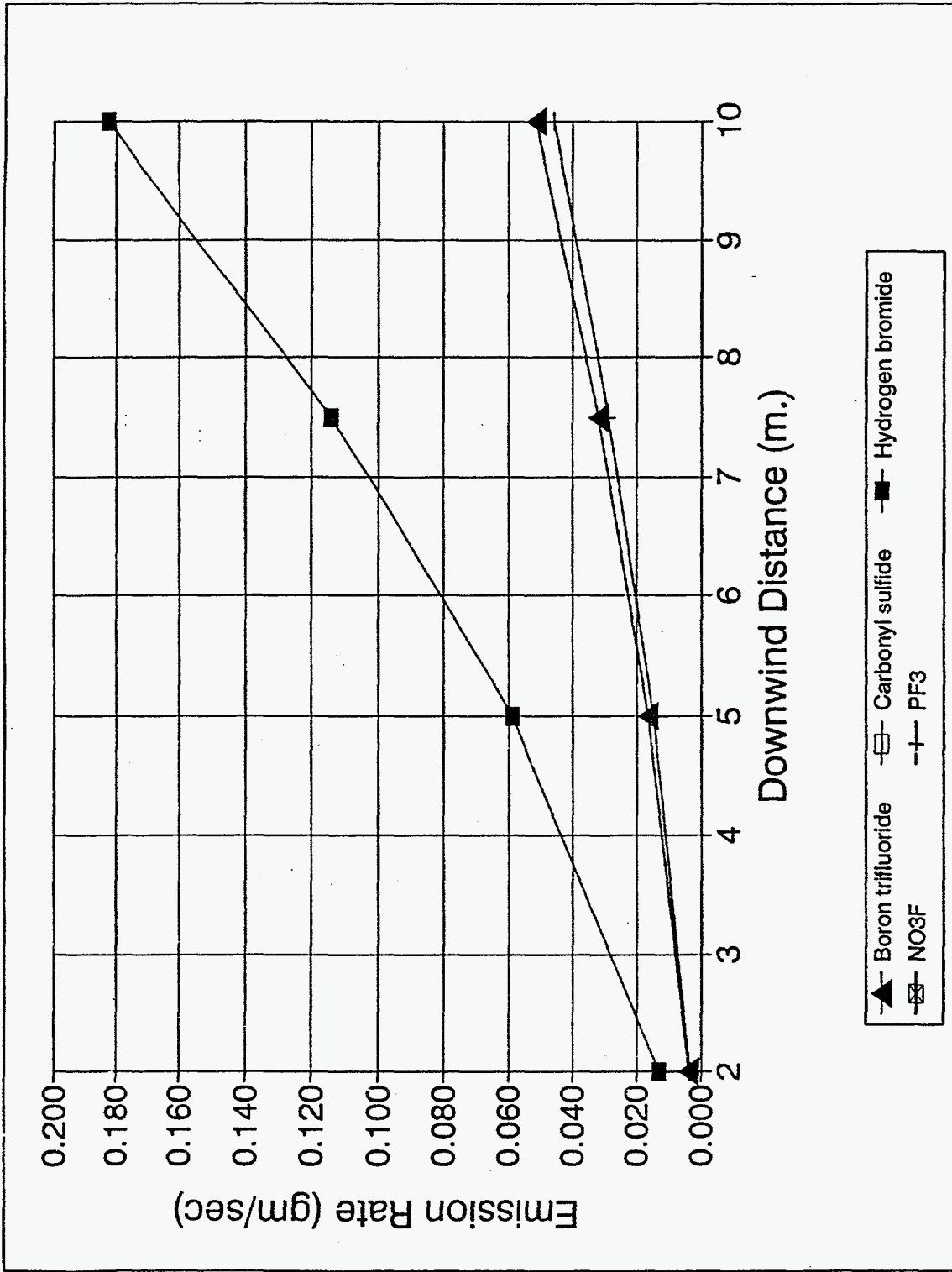


Figure 11



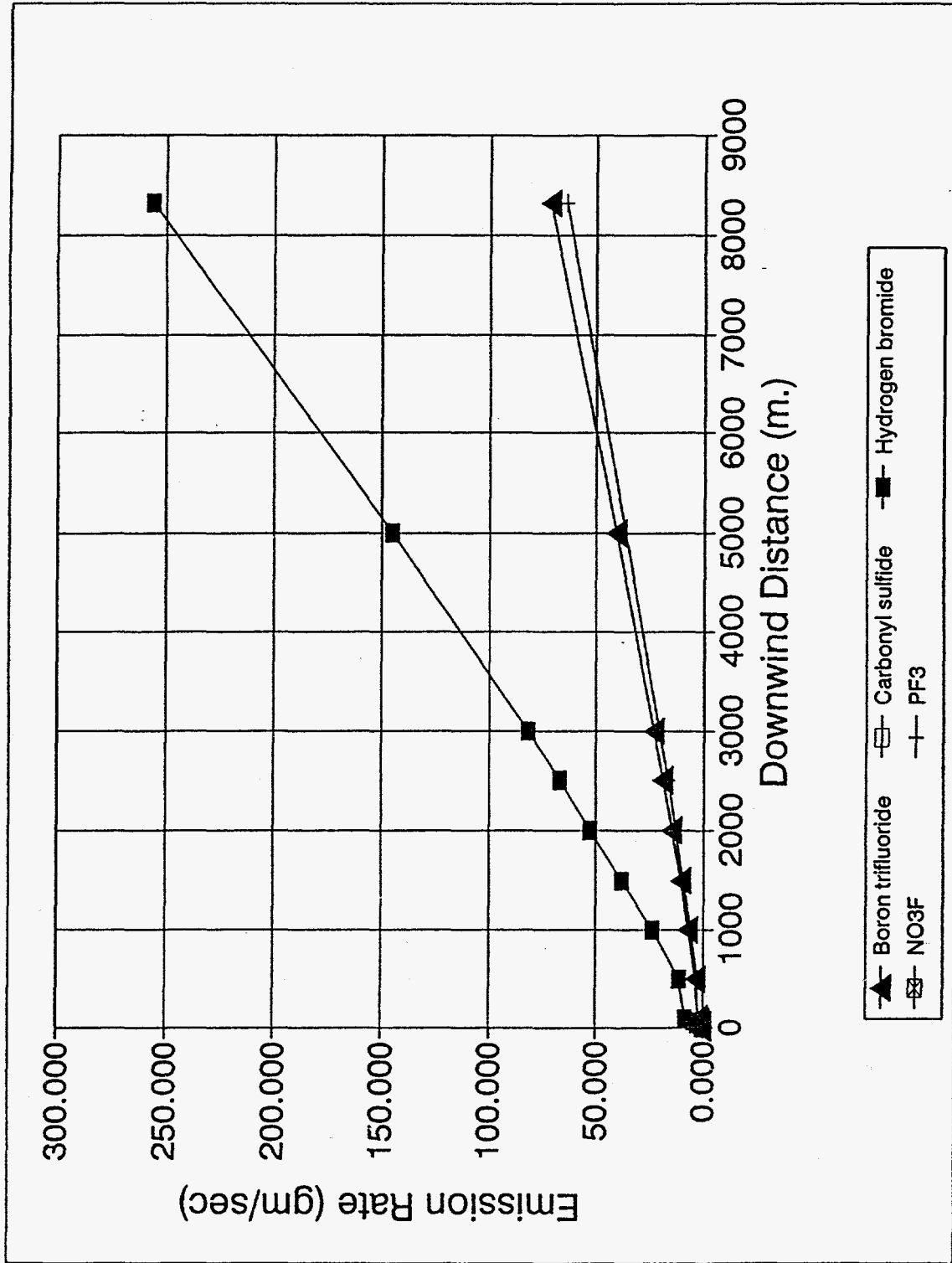


Figure 12

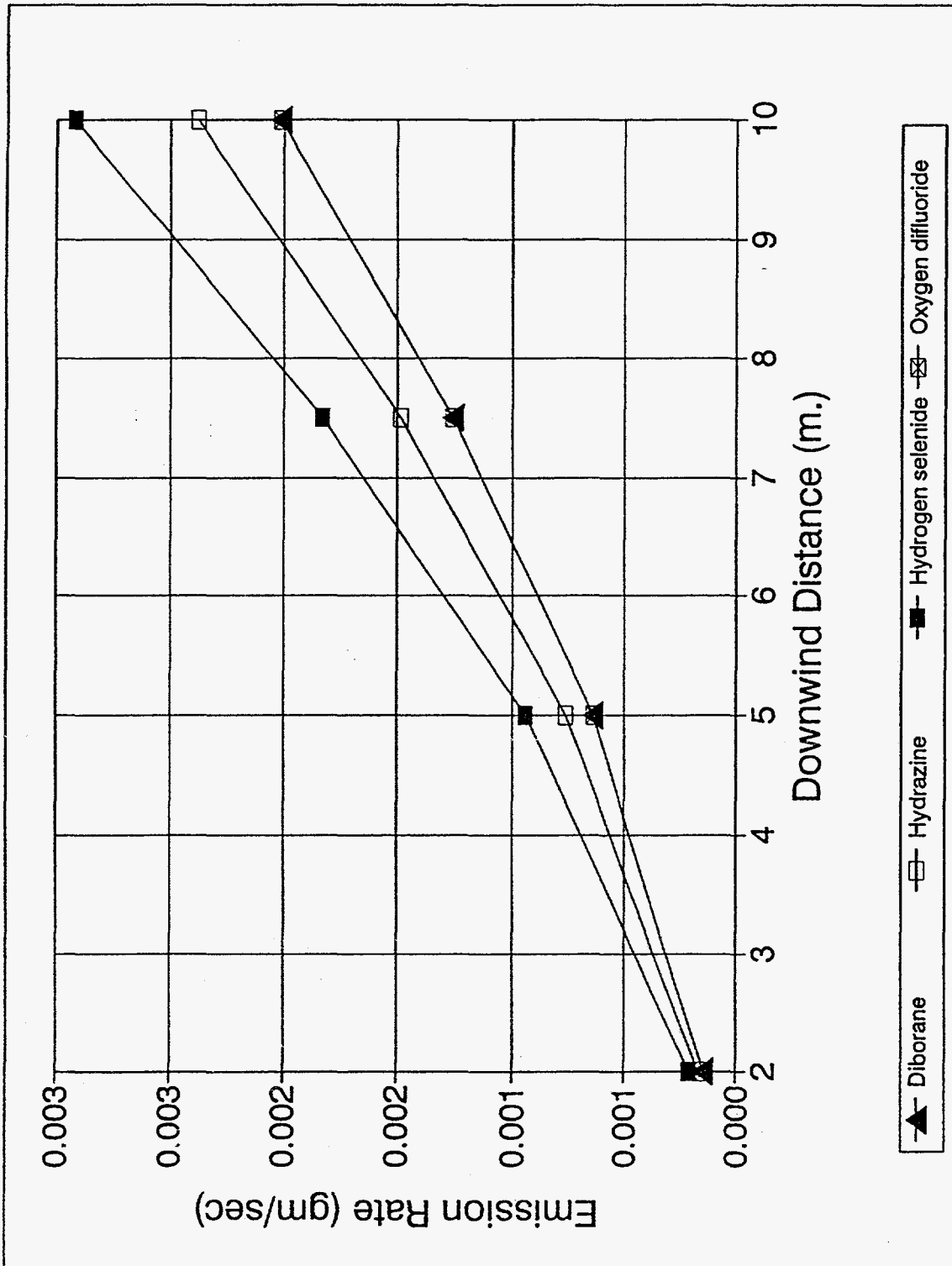


Figure 13

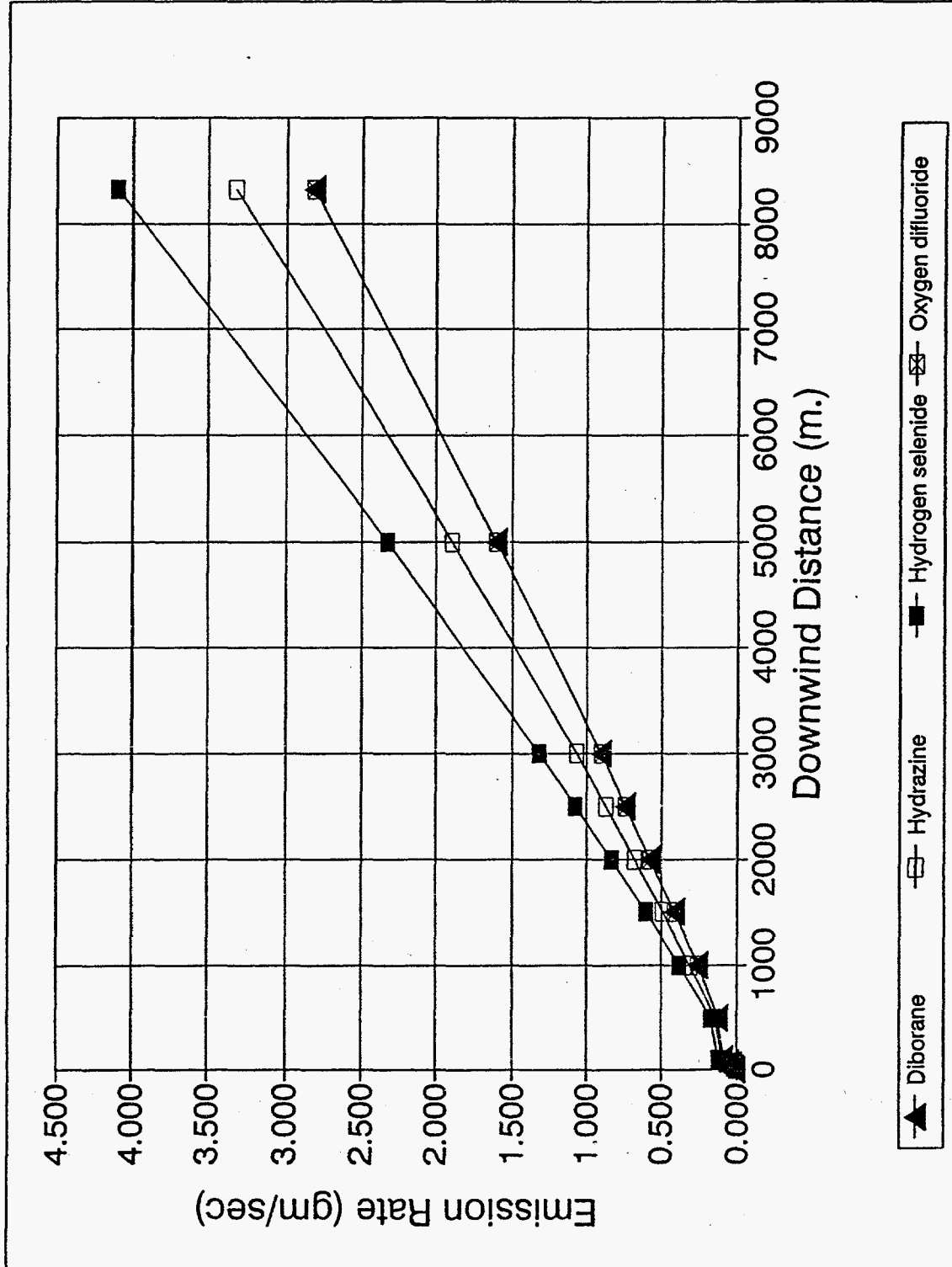


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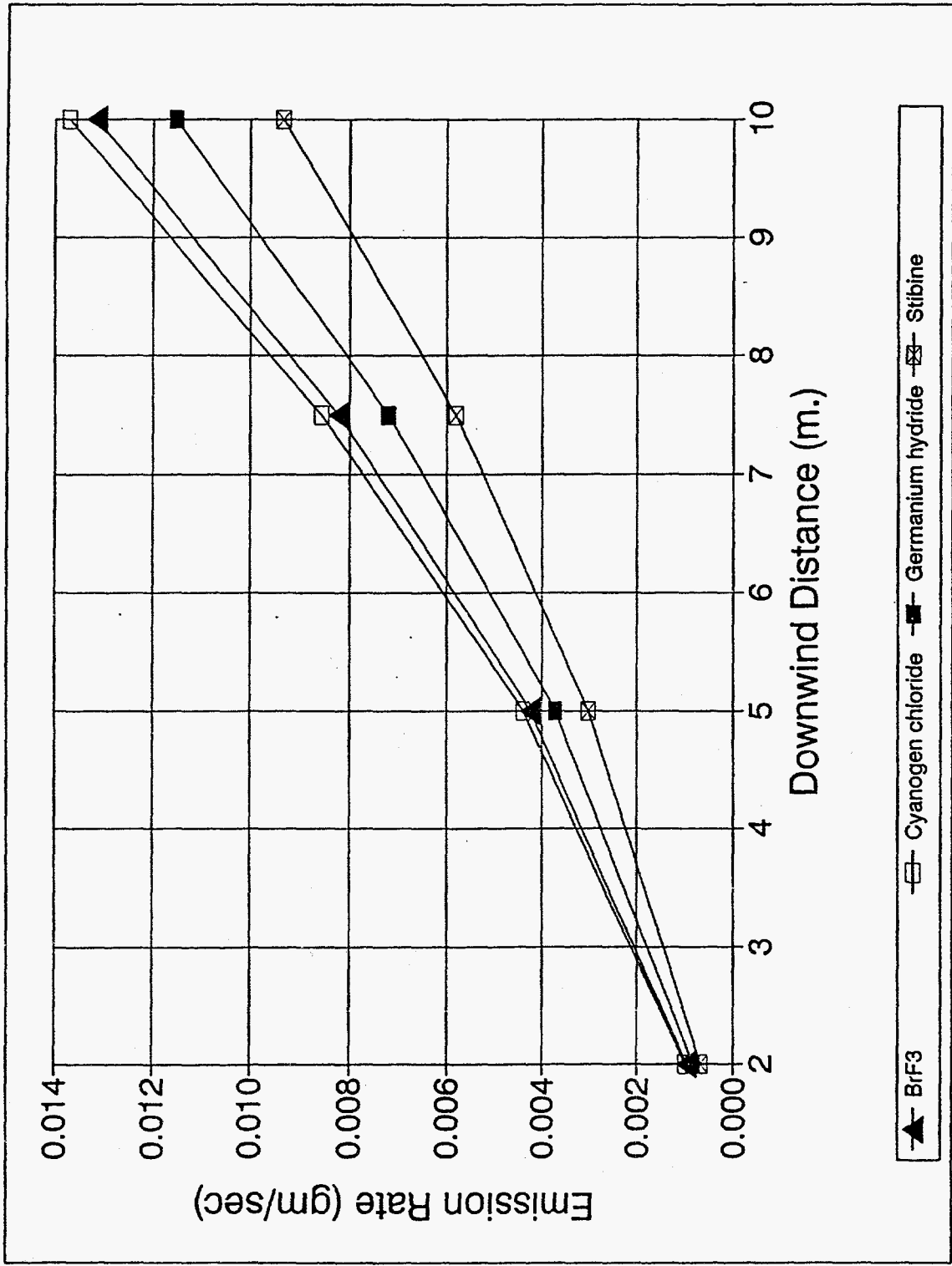


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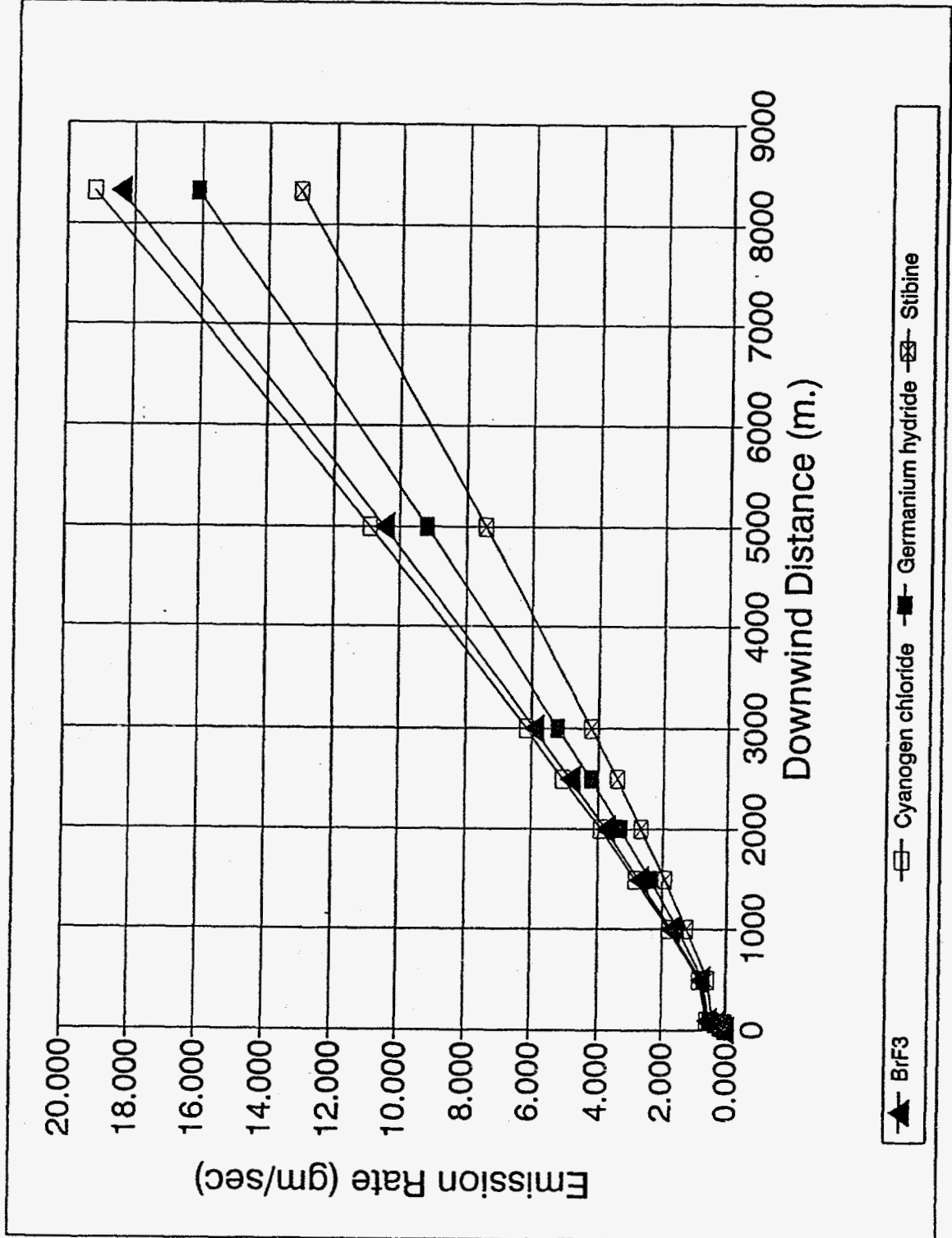


Figure 16

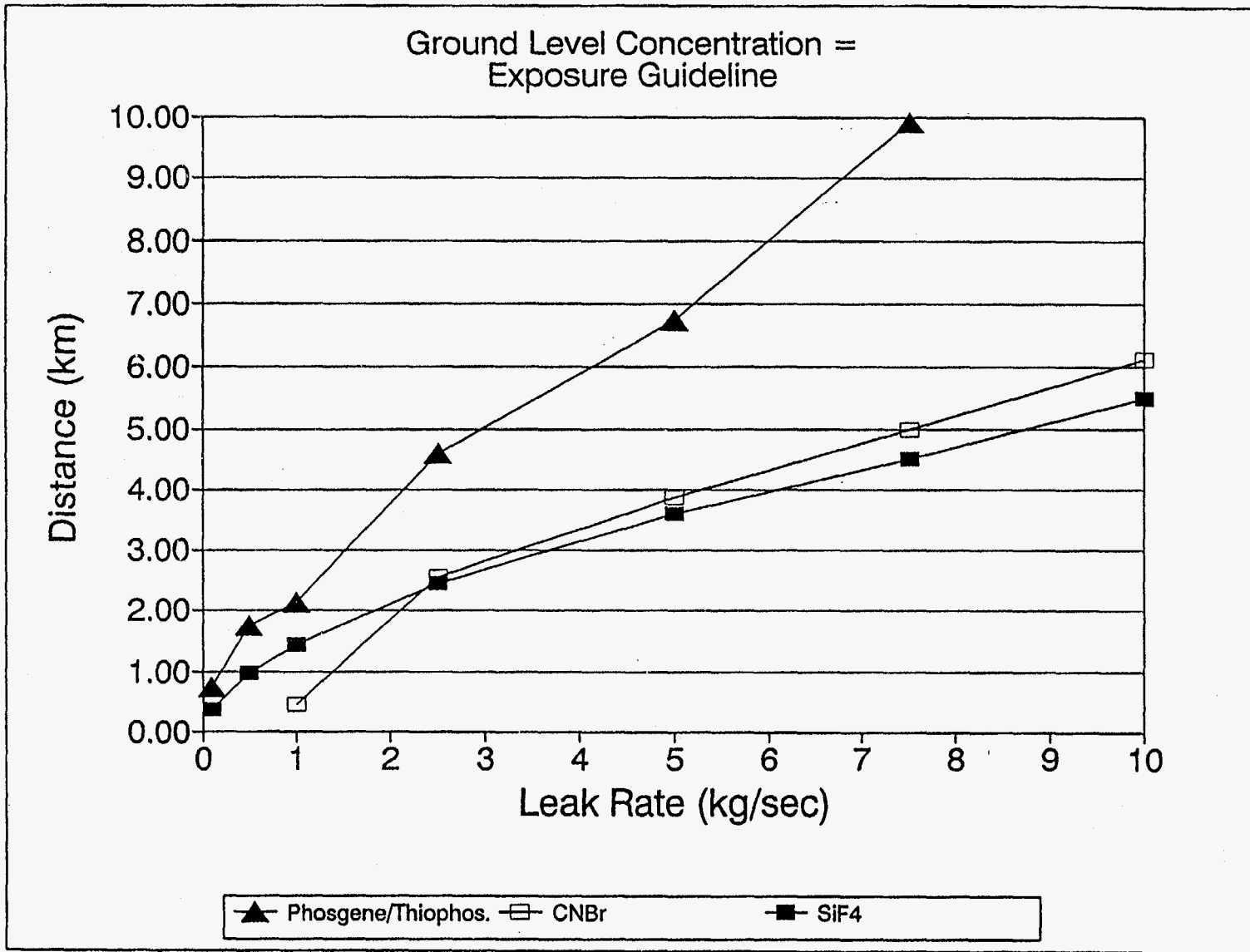


Figure 17

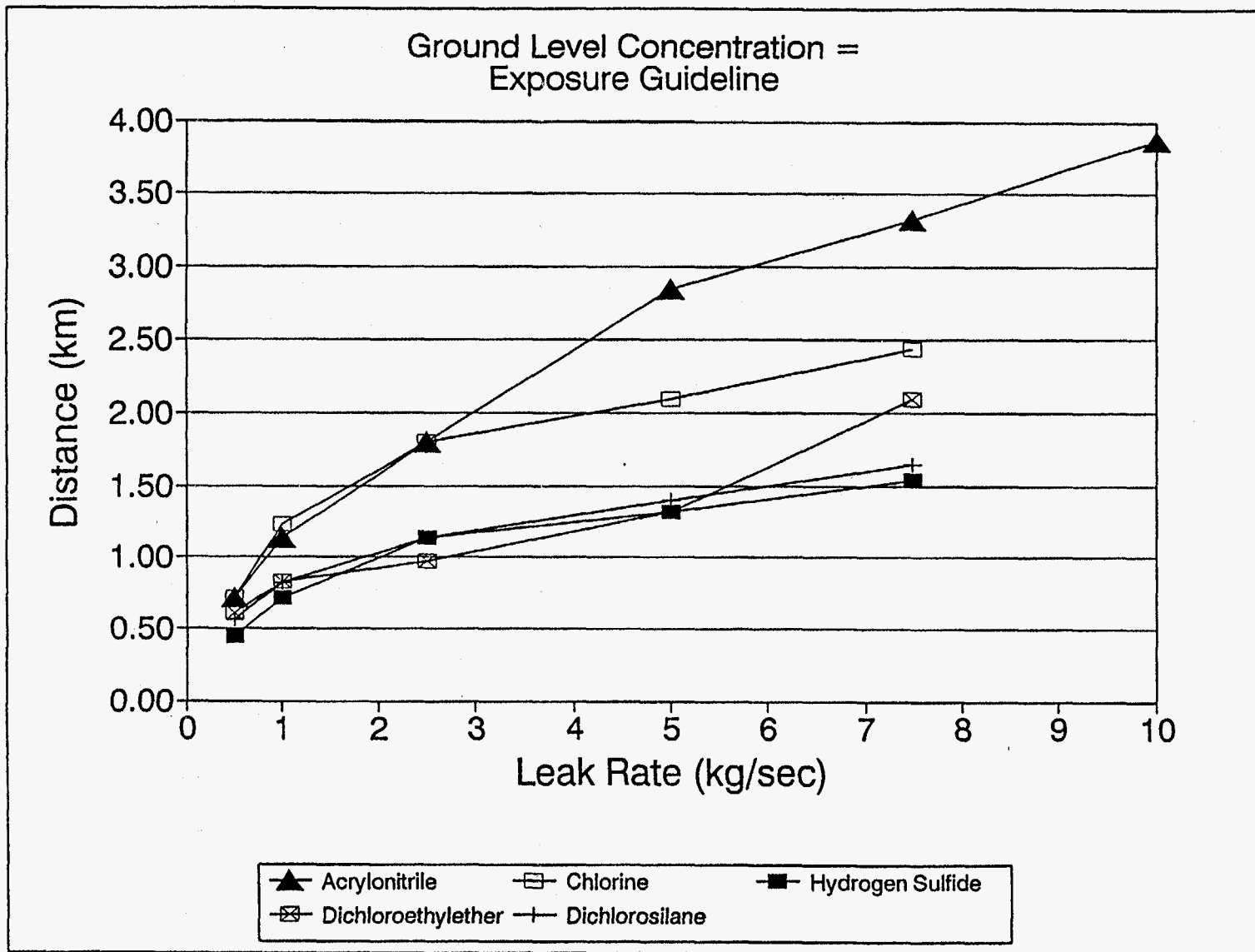


Figure 18

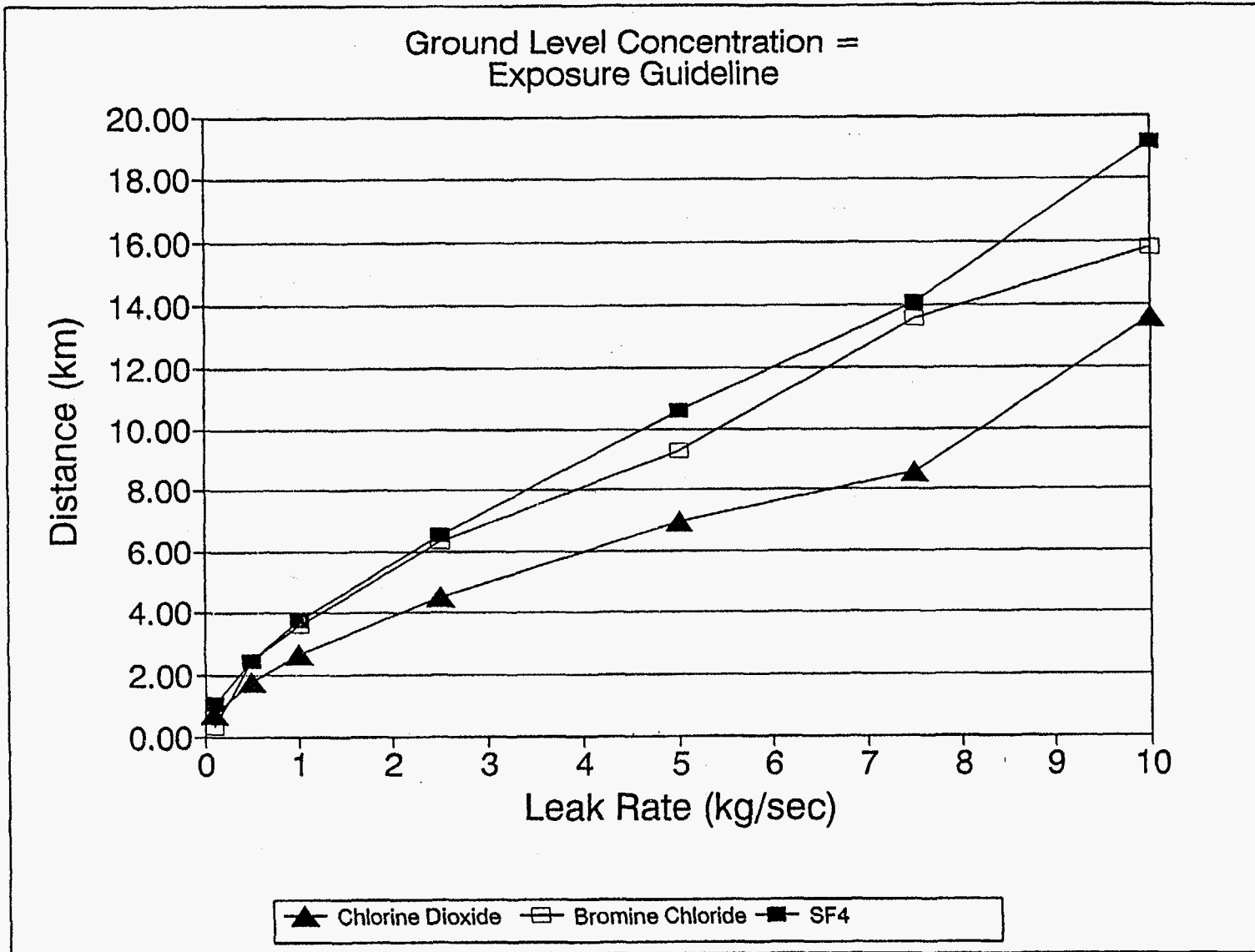


Figure 19



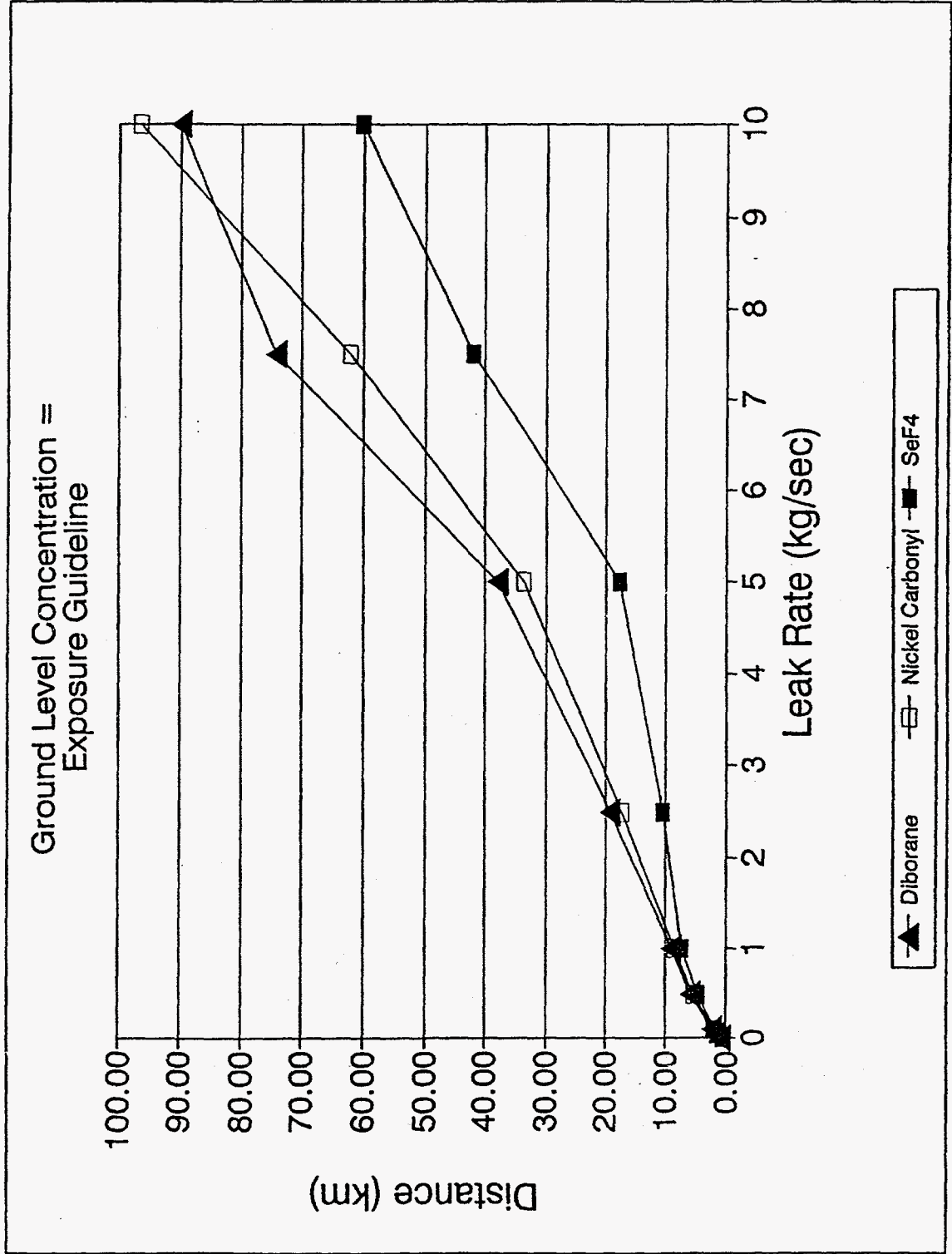


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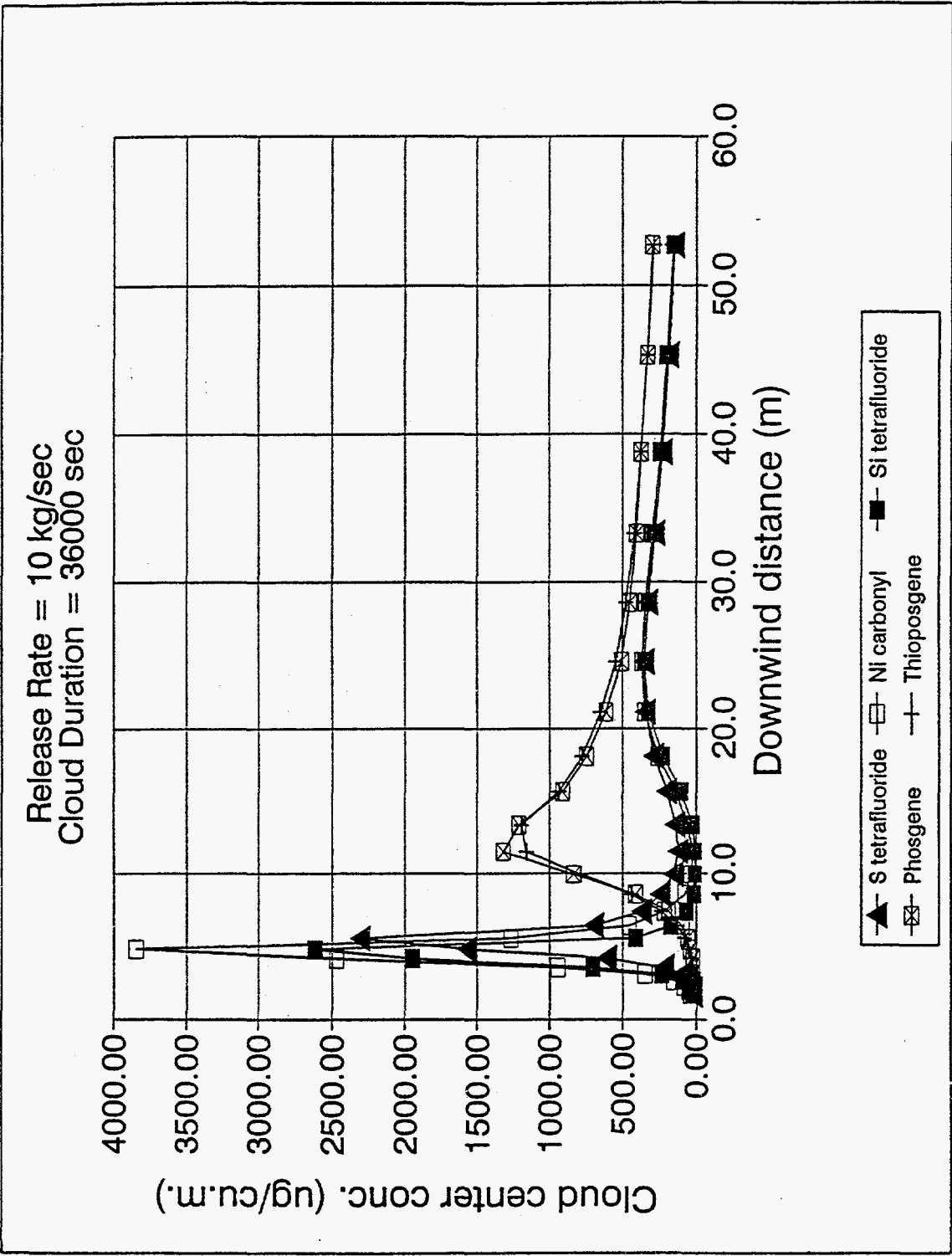


Figure 21

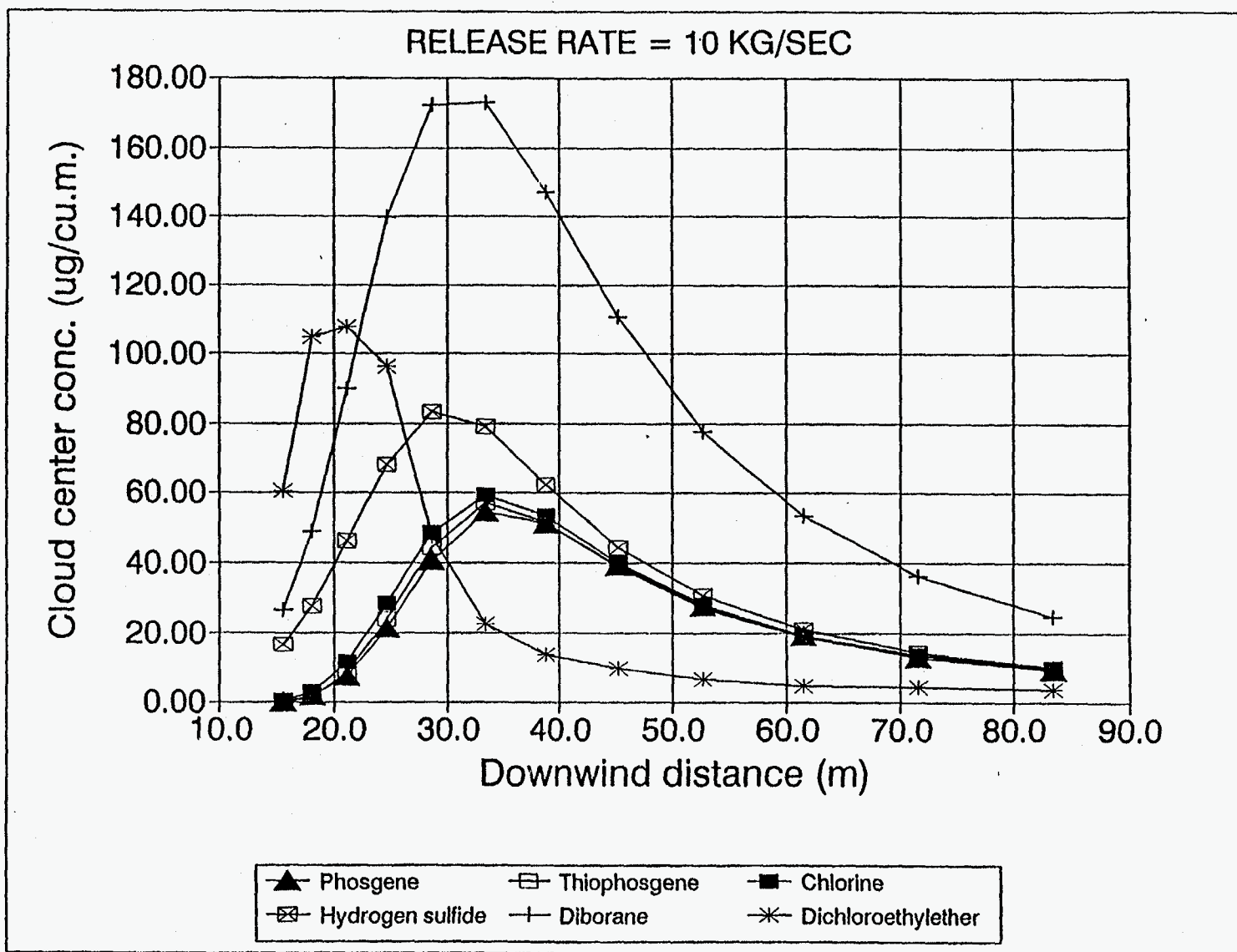


Figure 22

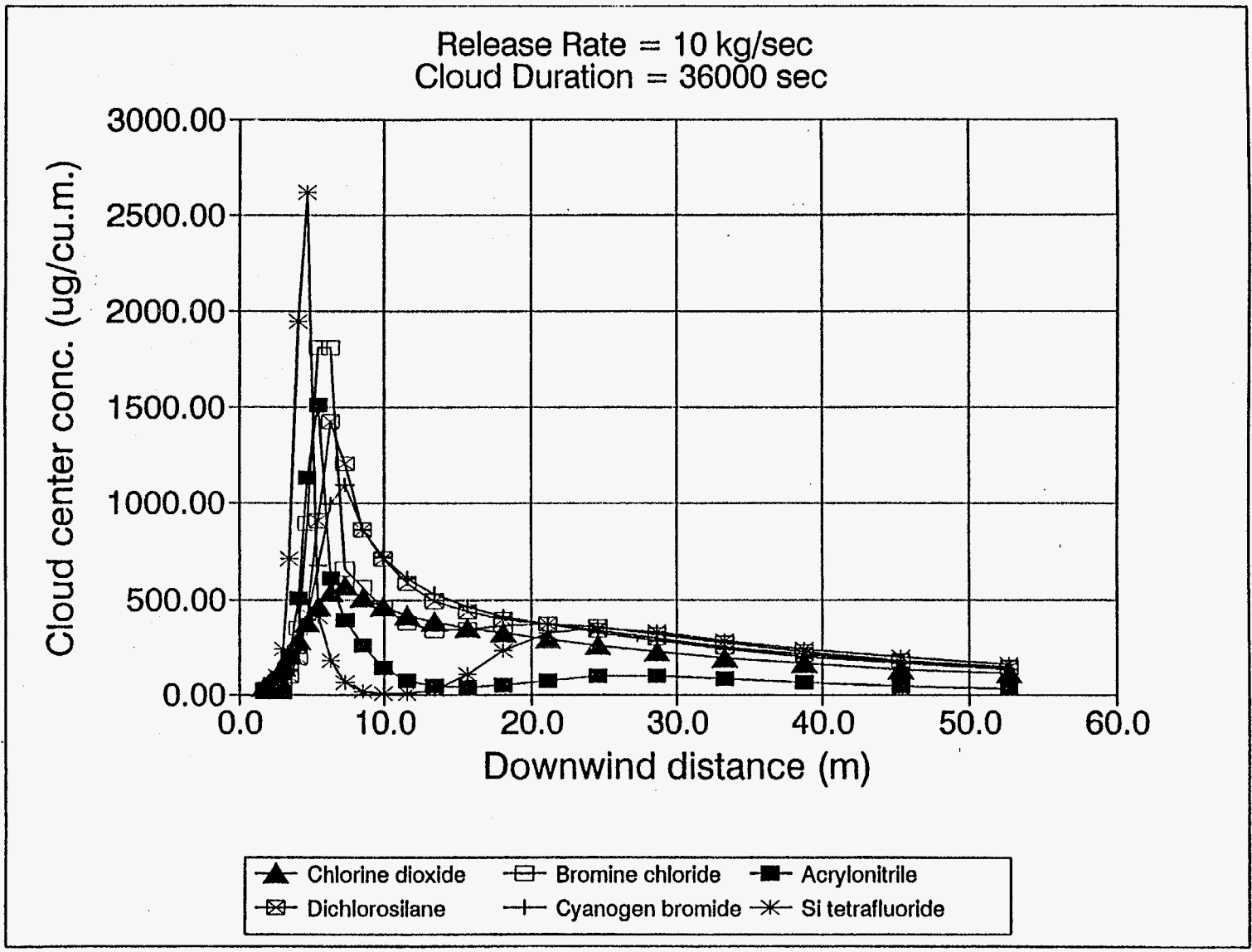


Figure 23

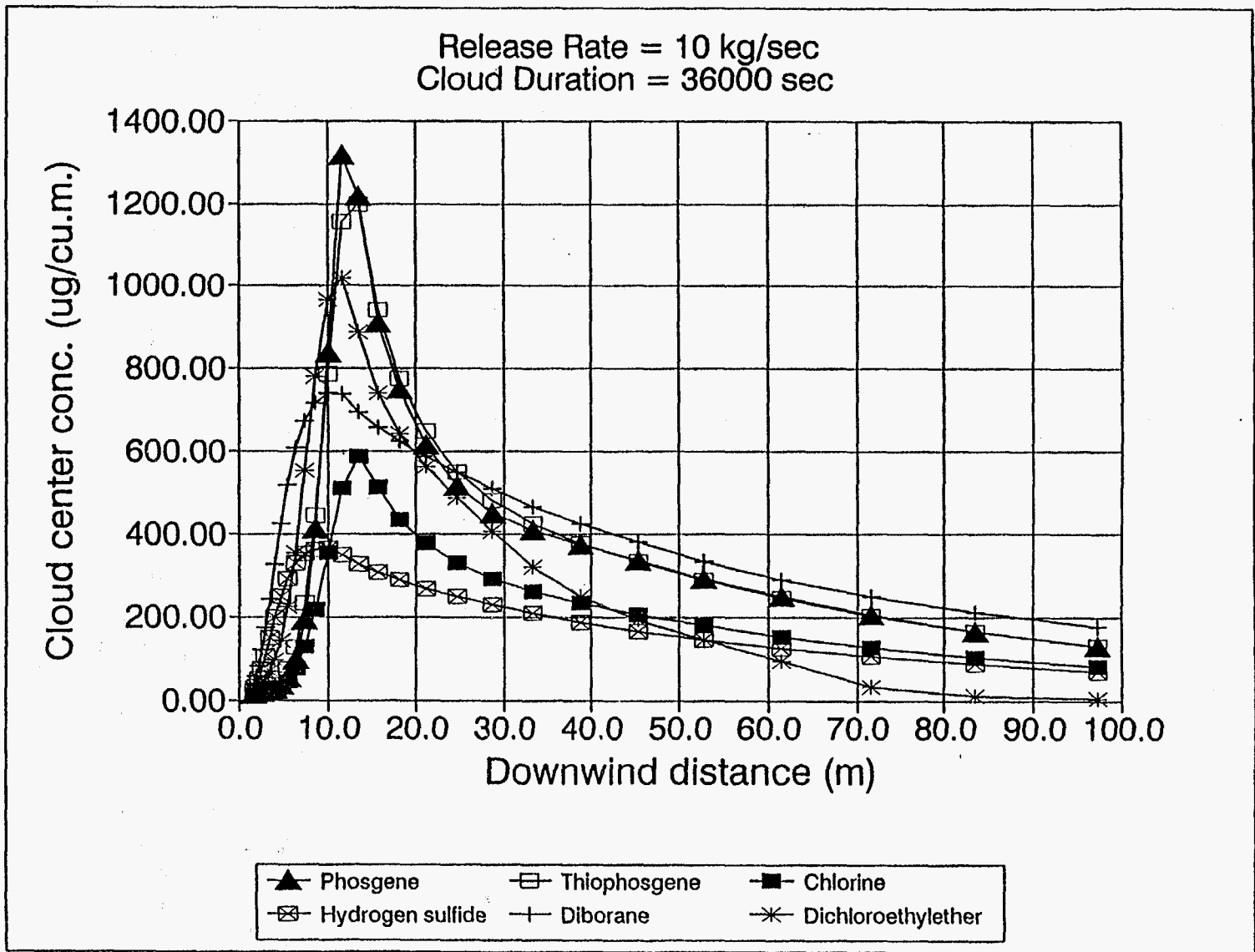


Figure 24

# LEAK RATE WHEN EPA GUIDELINE (TLV) IS MET AT 50 M DOWNWIND

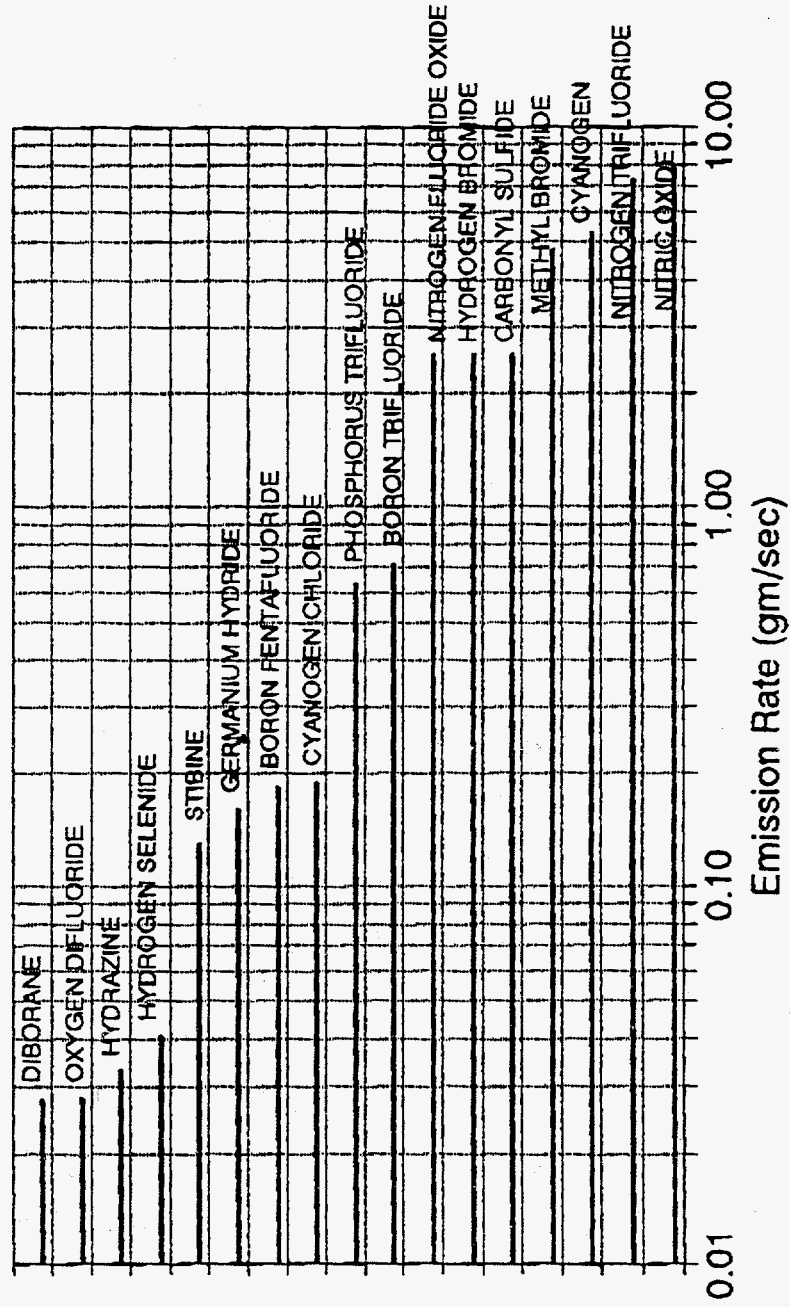


Figure 25

LEAK RATE WHEN EPA GUIDELINE (TLV)  
IS MET AT 1 KM DOWNWIND

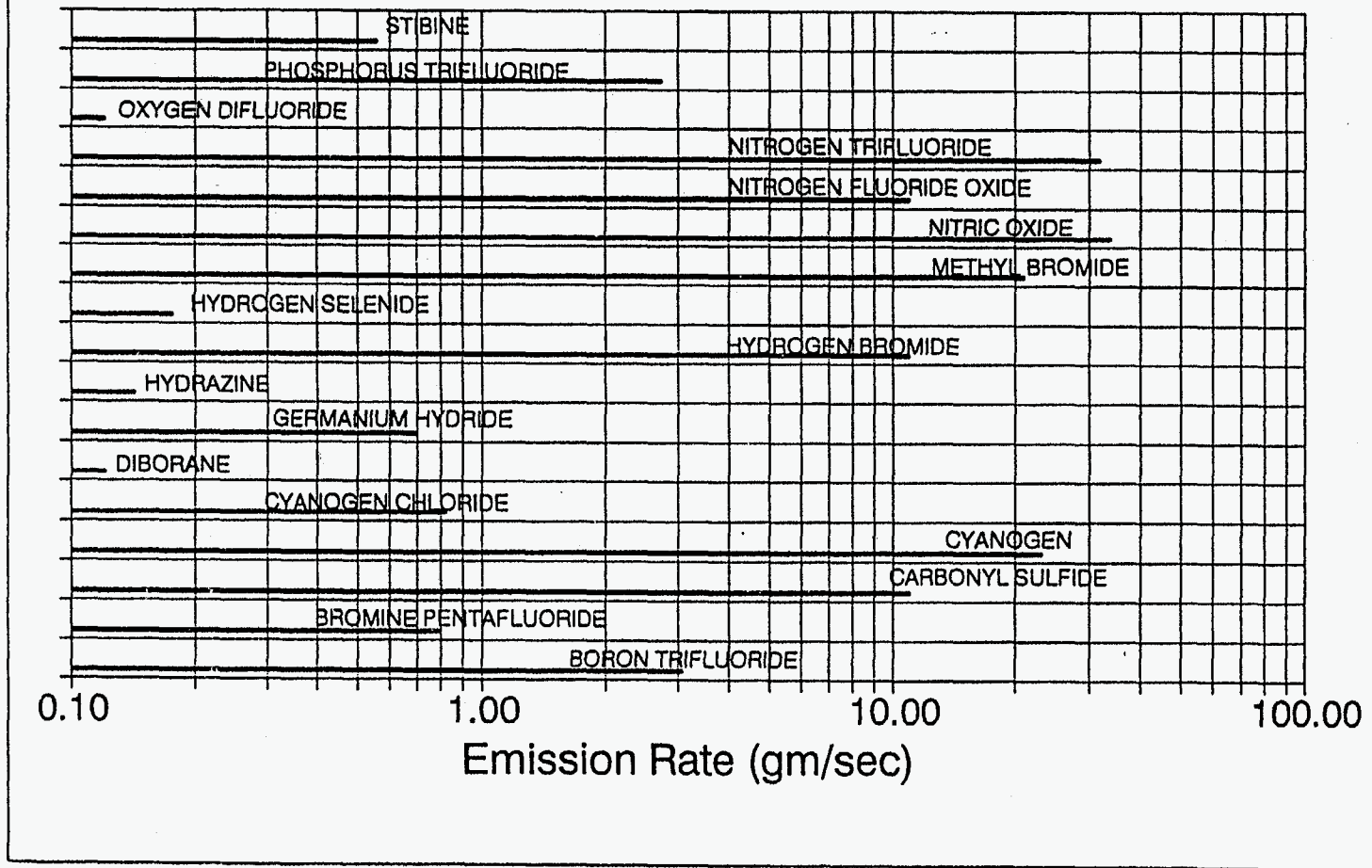


Figure 26

LEAK RATE WHEN EPA GUIDELINE (TLV)  
IS MET AT 8.33 KM (5 MILES) DOWNWIND

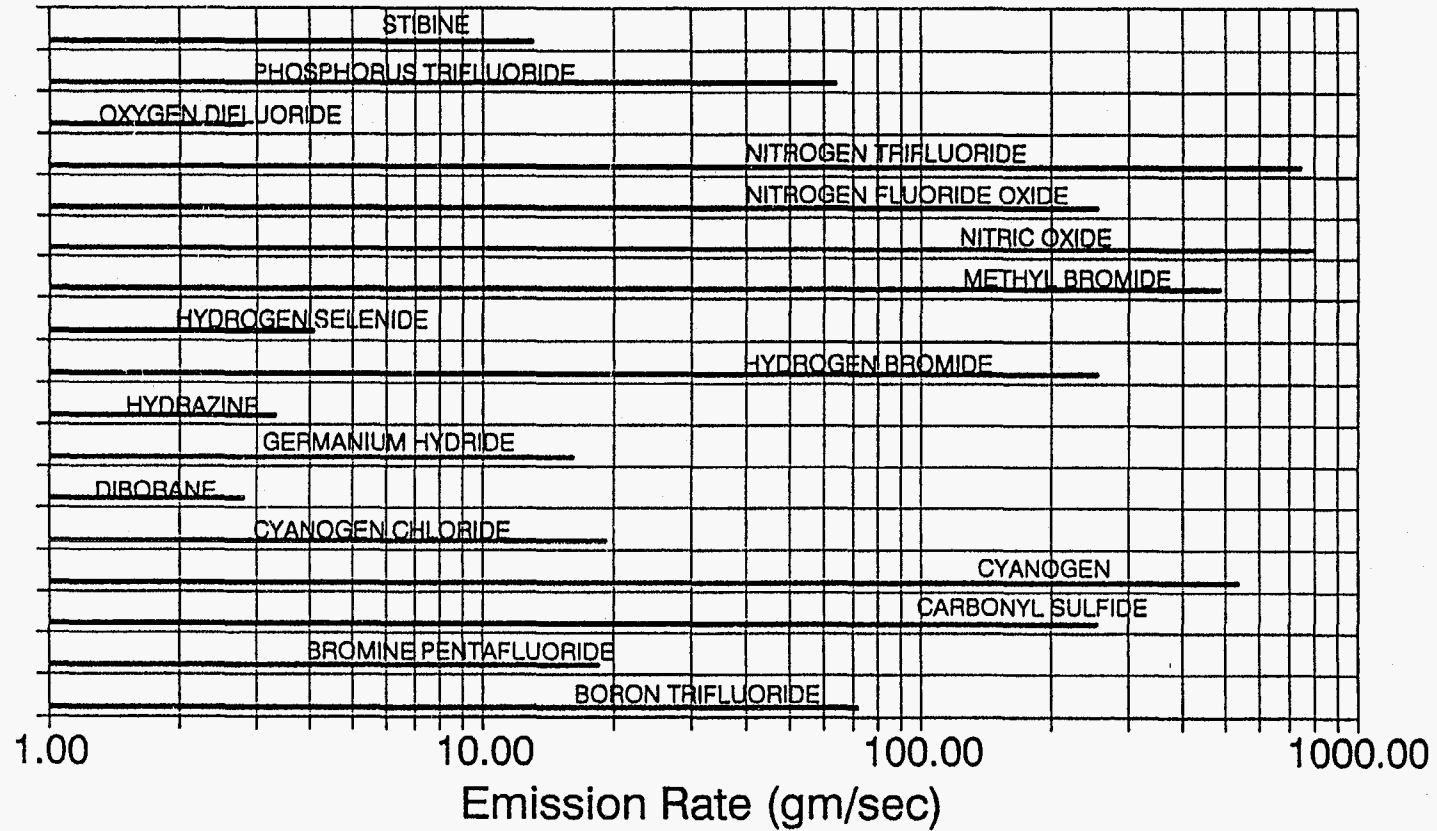


Figure 27



LEAK RATE WHEN EPA GUIDELINE  
(ERPG2, EEGL, STEL) IS MET AT 50 M.

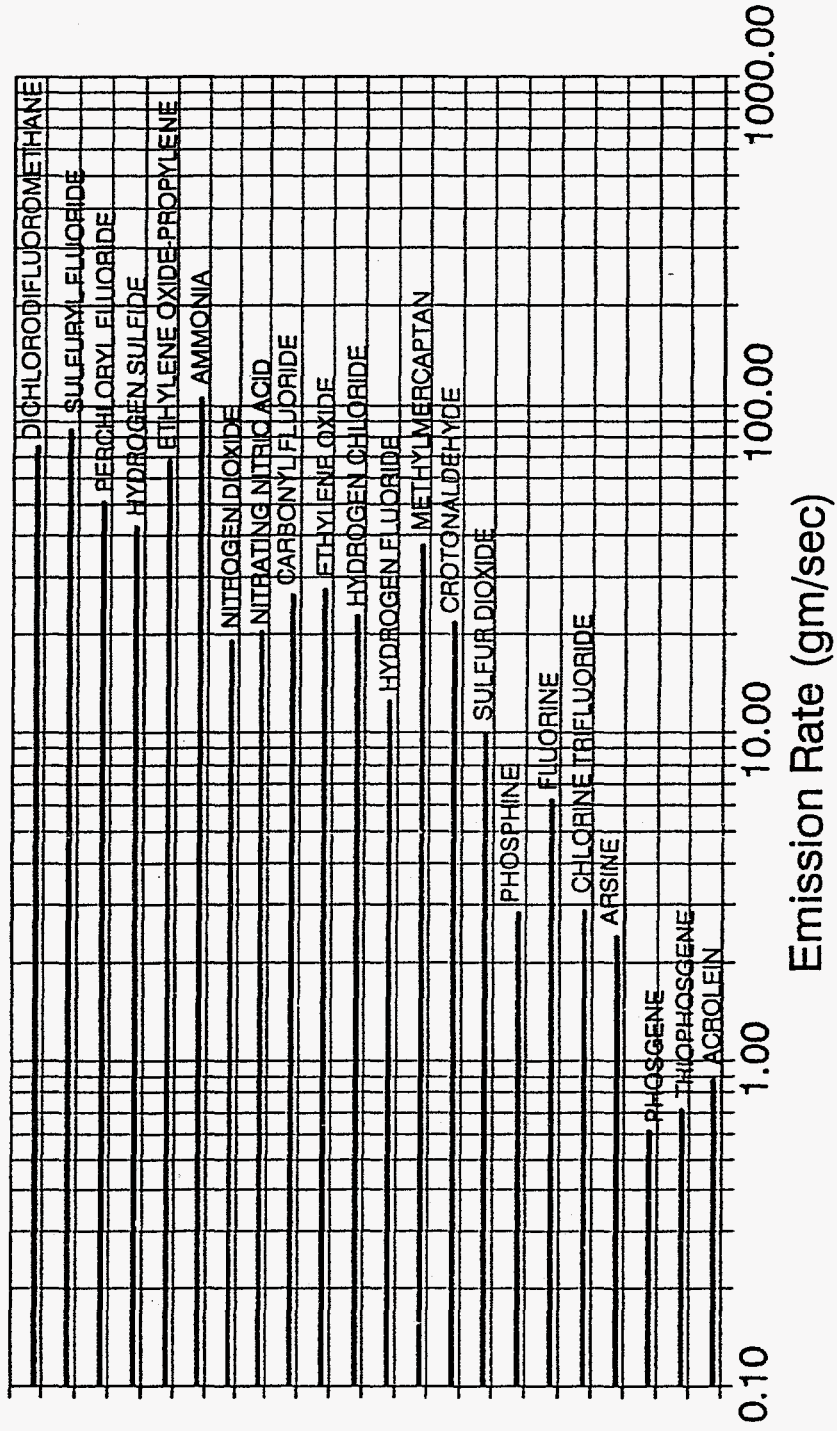


Figure 28

LEAK RATE WHEN EPA GUIDELINE  
(ERPG2, EEGL, STEL) IS MET AT 1 KM.

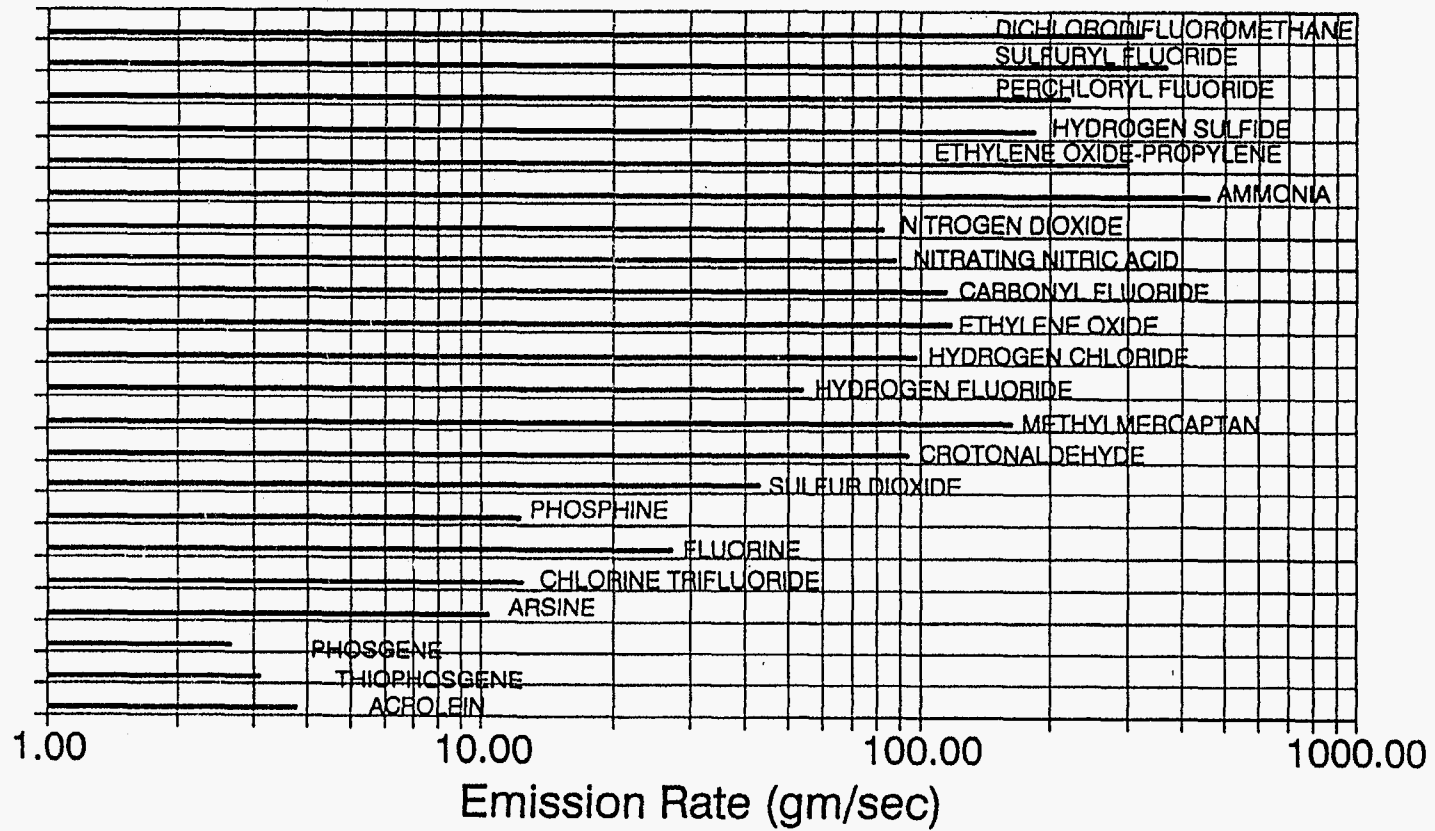


Figure 29

LEAK RATE WHEN EPA GUIDELINE  
(ERPG2, EEGL, STEL) IS MET AT 8.33 KM.

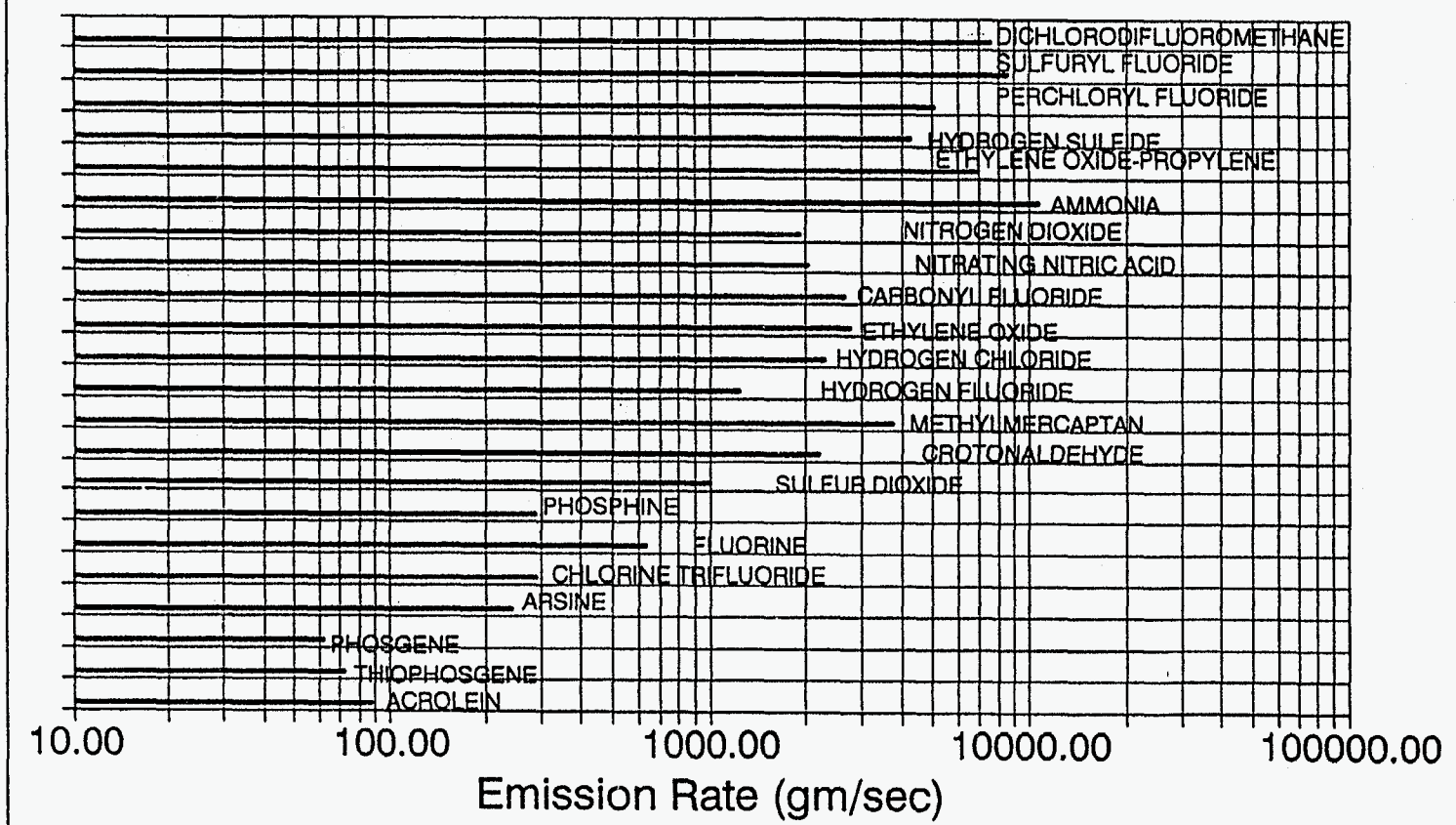


Figure 30

LEAK RATE WHEN EPA GUIDELINE IS MET  
AT 1 KM DOWNWIND - DENSE GASES

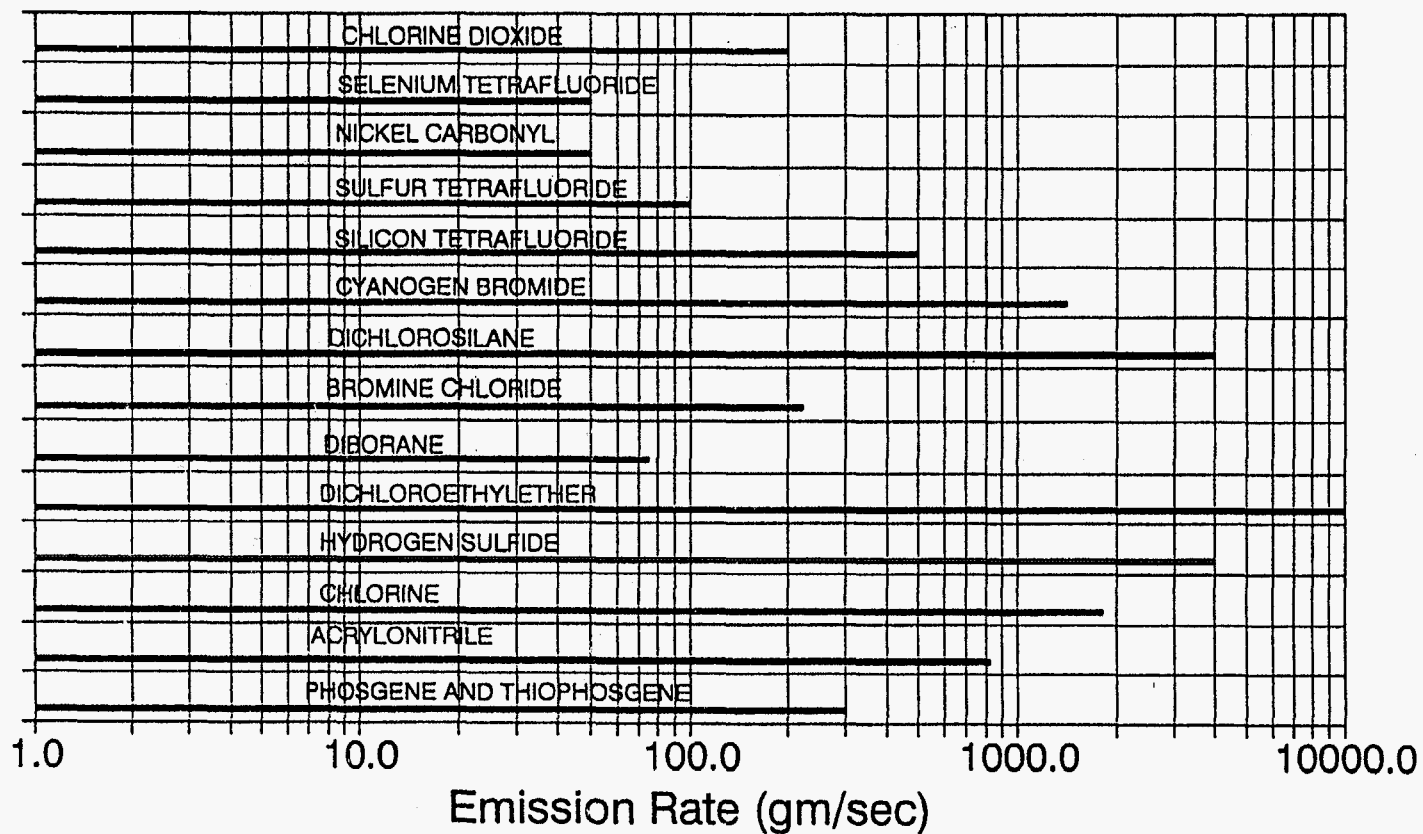


Figure 31

LEAK RATE WHEN EPA GUIDELINE IS MET  
AT 8 KM DOWNWIND - DENSE GASES

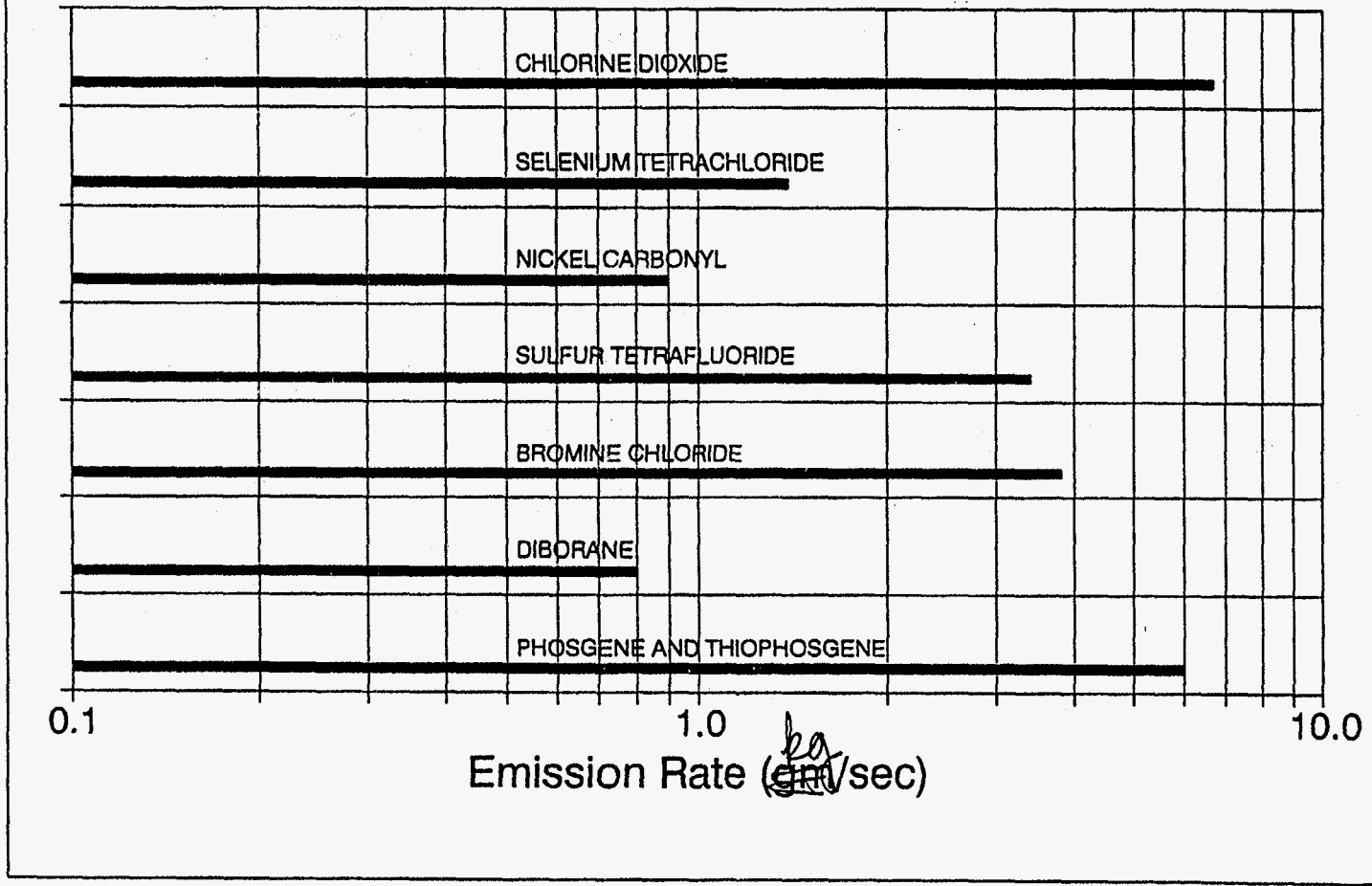


Figure 32

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