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MEXICO EMISSIONS INVENTORY PROGRAM MANUALS

VOLUME II – EMISSIONS INVENTORY FUNDAMENTALS

FINAL

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and

Binational Advisory Committee

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The *Mexico Emissions Inventory Program Manuals* were the result of efforts by several participants. The Binational Advisory Committee (BAC) guided the development of these manuals. The members of the BAC were:

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PREFACE

Air pollution can negatively impact public health when present in the atmosphere in sufficient quantities. Most rural areas rarely experience air quality problems, while elevated concentrations of air pollution are found in many urban environments. Recently, there has been an increasingly larger degree of urbanization and industrial activity throughout Mexico, resulting in air quality impairment for several regions.

Air pollution results from a complex mix of literally thousands of sources ranging from industrial smoke stacks and motor vehicles, to the individual use of grooming products, household cleaners, and paints. Even plant and animal life can play an important role in the air pollution problem. The complex nature of air pollution requires the development of detailed plans on a regional level that provide a full understanding of the emission sources and methods for reducing the health impacts associated with exposure to air pollution. Example air quality planning activities include:

- Application of air quality models;

- Examination of source attribution for emissions control where deemed necessary;

- Development of emission projections to examine possible changes in future air quality;

- Analysis of emission trends; and

- Analysis of emissions transport from one region to another.

Development of fundamentally sound emissions inventories is a key need for each of these air quality management and planning functions.
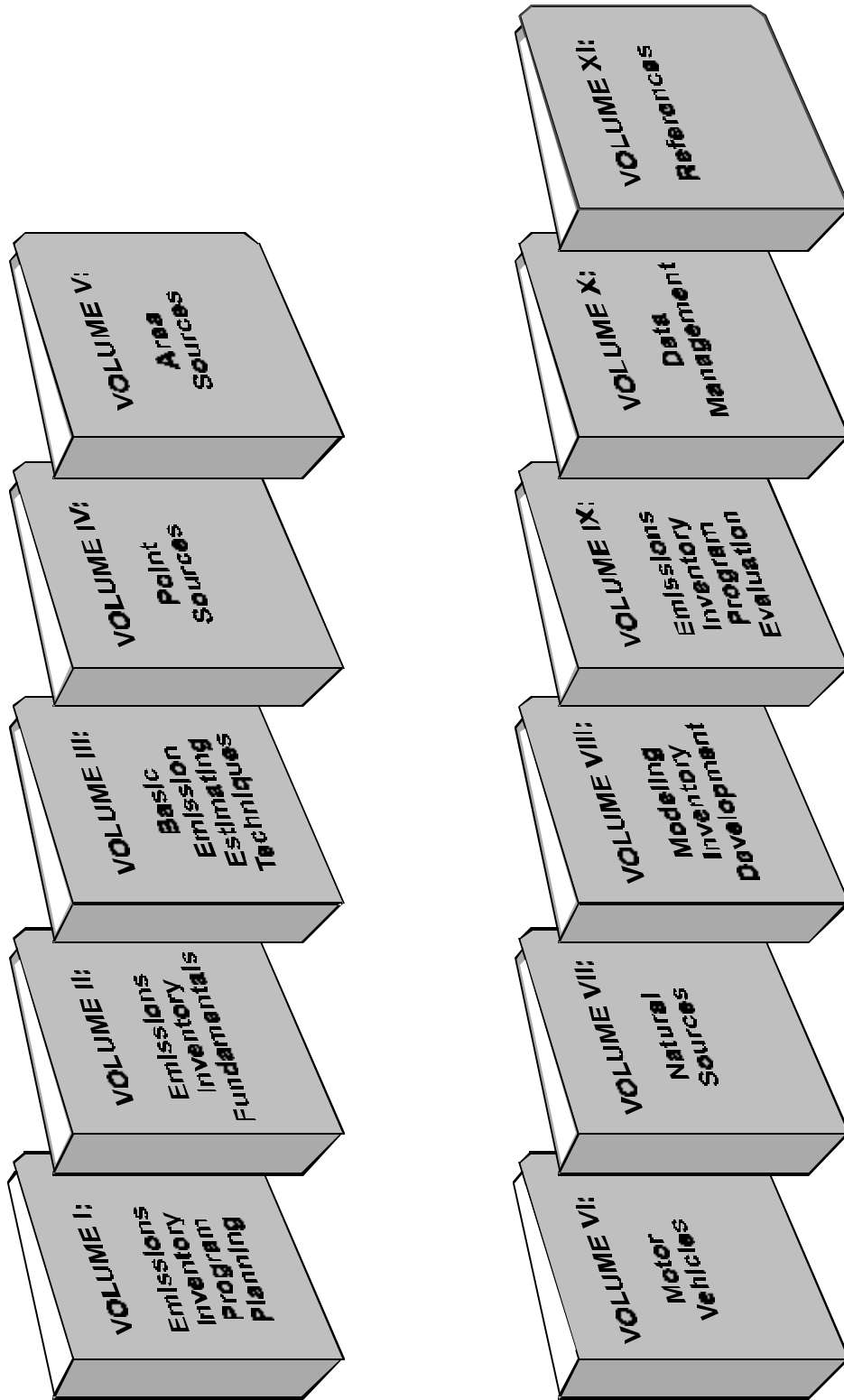
Developing emission estimates to meet air quality planning needs requires continual development and refinement; "one time" inventory efforts are not conducive to the

air quality planning process. For lasting benefit, an *inventory program* must be implemented so that accurate emission estimates can be developed for all important geographic regions, refined over time, and effectively applied in the air quality planning and monitoring process. Consequently, a set of inventory manuals will be developed that can be used throughout the country to help coordinate the development of consistent emission estimates. These manuals are intended for use by local, state, and federal agencies, as well as by industry and private consultants. The purpose of these manuals is to assist in implementing the inventory program and in maintaining that program over time so that emissions inventories can be developed in periodic cycles and continually improved.

The manuals cover inventory program elements such as estimating emissions, program planning, database management, emissions validation, and other important topics. Figure 1 shows the series of manuals that will be developed to support a complete inventory program. The main purpose of each manual or volume is summarized below.

Volume I—Emissions Inventory Program Planning. This manual addresses the important planning issues that must be considered in an air emissions inventory program. Program planning is discussed not as an "up-front" activity, but rather as an ongoing process to ensure the long-term growth and success of an emissions inventory program. *Key Topics*: program purpose, inventory end uses, regulatory requirements, coordination at federal/state/local levels, staff and data management requirements, identifying and selecting special studies.

Volume II—Emissions Inventory Fundamentals. This manual presents the basic fundamentals of emissions inventory development and discusses inventory elements that apply to multiple source types (e.g., point and area) to avoid the need for repetition in multiple volumes. *Key Topics*: applicable regulations, rule effectiveness, rule penetration, pollutant definitions (excluding nonreactive volatile), point/area source delineation, point/area source reconciliation.

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VOLUME XI:
References

VOLUME V:
Area
Sources

VOLUME X:
Data
Management

VOLUME IV:
Point
sources

VOLUME IX:
Emissions
Inventory
Program
Evaluation

VOLUME III:
Basic
Emission
Estimating
Techniques

VOLUME VIII:
Modelling
Inventory
Development

VOLUME II:
Emissions
Inventory
Fundamentals

VOLUME VII:
Natural
Sources

VOLUME I:
Emissions
Inventory
Program
Planning

VOLUME VI:
Motor
Vehicles

Figure 1. Mexico Emissions Inventory Program Manuals

Volume III—Basic Emission Estimating Techniques. This manual presents the basic methodologies used to develop emission estimates, including examples and sample calculations. Inventory tools associated with each methodology are identified and included in Volume XI (References). *Key Topics*: source sampling, emissions models, surveying, emission factors, material balance, and extrapolation.

Volume IV—Emissions Inventory Development: Point Sources. This manual provides guidance for developing the point source emissions inventory. A cross-reference table is provided for each industry/device type combination (e.g., petroleum refining/combustion devices) with one or more of the basic methodologies presented in Volume III. *Key Topics*: cross-reference table, stack parameters, control devices, design/process considerations, geographic differences and variability in Mexico, quality assurance/quality control (QA/QC), overlooked processes, data references, and data collection forms.

Volume V—Emissions Inventory Development: Area Sources (Includes Non-Road Mobile). This manual provides guidance for developing the area source emissions inventory. After the presentation of general area source information, a table is provided to cross-reference each area source category (e.g., asphalt application) with one or more of the basic methodologies presented in Volume III. Then, source category-specific information is discussed for each source category defined in the table. *Key Topics*: area source categorization and definition, cross-reference table, control factors, geographic differences and variability in Mexico, QA/QC, data references, and data collection forms (questionnaires).

Volume VI—Emissions Inventory Development: Motor Vehicles. Because motor vehicles are inherently different from point and area sources, the available estimation methods and required data are also different. To estimate emissions from these complex sources, models are the preferred estimation tool. Many of these models utilize extensive test data applicable to a given country or region. This manual focuses primarily on the data development phase of estimating motor vehicle emissions. *Key Topics*: available estimation methods, primary/secondary/tertiary data and information, source categorization, emission factor sources, geographic variability within Mexico, and

QA/QC.

Volume VII—Emissions Inventory Development: Natural Sources.
This manual provides guidance for developing a natural source emissions inventory (i.e.,
biogenic volatile organic compound [VOC] and soil nitrogen oxide [NO$_x$]). In addition, this
manual includes the theoretical aspects of emission calculations and discussion of specific
models. *Key Topics*: source categorization and definition, emission mechanisms, basic
emission algorithms, biomass determination, land use/land cover data development,
temporal and meteorological adjustments, and emission calculation approaches.

Volume VIII—Modeling Inventory Development. This manual provides
guidance for developing inventory data for use in air quality models and addresses issues
such as temporal allocation, spatial allocation, speciation, and projection of emission
estimates. *Key Topics*: definition of modeling terms, seasonal adjustment, temporal
allocation, spatial allocation, chemical speciation, and projections (growth and control
factors).

Volume IX—Emissions Inventory Program Evaluation. This manual
consists of three parts: QA/QC, uncertainty analysis, and emissions verification. The
QA/QC portion defines the overall QA/QC program and is written to complement source
specific QA/QC procedures written into other manuals. The uncertainty analysis includes
not only methods of assessing uncertainty in emission estimates, but also for assessing
uncertainty in modeling values such as speciation profiles and emission projection factors.
 The emissions verification section describes various analyses that can be performed to
examine the accuracy of the emission estimates. Examples include receptor modeling
and trajectory analysis combined with specific data analysis techniques. *Key Topics*:
description of concepts and definition of terms, inventory review protocol, completeness
review, accuracy review, consistency review, recommended uncertainty methodologies,
and applicable emission verification methodologies.

Volume X—Data Management. This manual addresses the important needs associated with the data management element of the Mexico national emissions inventory program. *Key Topics*: general-purpose data management systems and tools, specific-purpose software systems and tools, coding system, confidentiality, electronic submittal, frequency of updates, recordkeeping, Mexico-specific databases, and reports.

Volume XI—References. This manual is a compendium of tools that can be used in emissions inventory program development. Inventory tools referenced in the other manuals are included (i.e., hardcopy documents, electronic documents, and computer models).

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APPENDIX A: NON-REACTIVE HYDROCARBONS

APPENDIX B: HAZARDOUS AIR POLLUTANTS

FIGURES AND TABLES

ACRONYMS

ARB	Air Resources Board
Btu	British thermal unit
C	Celsius
CAS	Chemical Abstract Service
CATEF	California Air Toxics Emission Factor Database
Cd	cadmium
CFC	chlorofluorocarbon
CFR	Code of Federal Regulations
CH_4	methane
CO	carbon monoxide
CO_2	carbon dioxide
Cu	copper
EC	elemental carbon
EtO	ethylene oxide
F	Fahrenheit
FIRE	Factor Information Retrieval System
g	gram
H_2SO_4	sulfuric acid
HAP	hazardous air pollutant
HC	hydrocarbons
HCFC	hydrochlorofluorocarbon
HDDV	heavy duty diesel vehicle

HDGV	heavy duty gas vehicle
HFC	hydrofluorocarbon
Hg	mercury
hr	hour
kg	kilogram
km	kilometer
LDDT	light duty diesel truck
LDDV	light duty diesel vehicle
LDGT	light duty gas truck
LDGV	light duty gas vehicle
LPG	liquefied petroleum gas
MC	motorcycle
Mg	megagram (i.e., 10^6 g = 1 metric ton)
N_2	nitrogen
N_2O	nitrous oxide
NH_3	ammonia
NH_4NO_3	ammonium nitrate
$(NH_4)_2SO_4$	ammonium sulfate
NMHC	non-methane hydrocarbons
NMOC	non-methane organic compounds
NMOG	non-methane organic gases
NO	nitric oxide
NO_2	nitrogen dioxide
NO_x	nitrogen oxides

O_3	ozone
OC	organic carbon
ODS	ozone depleting substances
OH	hydroxyl radical
Pb	lead
PFC	perfluorocarbon
PM	particulate matter
$PM_{2.5}$	particulate matter of aerodynamic diameter or 2.5 microns or less
PM_{10}	particulate matter of aerodynamic diameter or 10 microns or less
POTW	publicly owned treatment works
ppm	parts per million
QA	quality assurance
QC	quality control
ROG	reactive organic gases
SO_2	sulfur dioxide
SO_3	sulfur trioxide
SO_4^{2-}	sulfate
SO_x	sulfur oxides
SP	suspended particulate
THC	total hydrocarbons
TOC	total organic compounds
TOG	total organic gases
TSP	total suspended particulate
U.S.	United States

U.S. EPA	United States Environmental Protection Agency
UTM	Universal Transverse Mercator
VMT	vehicle miles traveled
VOC	volatile organic compounds
yr	year
μm	micrometer (micron)

1.0 INTRODUCTION

This manual presents fundamental concepts that underlie the development of emissions inventories. In general, these concepts apply to every emissions inventory -- from facility-level emission estimates to large-scale regional modeling inventories. These fundamental concepts represent basic background information that should be established prior to beginning actual data collection and emissions estimation. Some concepts will be used in every type of inventory, while other concepts may only be used in certain limited types of inventories. Specific details will vary for individual inventories, as well as the total level of effort. However, these fundamental concepts should be considered in every inventory effort to ensure a successfully completed inventory.

The remainder of this manual is organized as follows:

- Section 2.0 presents the technical steps of emissions inventory development and provides a brief explanation of each step;

- Section 3.0 addresses the importance of identifying the purposes of an emissions inventory;

- Section 4.0 provides a detailed description of various inventory pollutants;

- Section 5.0 discusses the various inventory source categories;

- Section 6.0 presents other necessary inventory characteristics;

- Section 7.0 discusses the concept of emissions inventory improvement through iteration; and

- Section 8.0 contains references.

2.0   TECHNICAL STEPS OF EMISSIONS INVENTORY DEVELOPMENT

The technical steps conducted during emissions inventory development are presented in Figure 2-1. The following paragraphs briefly describe each of these steps and identify other manuals from this series that can be consulted for further information. Supplemental information can be found in U.S. Environmental Protection Agency (U.S. EPA) documents (U.S. EPA, 1991a; EIIP, 1997).

Identify purpose of emissions inventory. As the first technical step of inventory development, it is crucial to identify the purpose or end use of the emissions inventory. The overall purpose will help determine many of the other subsequent steps. If the purpose is not clearly identified, then it is possible that the completed inventory will not meet its required needs. For example, the data needs for the development of a modeling inventory are significantly different than those for other types of inventories. Consideration should also be given to future inventory uses, as well as uses on a larger geographic scale. Further discussion of this step can be found in Section 3.0 of this manual.

Define needed emissions inventory characteristics. Every emissions inventory has several characteristics that describe the fundamental nature of the inventory (e.g., pollutant types, source types, base year, etc.). Ten separate inventory characteristics are identified in Figure 2-1. Some inventories may require conducting activities for only a few of these characteristics, while others may need all of them.   Most of these characteristics will be determined by the purpose of the inventory (e.g., an ozone inventory will need to include TOG, CO, and NO_x as inventoried pollutants). Therefore, decisions are made that define each of the characteristics for an inventory.   Additional information regarding the characteristics of emissions inventories is provided in Sections 4.0, 5.0, and 6.0.

Identify purpose of emissions inventory

Define needed emissions inventory characteristics

Pollutant Types	Source Types	Base Year	Time Characteristics	Spatial Characteristics	Species Resolution	Quality Assurance (QA)	Data Management	Projections	Uncertainty Estimation

Determine emissions inventory data sources	⟷	Select emission estimating techniques and methods

Collect emissions-related data QA✓	⟷	Collect activity data QA✓

Calculate emission estimates   QA✓

Perform necessary inventory modeling   QA✓

Evaluate the reasonableness and uncertainty of emissions inventory results

Store electronic data

Document results

Determine emissions inventory data sources/Select emission estimating techniques and methods. Once the required characteristics have been established, it is necessary to determine the sources of emissions-related data and select the emission estimating techniques and methods. These two steps are usually interrelated. In some situations, data availability will determine which estimating methods are feasible. In other instances, a desired technique will indicate which types of data must be collected. Data sources are discussed in detail in Volumes IV-VII of the Manual series (*Point Source, Area Source, Motor Vehicle, and Natural Source Inventory Development*). Specific emission estimating techniques are described in Volume III of the Manual series (*Basic Emission Estimating Techniques*).

Collect emissions-related data/Collect activity data. After the data sources and estimation methodologies have been identified, it is appropriate to collect relevant data. Emissions-related data include emissions factors, source test data, and emission factor model parameters. Some emissions-related data may already exist; other data may need to be developed for use in a specific inventory. Activity data typically include information such as hours of operation, fuel consumption, and other measures of process activity for identified sources. Because both emissions-related data and activity data are needed to estimate emissions, these two steps are often performed simultaneously. Both emissions-related data and activity data are discussed in detail in Volumes IV-VII of the Manual series (*Point Source, Area Source, Motor Vehicle, and Natural Source Inventory Development*).

Calculate emission estimates. Once all necessary data have been collected, it is necessary to perform the specific emission calculations. These calculations are performed as required by the selected emission estimating technique or methodology. Typically, these emission calculations are done electronically, particularly for more complex emissions inventories. Details related to emission calculations can be found in Volumes IV-VII of the Manual series (*Point Source, Area Source, Motor Vehicle, and*

Natural Source Inventory Development). Issues related to emission calculations, such as rule effectiveness and rule penetration, are also discussed in Volume III of the Manual series (*Basic Emission Estimating Techniques*). Rule effectiveness quantifies the ability of a regulatory program to achieve the required emissions reductions, while rule penetration measures the extent to which a regulation covers emissions from all sources within a source category.

Perform necessary modeling. After the emissions have been calculated, inventory modeling is performed if necessary. The modeling may include spatial and temporal distribution, species resolution, and emissions projections. Further discussion of modeling can be found in Volume VIII of the Manual series (*Modeling Inventory Development*).

Quality assurance. Quality assurance (QA) is not included as its own box in Figure 2-1 because it is an integral element of the entire emissions inventory development process. QA should be performed throughout the emissions inventory process. In particular, it should begin with the collection of emissions-related and activity data and continue through the emission calculations and the entire modeling process. This concept is indicated with multiple "QA checkmarks" in Figure 2-1. QA is discussed in Volume IX of the Manual series (*Emissions Inventory Program Evaluation*).

Evaluate the reasonableness and uncertainty of emissions inventory results. After the inventory has been completed, it is necessary to examine the inventory and evaluate the reasonableness and uncertainty of the results. Comparisons to expectations, previous experience, and similar inventories developed previously or for other geographic regions would be valuable at this time. Also, an examination of the inventory's uncertainty will reveal its strong areas, as well as those areas that could be the focus of future improvements. These issues are discussed in Volume IX of the Manual series (*Emissions Inventory Program Evaluation*).

Store electronic data. One of the final steps of emissions inventory

development is the electronic storage of the inventory and related data. The integrity of the emissions inventory must be maintained as the basis for future inventory development. Electronic storage of data is addressed in Volume X of the Manual series (*Data Management*).

Document results. The last step of emissions inventory development is the documentation of results. In addition to the actual inventory results, the documentation should also include the methodologies, data, and assumptions that were used in the development process. In general, enough documentation should be provided to allow others to reproduce and analyze the inventory results. Inventory documentation serves as an important reference for future inventory efforts.

As can be seen by the brief descriptions given above, the Mexico Emissions Inventory Program Manuals provide comprehensive support for the technical steps associated with emissions inventory development.

3.0 PURPOSE OF AN EMISSIONS INVENTORY

As previously shown in Figure 2-1, the first technical step of emissions inventory development is the identification of the inventory purpose. Defining the inventory purpose is crucial to the success of inventory development, and it is important that it not be overlooked in the "rush" to begin the emissions inventory. The general nature as well as most of the characteristics of an emissions inventory are ultimately determined by its purpose. In many instances, an inventory will be constructed to meet two or three major purposes.

The purpose to be achieved by an emissions inventory will define the inventory's characteristics as well as subsequent steps of data collection and potential inventory modeling. For this reason, it is critical to reach agreement on all of the potential uses for the inventory. It is also important that the purpose of the inventory be identified before any substantive work is begun on the inventory. Otherwise, some of the work performed may not be of value for the inventory.

Furthermore, it is critical that the purpose of an emissions inventory be explicitly identified. This purpose is the "guiding principle" of the inventory and defines all of the appropriate steps to be performed during development of the inventory. A complete assessment of the inventory's purposes will ensure that the inventory proceeds along a development path fully consistent with its intended uses. Typically, the purposes of an inventory are described in a planning document that is prepared at the beginning of an emissions inventory effort. This planning document is sometimes termed a work plan or inventory protocol. In addition to the inventory purpose, the planning document will include a description of relevant inventory characteristics, as well as proposed technical steps. The planning document provides up-front guidance for the inventory developers and helps

ensure successful inventory development.

There are many different inventory purposes which will vary depending upon specific needs and circumstances. For example, the purpose of an inventory for a single manufacturing facility is significantly different from the purpose of a large-scale regional modeling inventory. The inventory for the manufacturing facility might be used to determine compliance with specific regulations, whereas the regional modeling inventory might be constructed to support an air quality assessment of multiple source impacts. Several common reasons for developing inventories include the following:

- To estimate air quality impacts through modeling studies;

- To determine the applicability of permit and other regulatory requirements;

- To determine source compliance with permit conditions;

- To estimate changes in source emissions for permit applications;

- To determine the technical specifications of emission control equipment;

- To track emission levels over time;

- To identify emission contributions by source category or specific source;

- To identify potential emission trading opportunities;

- To meet emission reporting requirements; and

- To satisfy regulations requiring the development of comprehensive emission inventories.

All of the reasons given above for developing emissions inventories ultimately contribute to the process of air quality management.

As shown in Figure 3-1, the identification of the inventory purpose requires the input and opinions of many people. First, the input of the end-users of the emissions

inventory is crucial. The desired end use, as well as the ease of use, often will be significant factors for consideration in the development of an emissions inventory. Moreover, because emissions inventories play a central role in air quality planning, the input of regulatory and governmental agencies responsible for air quality and related policy should be solicited. In many situations, these agencies' needs and objectives will be the key driving force behind a specific inventory. Relevant Mexico air quality regulations are discussed in Volume I of this Manual series, *Emissions Inventory Program Planning.* Finally, the input of those constructing the emissions inventory, including government, industry, and contractor staff, will be important. These individuals must clearly understand the purposes of the inventory so that their inventory results will meet each of the needs. In the end, the synthesis of all participants' ideas will define the purposes for the inventory.
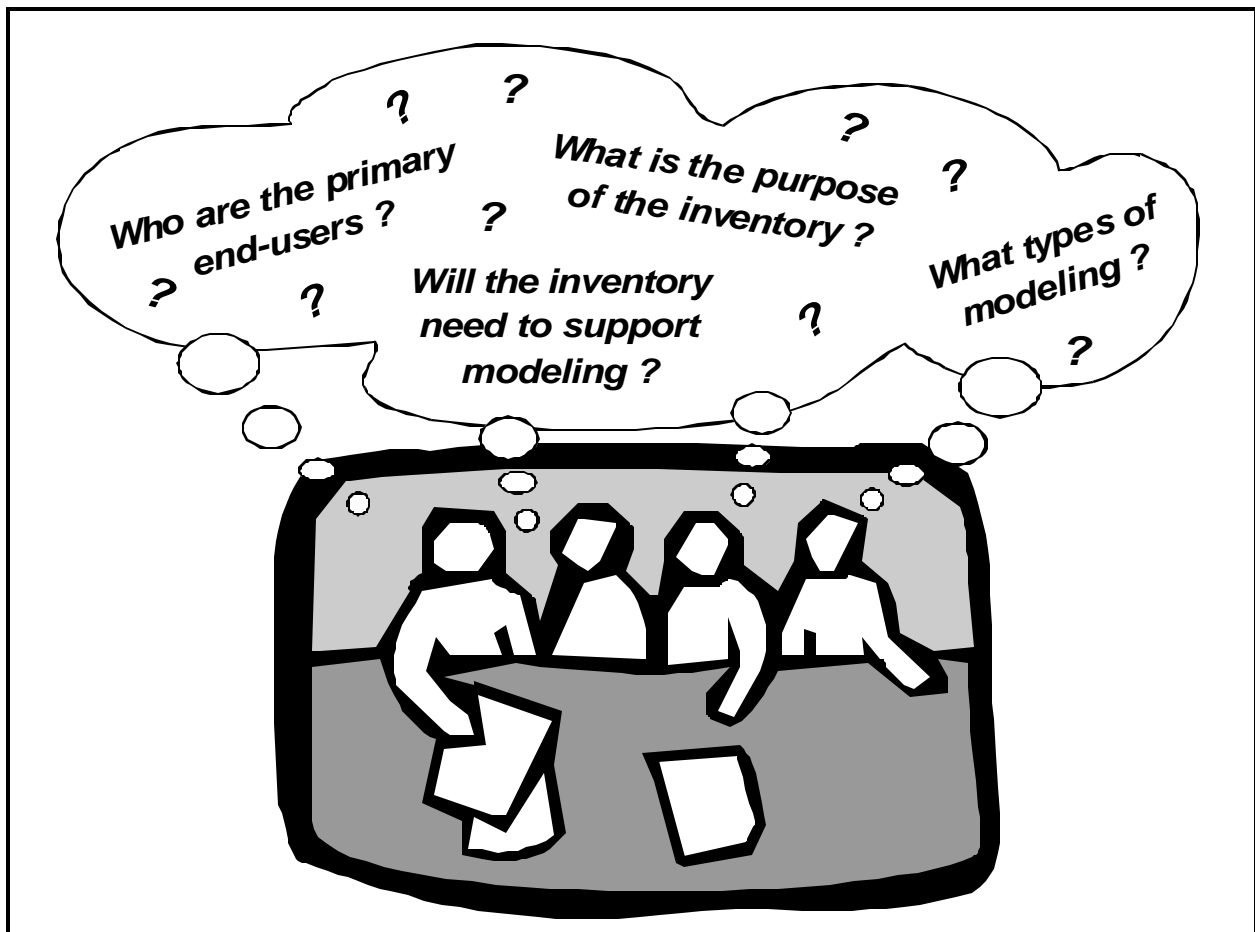
Figure 3-1. Identification of the Inventory Purpose

Further, the purpose of an emissions inventory should address present <u>and</u> future air quality needs. An attempt should be made to identify future air quality needs during the scoping of the inventory. Sometimes these future needs will be difficult to project. In other cases, however, future needs will be clearer, and a small expansion of resources might significantly increase the ultimate utility of the inventory.

The determination of the purposes of an emissions inventory need not require a significant level of effort. A reasonable amount of time and effort invested at the beginning of the process to identify uses and establish the inventory purpose will help ensure the development of useful inventory data and information. With explicit purposes identified, the resulting inventory is much more likely to satisfy each of the expected uses of the data set.

4.0   INVENTORY POLLUTANTS

In general, an air pollutant may be defined as any substance released to the atmosphere that alters the air's natural composition and may result in adverse effects to humans, animals, vegetation, or materials. The established purposes of an emissions inventory will determine which pollutants should be included in the inventory. For example, a criteria pollutant inventory would include total organic gases (TOG), carbon monoxide (CO), nitrogen oxides (NO_x), sulfur oxides (SO_x), particulate matter with an aerodynamic diameter less than 10 microns (PM_{10}), and lead (Pb). An ozone inventory, however, would focus on the precursors of ozone, namely TOG, CO, and NO_x. Finally a visibility inventory would include SO_x, NO_x, fine particulate matter (aerodynamic diameter less than 2.5 microns—$PM_{2.5}$), elemental carbon (EC), organic carbon (OC), and ammonia (NH_3) emissions.

Once it has been determined which pollutants should be included in the inventory, it is important to clearly <u>define</u> each pollutant. It is essential that each pollutant be clearly defined so that all collected data are consistent and yield accurate emission results of the desired pollutant. Though "conventional pollutant terminology" exists, it is recommended that all pollutants be clearly defined in writing at the beginning of an inventory effort, in order to reduce confusion regarding pollutants to be inventoried. Also, many pollutants are defined by their chemical names, which often may have synonyms and trade names. Trade names are often given to mixtures by manufacturers to obscure proprietary information, and the same components may have several trade names. For example Freon 11 is the commercial name for trichlorofluoromethane (CFC-11). In order to guarantee use of the proper chemical identification, the Chemical Abstract Service (CAS) number for the chemical should be consulted along with the list of synonyms. Finally, suppose it is only stated that a given inventory is to include "particulate" emissions. Then, different inventory developers might develop emission estimates of total particulate matter

(PM), particulate matter with an aerodynamic diameter less than 10 microns (PM$_{10}$), or PM$_{2.5}$. A significant amount of extra time and effort would be required to convert these different types of "particulate" emissions to the desired common basis. By explicitly defining the pollutants at the start of the inventory, this wasted effort could be avoided.

Sections 4.1—4.9 provide detailed definitions for commonly inventoried pollutants or pollutant categories.

4.1   <u>Total Organic Gases/Reactive Organic Gases</u>

Many different sources emit organic gases to the atmosphere. In general, however, organic gases are emitted from either combustion sources or evaporation sources. Collectively, the compounds that comprise hydrocarbon emissions are known as total organic gases (TOG). The concept of TOG includes all carbonaceous compounds except carbonates, metallic carbides, CO, carbon dioxide (CO$_2$), and carbonic acid. TOG are sometimes also referred to as total organic compounds (TOC), but usually only when discussed in an air quality context.

Some of the compounds in this pollutant category include aldehydes such as formaldehyde and acetaldehyde which are respiratory tract irritants as well as cancer-causing chemicals. Benzene, also a cancer-causing chemical, may be present as well. Short-term exposure to these chemicals may result in irritation of the respiratory tract. The potential for increased cases of cancer also exists for long-term exposures to some TOG species.

From an air quality perspective, it is important to note that some of the TOG emitted to the atmosphere have limited, or no, photochemical reactivity. Consequently, they do not participate in the formation of ozone. The U.S. EPA has identified the following compounds that have negligible, or no, photochemical reactivity:

- Methane;

- Ethane;

- Acetone;

- Perchloroethylene (tetrachloroethylene);

- Methylene chloride (dichloromethane);

- Methyl chloroform (1,1,1-trichloroethane);

- Various chlorofluorocarbons (CFCs);

- Various hydrochlorofluorocarbons (HCFCs);

- Various hydrofluorocarbons (HFCs); and

- Various perfluorocarbons (PFCs).

Additional information on these compounds, and a listing of a few more uncommon non-photochemically reactive compounds, can be found in the U.S. *Code of Federal Regulations* (CFR, 1997). This listing of non-reactive compounds is updated periodically as U.S. EPA designates new non-reactive compounds. The current listing is provided in Appendix A.

Chemicals considered to be photochemically reactive are termed reactive organic gases (ROG). By definition, therefore, ROG is a subset of TOG. ROG are photochemically reactive chemical gases, composed of hydrocarbons that may contribute to the formation of smog.

ROG are also sometimes referred to as volatile organic compounds (VOC). Emission factors published in U.S. EPA's AP-42 (AP-42, 1995) are presented almost exclusively for VOC. Other hydrocarbon definitions that occasionally appear in air quality and emission factor literature include: non-methane organic gases (NMOG), non-methane hydrocarbons (NMHC), total hydrocarbons (THC), and hydrocarbons (HC). Figure 4-1 graphically illustrates the relationship between these various hydrocarbon definitions. The shaded areas in Figure 4-1 indicate the compounds included in each definition. The definitions for NMOG, NMHC, THC, and HC are generally used for combustion processes only.

It is recommended that both TOG and ROG emission estimates be

developed, so that the user may have the flexibility to choose the pollutant group that is needed for a particular inventory purpose. If emission factors for other less common hydrocarbons are used, they must
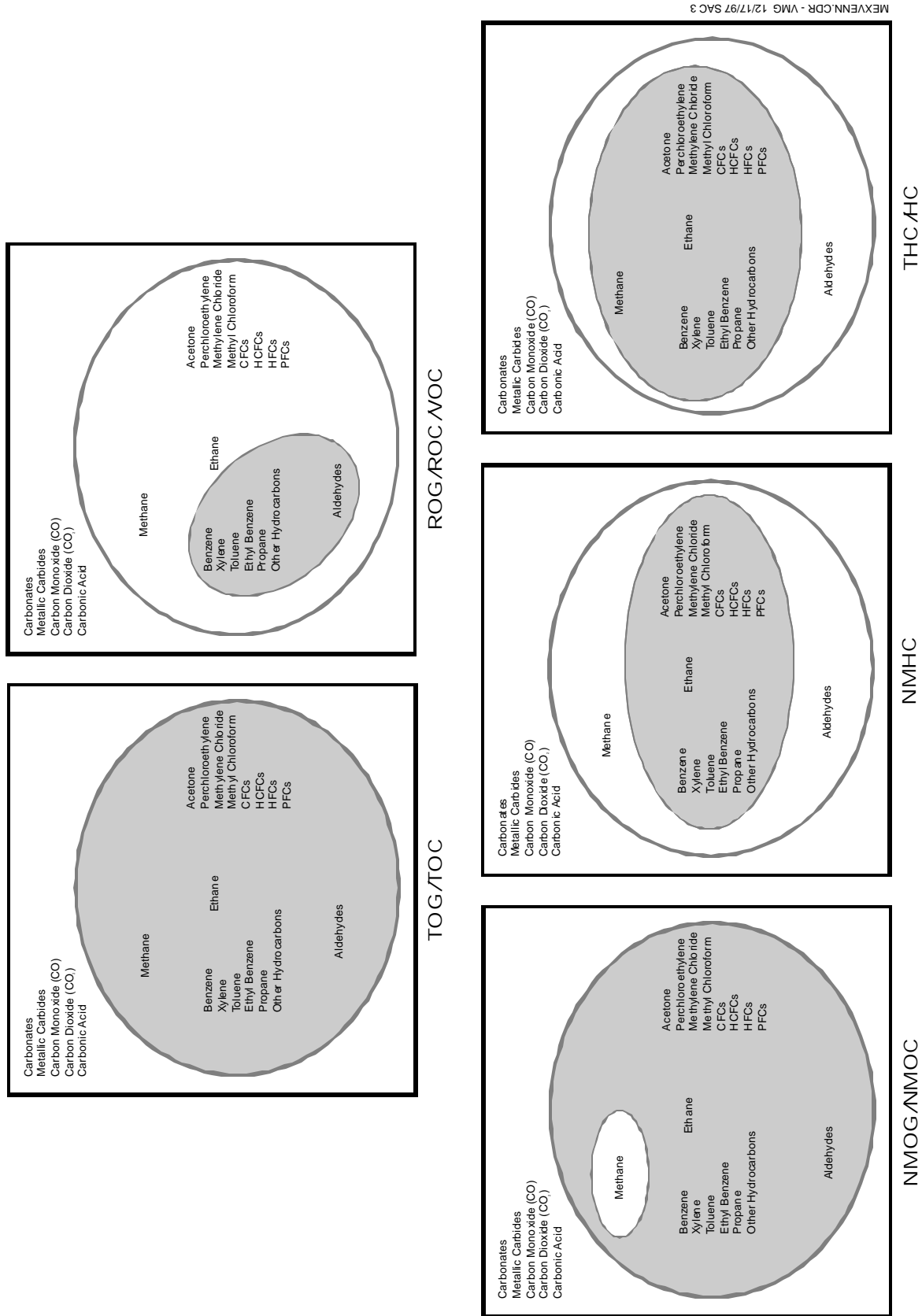
Figure 4-1. Description of Hydrocarbon Definitions

be adjusted to TOG and ROG to account for the presence/absence of methane, ethane, and aldehydes as shown in Figure 4-1. At first it may seem unnecessary to inventory TOG, but developing TOG emission estimates can facilitate a number of reporting functions for such emissions as greenhouse gases and air toxics. In addition, TOG emissions are better suited for use in three dimensional grid models used to simulate ozone and aerosol formation. This is because the models contain chemical mechanisms that use emission estimates based upon speciated TOG profiles.

4.2   Carbon Monoxide

Carbon monoxide (CO) is a colorless, odorless gas resulting from the incomplete combustion of fossil fuels. A significant amount of the CO emitted in urban areas is produced by motor vehicles. Exposure of non-smokers to CO at levels below 15 to 20 ppm does not appear to produce adverse health effects. At levels above this, the carboxyhemoglobin in the blood rises causing adverse effects on the nervous system and the cardiovascular system. Smokers have a higher carboxyhemoglobin level to begin with, so they may experience adverse effects from lower ambient levels of CO.

4.3   Nitrogen Oxides

Nitrogen oxides (NO_x) is a general term that includes nitric oxide (NO), nitrogen dioxide (NO_2), and other less common oxides of nitrogen. Nitrogen oxides are typically created during combustion processes and are ozone precursors. They are usually removed from the atmosphere by wet and dry deposition. NO is not expected to cause any adverse health effects at ambient air concentrations. Exposure to NO_2 can cause irritation of the respiratory tract and if the exposure continues, decrements in lung function can occur.

The primary NO_x combustion product is NO. However, NO_2 and other nitrogen oxides are usually emitted at the same time, and these may or may not be distinguishable in available test data. They are usually in a rapid state of flux, with NO_2 being the ultimate

oxidation product emitted or formed shortly downstream of the combustion process. The general convention followed is to report the pollutant distinctions wherever possible, but to report total NO_x on the basis of the molecular weight of NO_2.

NO_x is formed in external combustion in primarily two ways: thermal NO_x and fuel NO_x. Thermal NO_x is formed when nitrogen and oxygen in the combustion air react at high temperatures in the flame. Fuel NO_x is formed by the reaction of any nitrogen in the fuel with combustion air. Thermal NO_x is the primary source of NO_x in natural gas and light oil combustion, and the most significant factor affecting its formation is flame temperature. Excess air level and combustion air temperature also are factors in the formation of thermal NO_x. Fuel NO_x formation is dependent on the nitrogen content of the fuel and can account for as much as 50% of the NO_x emissions from the combustion of high-nitrogen fuels, primarily coal and heavy oils.

4.4   <u>Sulfur Oxides</u>

Sulfur oxides (SO_x) is a general term pertaining to compounds of sulfur dioxide (SO_2), and other oxides of sulfur. Sulfur dioxide is a strong smelling, colorless gas that is formed by the combustion of sulfur-containing fossil fuels. Sulfur oxides are respiratory irritants and can cause an asthma-like response or aggravate an existing asthma condition. Signs of exposure to high ambient concentrations can include coughing, runny nose, and shortness of breath. These responses may be more severe in smokers.

Power plants, which may use coal or fuel oil high in sulfur content, can be major sources of SO_2. Emitted SO_2 sometimes oxidizes to sulfur trioxide (SO_3) and then to sulfuric acid ($H_2 SO_4$) or sulfate (SO_4^{2-}) aerosols. The general convention is to report the pollutant distinctions wherever possible, but to report total SO_x on the basis of the molecular weight of SO_2. The quantity of SO_x emissions from combustion sources is dependent upon the sulfur content of the fuel used.

Sulfur oxides contribute to the problem of acid deposition. Acid deposition is a comprehensive term for the ways that acidic compounds deposit from the atmosphere to the earth's surface. It can include wet deposition by means of acid rain, fog, and snow; and dry deposition of acidic particles (aerosols). Acid rain refers to precipitation that has a pH of less than 5.6. Neutral precipitation would have a pH of 7; however, the "natural" activity of rainwater has been estimated to be pH 5.6 when in equilibrium with the average atmospheric concentration of CO_2 (330 ppm) (Seinfeld, 1986). Principal components of acid rain typically include nitric and sulfuric acid. These may be formed by the combination of nitrogen and sulfur oxides with water vapor in the atmosphere. In addition, sulfate particles also tend to have a small size (0.2—0.9 µm diameter). Consequently, they can be a significant component of fine particulate and adversely affect visibility.

4.5   **Particulate Matter**

Particulate matter (PM) refers to any airborne solid or liquid particles of soot, dust, aerosols, fumes, and mists. Some classifications of PM include total particulate; primary and secondary particulate; total suspended particulate (TSP), suspended particulate (SP), PM_{10} and $PM_{2.5}$; and filterable and condensable particulate.

Primary particulate matter includes solid, liquid, or gaseous material emitted directly from the process or stack that would be expected to become a particulate at ambient temperature and pressure. Secondary particulate matter is an aerosol that was formed from gaseous material through atmospheric chemical reactions. Figure 4-2 illustrates the concepts of primary and secondary particulate matter. All PM emission factor references (e.g., AP-42) contain emission factors for primary particulate matter; therefore, the term "total PM" is used to describe emissions that represent only primary particulate matter.

TSP consists of all matter emitted from sources as solid, liquid, and vapor forms, but existing or "suspended" in the air as particulate solids or liquids. TSP may include particles
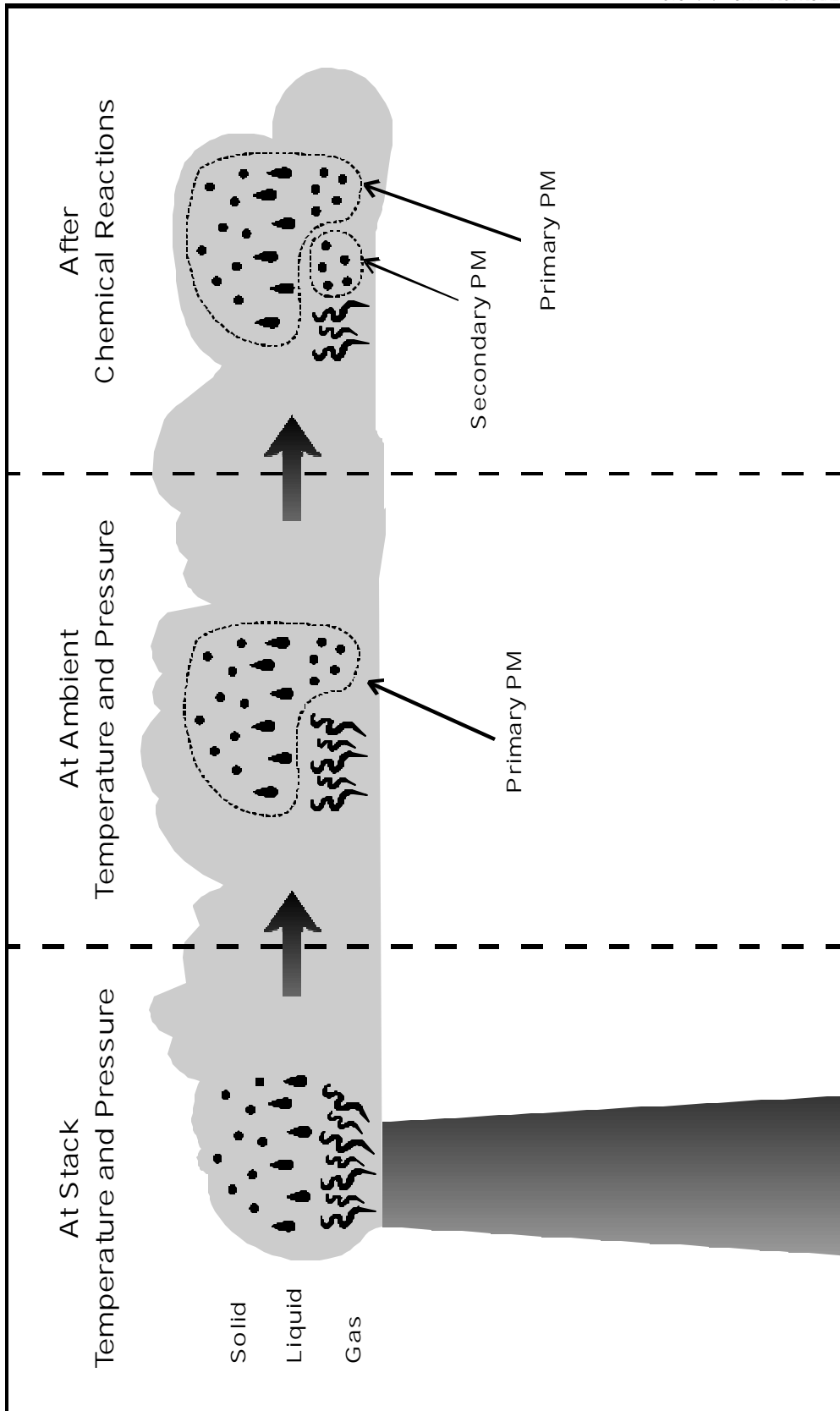
Figure 4-2. Primary and Secondary Particulate Matter

with an aerodynamic diameter up to 100 micrometers (μm); particles larger that 100 μm tend to settle out rapidly and should not be considered air emissions. Particles between 30 and 100 μm in diameter also typically undergo impeded setting. SP is usually defined as all particles with diameter less than 30 μm and is often used as a surrogate for TSP. PM_{10} describes primary particulate matter emissions smaller than 10 μm in aerodynamic diameter. Similarly, $PM_{2.5}$ is primary particulate matter smaller than 2.5 μm in aerodynamic diameter. TSP, PM_{10}, and $PM_{2.5}$ are demonstrated in Figure 4-3. The small size of PM_{10} or $PM_{2.5}$ particles allows them to easily enter the air sacs deep in human lungs where they may be deposited and result in adverse health effects. PM may cause coughing, wheezing, and respiratory function changes as well as changes in the lung itself. Increased levels of PM are believed to be responsible for increased mortality and morbidity in those with preexisting cardiovascular and/or respiratory conditions. However, it has been difficult to establish levels at which adverse effects occur because of other chemicals present which may be responsible for some of the adverse effects seen. In addition, $PM_{2.5}$ emissions are also a visibility concern.

In AP-42, total particulate emission factors may be split into filterable and condensable particulate emission factors. The filterable portions include material that is smaller than the stated size and is collected on the filter of the particulate sampling train. Unless noted, it is reasonable to assume that the emission factors in AP-42 for processes that operate above ambient temperatures are for filterable particulate, as defined by U.S. EPA Method 5 or its equivalent (a filter temperature of 121°C [250°F]). The condensable portions of the particulate matter consist of vaporous matter at the filter temperature that is collected in the sampling train impingers and is analyzed by U.S. EPA Method 202 or its equivalent. Total particulate emission factors are the sum of filterable and condensable particulate emission factors.

4.6   <u>Ozone</u>

Ozone (O_3) is a strong smelling, pale blue, reactive toxic chemical gas consisting of three oxygen atoms. It is the most abundant photochemical oxidant. Ozone

and other

TSP = ●•• (Includes all particulate matter ≤100 μm)

PM₁₀ = •• (Includes all particulate matter ≤10 μm)

PM₂.₅ = • (Includes all particulate matter ≤2.5 μm)

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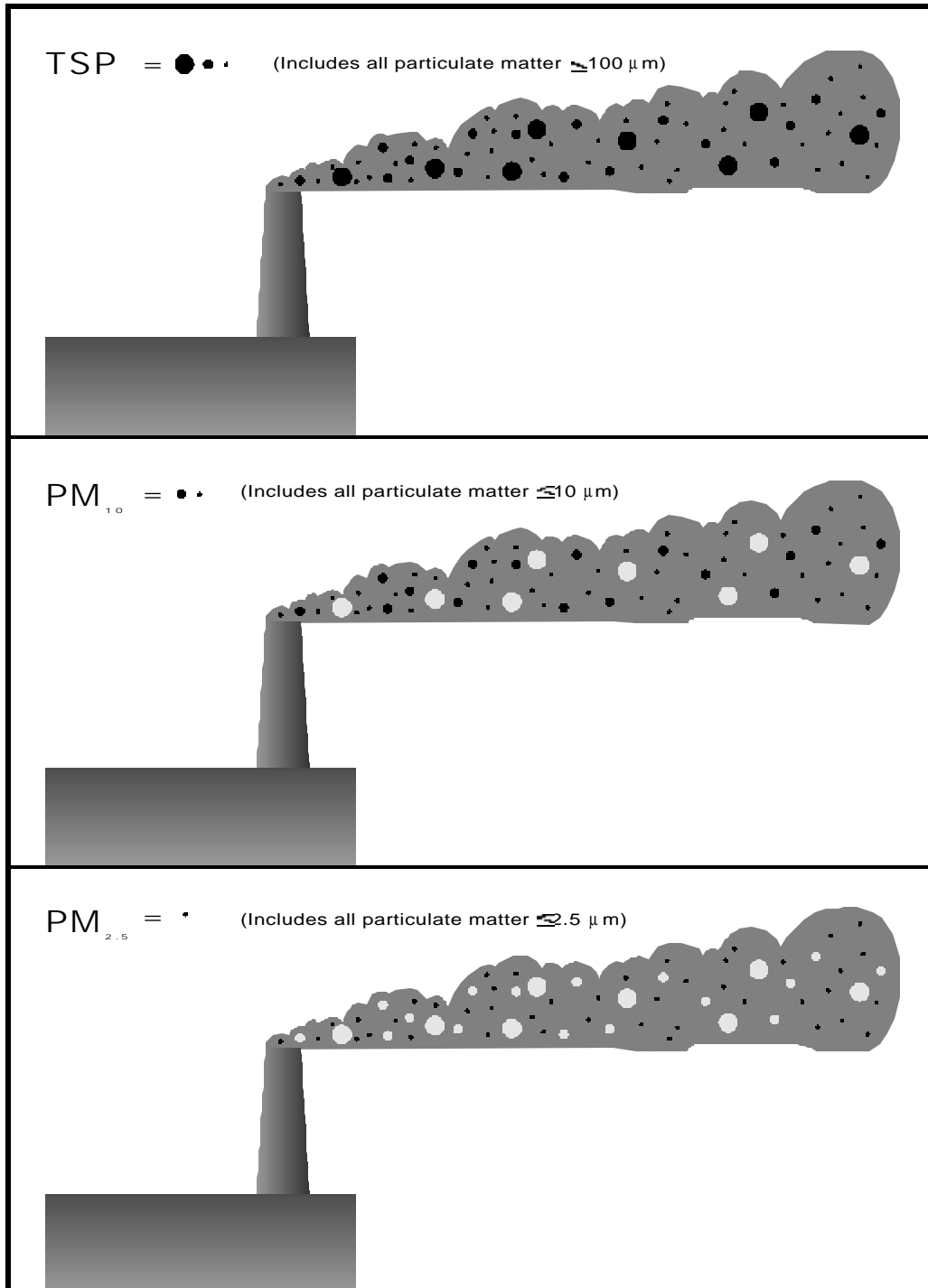
Figure 4-3. TSP, PM₁₀, and PM₂.₅

photochemical oxidants are not directly emitted to the atmosphere; instead, they are formed by the chemical reactions of hydrocarbons, CO, and NO_x in the presence of sunlight. Therefore, ozone is not estimated in emissions inventories. Its precursors, however, are estimated.

The general chemical equations describing ozone formation are presented below:

$$HO + RH \rightarrow H_2O + R \quad \text{(R = alkyl group)}$$
$$R + O_2 \rightarrow RO_2$$
$$RO_2 + NO \rightarrow RO + NO_2$$
$$NO_2 + h\nu \rightarrow NO + O \quad (h\nu = \text{ultraviolet photon})$$
$$O + O_2 + M \rightarrow O_3 + M \quad \text{(M = third-body molecule)}$$
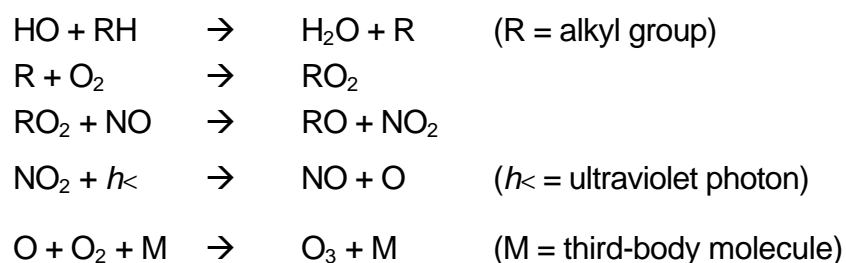
Ozone and other photochemical oxidants are irritants that can have adverse effects on the lung. Exposure to high ambient levels can cause decrements in lung function. Shallow, rapid breathing; bronchitis; and emphysema are among the adverse health effects that may occur as a result of exposure to ozone. In addition, ozone is very effective in deteriorating rubber and other materials.

4.7 <u>Visibility Species</u>

Visibility degradation is caused by fine particles that absorb or scatter light in a direction different from that of the incident light. Some of these particles (primary particles) are emitted directly to the atmosphere; others (secondary particles) are formed in the atmosphere from gaseous precursors.

The extinction coefficient, the fraction of light that is attenuated by scattering or absorption as the light beam traverses a unit of atmosphere, is used in visibility measurements. The extinction coefficient indicates the rate at which energy is lost or redirected due to interactions with gases and suspended particles in the atmosphere. Particles with higher extinction coefficients will cause more visibility degradation.

The magnitude of these visibility degradation effects depends on several factors such as the size and composition of the particles and the wavelength of the incident light. Therefore, not all species have the same impact on visibility. The major sources of visibility impairment are organic carbon (OC), elemental carbon (EC) or soot, sulfates, and nitrates. Organic carbon and elemental carbon are significant sources of visibility degradation because they both scatter <u>and</u> absorb light. OC and EC are emitted as primary particles. All of the other visibility species mainly scatter light and are typically secondary particles formed from gaseous precursors. Sulfates and nitrates are primarily the results of various chemical reactions on SO_x and NO_x emissions. Ozone precursors may be also important because secondary aerosol is one of the end products from the photochemical smog cycle. Finally, ammonia (NH_3) is frequently considered as a visibility species because of its interaction with SO_x and NO_x to form ammonium sulfate, $(NH_4)_2 SO_4$, and ammonium nitrate, NH_4NO_3.

Particles and their precursors can remain in the atmosphere for several days and can be carried great dstances downwind from their sources to affect visibility in remote areas. The emissions from many sources may mix together during transport to form a uniform widespread haze commonly known as regional haze. Changes in meteorological conditions, sunlight, and the size and proximity of emission sources are a few of the factors that will vary the degree of visibility impairment over time and from place to place.

4.8   <u>Air Toxics/Hazardous Air Pollutants</u>

Air toxics is a general term used to refer to a harmful chemical or group of chemicals in the air. They are sometimes called hazardous air pollutants (HAPs). They are considered air toxics because they either have shorter term (acute) effects or long term (chronic) effects. This pollutant category encompasses many chemicals with varying effects and concentrations at which those effects might occur. They range from cancer-causing chemicals such as 1,3-butadiene and vinyl chloride, to chemical solvents such as toluene and ethylbenzene which, at the concentrations found in ambient air, are likely to be limited

to irritant effects.

Air toxics can exist in gaseous or particulate form. A few examples of common gaseous air toxics are benzene, toluene, xylene, and ethylbenzene. There are also a limited number of gaseous hazardous or toxic compounds that may not be TOG such as ammonia and chlorine. Many of the particulate air toxics are heavy metals such as lead, chromium, and cadmium. Appendix B contains a listing of the 189 U.S. Federal Hazardous Air Pollutants. This listing is not an exhaustive list of air toxics; in some inventory applications, other chemicals may need to be considered as HAPs.

Air toxics emissions should ideally be estimated using source test data or emission factors. Two possible sources of emission factors are U.S. EPA's Factor Information Retrieval System (FIRE) (U.S. EPA, 1995) and California Air Resources Board's (ARB) California Air Toxics Emission Factor Database (CATEF) (ARB, 1996). Additional engineering judgment is required to determine whether a particular emission factor is applicable for a given source. When air toxic emission factors are not available, then it is necessary to combine the total TOG or PM emission estimates with speciation profiles to estimate emissions of individual air toxics. However, because speciation profiles were not developed with the intent of estimating individual air toxics emissions, this approach is not generally recommended.

4.9 <u>Greenhouse Gases</u>

The greenhouse effect is the trapping of incoming solar radiation by a combination of radiatively active gases (i.e., greenhouse gases). Light energy from the sun (short wavelength radiation) that passes through the earth's atmosphere is absorbed by the earth's surface and re-radiated into the atmosphere as heat energy (long wavelength radiation). The heat energy is then trapped by the atmosphere, creating a situation similar to what occurs in a greenhouse or a car with its windows rolled up. Many scientists believe that the emission of greenhouse gases (carbon dioxide [CO_2], methane [CH_4], nitrous

oxide [N_2O], chlorofluorocarbons [CFCs] and others) into the atmosphere may increase the greenhouse effect and contribute to global warming. Each of these greenhouse gases is described below.

Carbon dioxide (CO_2) is a colorless, odorless gas that occurs naturally in the earth's atmosphere. Significant quantities are also emitted into the air by fossil fuel combustion. The second most important source of global CO_2 emissions is from land use change and forests. Forests and other vegetation absorb CO_2 while growing. Therefore, loss of forest area (i.e., deforestation) leads to a reduction of CO_2 incorporation in future years or, in other words, a net increase of atmospheric CO_2. Cultivation or the burning and/or clearing of land for agricultural purposes can also result in an increase in the natural release or storage of CO_2 from soils (IPCC, 1993).

Methane (CH_4) is the most abundant and stable hydrocarbon gas in the atmosphere. The latest estimate of the atmospheric lifetime of methane is 11 years (IPCC, 1993). Chemical reactions involving methane in the troposphere can lead to ozone production, and reaction with the hydroxyl radical (OH) in the stratosphere results in the production of water vapor. This is important, because both ozone and water vapor are greenhouse gases, as is the final oxidation product of methane, carbon dioxide. Some important anthropogenic sources of methane emissions are coal mining operations, natural gas production, rice paddies, livestock, and biomass burning. Methane is also formed by decomposition of organic material by bacteria under anaerobic conditions (e.g., animal waste, domestic sewage treatment, and landfills).

Nitrous oxide (N_2O) is an important greenhouse gas with an atmospheric lifetime of about 110—168 years (WMO, 1992). After release it is practically inert and seldom involved in any chemical reactions in the troposphere. Nitrous oxide is also the primary source of NO_x in the stratosphere which is contributing to the depletion of stratospheric ozone. Over 20 percent of the total global N_2O emissions and 50 percent of the total N_2 emissions may be due to natural terrestrial emissions (IPCC, 1993). The most important anthropogenic source of N_2O is the increased use of nitrogen fertilizers. Nitrous oxide is produced naturally in soils by denitrification (i.e., the reduction of nitrite or nitrate to

gaseous nitrogen as N_2 or as a nitrogen oxide) and nitrification (i.e., the oxidation of ammonia to nitrate). Commercial nitrogen fertilizers provide an additional nitrogen source, thereby increasing the emissions of nitrous oxide from the soil. Other potentially significant sources of N_2O include fossil fuel combustion, biomass burning, and adipic acid production for the nylon industry. Recently, the importance of

mobile combustion as a source of N_2O emissions has been increasing due to the use of three-way catalysts to reduce NO_x emissions (De Soete, 1989).

Chlorofluorocarbons (CFCs) are any of a number of manmade substances consisting of chlorine, fluorine, and carbon. Some examples include dichlorodifluoromethane (CFC-12) and trichlorotrifluoroethane (CFC-113). CFCs are extremely stable due to full halogenation. They are also non-flammable and generally non-toxic at low doses. However, they have been identified as greenhouse gases, as well as ozone depleting substances (ODS). Because of the potential of ozone depletion, virtually all worldwide production of CFCs has ceased as set forth in the Montreal Protocol. CFCs have appropriate boiling points to make them excellent refrigerants. Their low surface tension and low viscosity make them ideal cleaning solvents. They also exhibit high evaporation rates and leave no residue. They are also used as inert carriers in ethylene oxide (EtO) sterilizers.

5.0 SOURCE CATEGORIES

Air pollution results from a complex mix of literally thousands of sources, ranging from industrial smoke stacks and motor vehicles to the individual use of household cleaners and paints. Even plant and animal life can play an important role in the air pollution problem. For emissions inventory purposes, emission sources are typically grouped into four different source types:

- Point sources;

- Area sources;

- Motor vehicle sources; and

- Natural sources.

This section provides a general description of these different types of emission sources, explains the concept of point/area source reconciliation, and presents a checklist of source categories that should be included (or at least considered) in every emissions inventory.

5.1 Point Sources

Volume IV of this Manual series, *Point Source Inventory Development,* presents detailed information about point sources. However, before beginning to develop a point source inventory, two important decisions must be made. First, a "point source" must be clearly defined (i.e., a point/area source delineation must be established). Second, the desired level of detail must be determined.

5.1.1 Point/Area Source Delineation

The division of emissions sources into "point" and "area" sources is arbitrary but necessary to allow for the efficient collection of information needed to support air quality programs. This division has important implications for both the development of regulatory programs and the amount and type of information needed to support those programs.

Detailed information on every "point" at which emissions are discharged to the atmosphere is desirable. While this would allow a detailed understanding of the characteristics of each such emission source, there is no practical way that such information can be collected. Treating all facilities as point sources may increase the accuracy of the inventory, but will require substantially more resources to compile and maintain the point source inventory. An alternative approach is to collect information on a simpler basis by aggregating related sources (e.g., all automobiles, all bakeries) into a single "area source."

In Mexico, point sources are defined in Article 6 of the *General Law for the Ecological Equilibrium and Environmental Protection on Air Pollution Control and Prevention* as any facility that is established in one place only, with the purpose of developing industrial or commercial processes, service works, or activities that generate or can generate air pollutant emissions (Fuente fija. Es toda instalación establecida en un solo lugar, que tenga como finalidad desarrollar operaciones o procesos industriales, comerciales, de servicios o actividades que generen o puedan generar emisiones contaminantes a la atmósfera).

As indicated in Article 111Bis of *the General Law for the Ecological Equilibrium and Environmental Protection* and Article 11 of the *Regulation of the General Law for the Ecological Equilibrium and Environmental Protection on Air Pollution Control and Prevention*, point sources under Federal jurisdiction include:

- The following industrial sectors: chemical, petroleum and petrochemical, paint and ink, automobile, cellulose and paper, iron and steel, glass, electricity generation, asbestos, cement and lime, and hazardous waste treatment;

- All facilities, projects, or activities (industrial, commercial, or service) conducted by Federal Public Administration entities;

- Facilities located in the Federal District adjoining zone; and

- Sources affecting the ecological equilibrium in an adjoining state or country.

These facilities must solicit a permit to operate through the Secretary (SEMARNAP). In addition, they must annually submit emission estimates and/or stack measurements for the facility.

Certain companies that have a microindustry certificate may be exempt from the licensing and operating certificate requirements for point sources if their activities are exempted in the *Agreement by which Point sources considered to be Small Businesses (microindustries) in Terms of the Law of the matter Published 17 May 1990 are Exempted from the Requirement of obtaining an Operating License (el Acuerdo por el que se Exceptúan del Trámite para la Obtención de la Licencia de Funcionamiento, a las Fuentes Fijas consideradas como Empresas Microindustriales en los Términos de la Ley en la materia publicado el 17 de Mayo de 1990).*

Point sources could also be specified in a number of other ways. These include defining a point source as follows (with all other sources included as area):

- Source of a given type (e.g., Fluidized Catalytic Cracking unit) or both type <u>and</u> size (e.g., boiler with heat input >10,000 British thermal units [Btu]/hr);

- Source that emits more than a specific amount of emissions determined on some consistent basis (e.g., boilers emitting more than 100 tons per year of NO_x);

- Every source (regardless of type, size or emissions) that is located in a facility of a given type (e.g., petroleum refinery) or type and size (e.g., steel foundry with steel production more than 1,000 tons/year); and

- Every source (regardless of type, size or emissions) that is located in a facility with more than a specified amount of emissions determined on some consistent basis.

Some examples of a consistent basis for determining the amount of emissions are:

- Actual emissions (what was actually emitted in some prior time period);

- Allowable emissions (the maximum that could be emitted under regulatory limits); and

- Potential emissions (what would be emitted if operated full time without control equipment).

In addition, these definitions can vary by regulatory region to account for different levels of severity of the air quality problem and/or the stringency of the regulatory program. As an example, a specific basis has been set in the United States for areas that exceed various ambient air quality standards. Depending upon the exceedance severity, the point source emissions cut-off is set at a different level. As a result, areas with the worst air quality have the lowest point source emissions cut-off. Furthermore, individual states have been encouraged to inventory sources below these cutoffs on an individual basis. The decision to set a lower cutoff depends on a number of local factors, usually available resources to obtain and manage the data.

Environmental programs in the United States have often used the last definition (i.e., facility-wide emission thresholds) based on actual emissions. These sources have been designated as "stationary sources" and are subject to more stringent regulations than sources that emit less. The United States Environmental Protection Agency (U.S. EPA) has expanded this regulatory definition into the realm of data management. U.S. EPA requires that state agencies submit data on the regulatory-defined stationary sources as "point sources"; all data on the remaining facilities must be submitted in aggregated form as "area sources."

As the Mexico emissions inventory program evolves, the established point source definition may be modified to add new significant sources that are identified or to eliminate insignificant sources. Again, the goal is to maximize the overall accuracy of the comprehensive emissions inventory (i.e., point, area, motor vehicle, and nature sources) within the allotted amount of available resources.

5.1.2   Level of Detail

Information on point sources is usually gathered by surveys. Point sources can be inventoried at the following three levels of detail (which are illustrated in Figure 5-1):

- Plant level, which denotes a plant or facility that could contain several pollutant-emitting activities;

- Point/stack level, where emissions to the ambient air occur; and

- Process level, representing the emission unit operations of a source category.

Whenever possible, emissions should be inventoried at the process level in order to support air quality activities such as regulatory development, compliance, tracking, and permitting. For example, identifying the processes or devices to which a future regulation might apply and then estimating the impact (i.e., costs and benefits) of that regulation would typically require estimating emissions for each process or device. Another equally important reason for collecting data at this level of detail is that it provides the agency with the information required to verify the facility-wide emissions estimates provided by the facility operators. Resource limitations, however, may dictate that emissions should be inventoried at the plant or point/stack level.

5.2   <u>Area Sources</u>

Area sources represent the emissions from sources that are too numerous and dispersed to efficiently include in a point source inventory. Collectively, however, area sources are significant emitters of air pollutants, and such pollutants must be included in an emissions inventory to ensure completeness. For example, gasoline stations and dry-cleaning establishments are often treated as area sources. Such facilities are typically not included in point source inventories because of the extensive effort that would be required to gather data and estimate emissions for each individual facility. Non-road mobile sources (e.g., industrial equipment, construction equipment, etc.)   are   often   included   with   stationary   area   sources
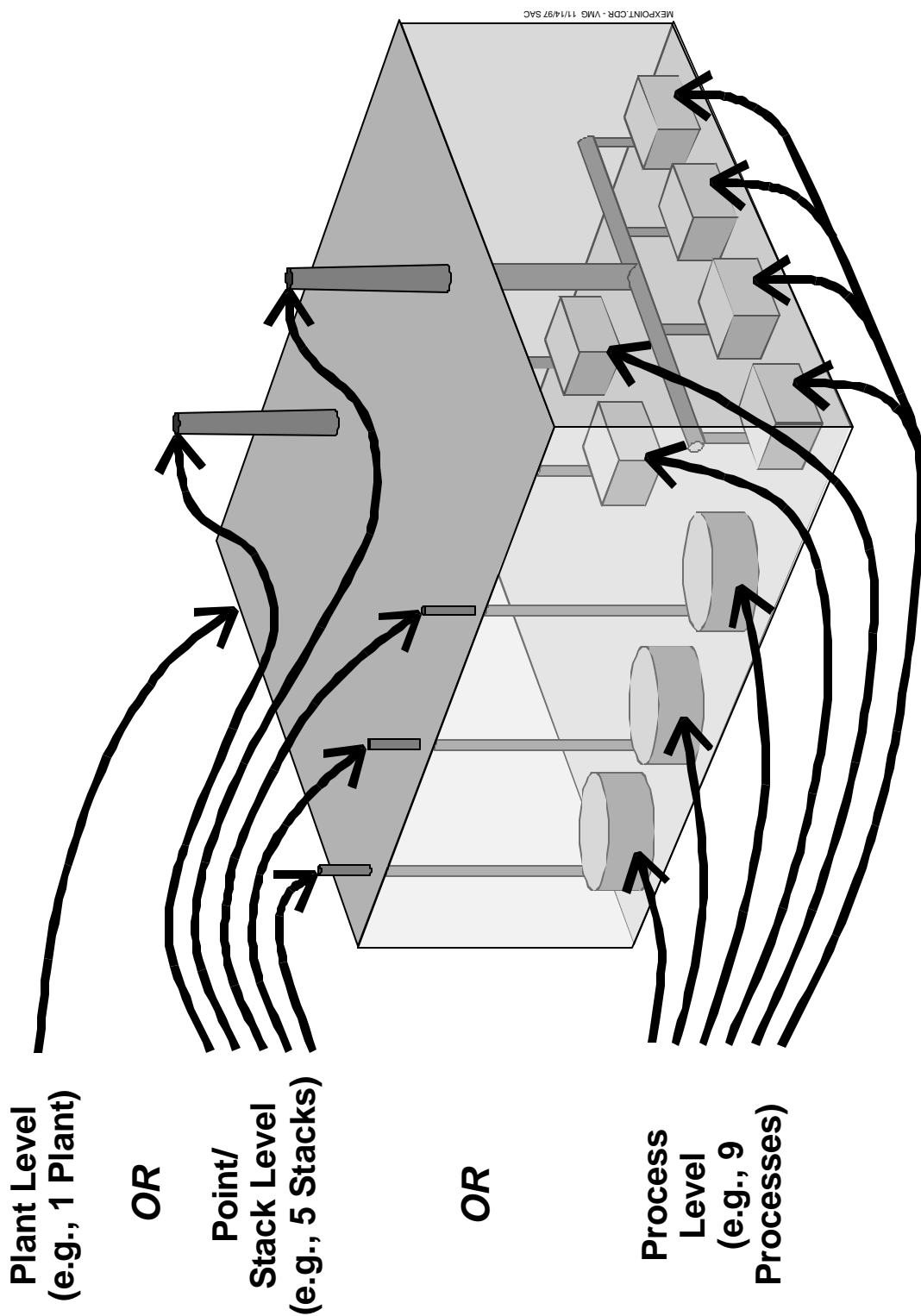
Figure 5-1. Different Point Source Inventory Levels

Plant Level (e.g., 1 Plant)

OR

Point/ Stack Level (e.g., 5 Stacks)

OR

Process Level (e.g., 9 Processes)

primarily because the methods used to estimate area and non-road mobile emissions are very similar. In contrast, the inventory methodology applied to motor vehicles is significantly different. More detailed information about area sources may be found in Volume V of this manual series, *Area Source Inventory Development.* Area source issues related specifically to emission calculations, such as rule effectiveness and rule penetration, are also discussed in Volume III of this Manual series, *Basic Emission Estimating Techniques.*

Instead of distinguishing between individual facilities and emitting devices as is done in point source inventories, area source inventories place emissions from similar sources into *categories*. An area source inventory generally consists of the following broad categories:

- Stationary source fuel combustion;
- Non-road mobile sources;
- Solvent use;
- Petroleum product storage and transport;
- Light industrial/commercial sources;
- Agriculture sources;
- Waste management sources; and
- Miscellaneous area sources.

Each of these categories is comprised of more specific source categories (e.g., organic solvent use includes commercial/consumer solvent use, dry cleaning, surface cleaning) that are defined by similar emission processes or a similarity in the methods that best estimate emissions. A comprehensive area source inventory may contain 150 or more individual source categories. For example, dry cleaning is typically represented by two or more source categories to account for the different solvents that are used (i.e., perchloroethylene versus petroleum-based solvents). Likewise, surface coating may have many source categories to account for the many different applications that exist (e.g., metal cans, metal coils, machinery, wood furniture, etc.).

Emissions from the broad source categories are produced through various mechanisms. Table 5-1 presents the different mechanisms associated with each broad

area source category; sample specific source categories are also included.

5.3   **Point and Area Source Reconciliation**

When a point source inventory and an area source inventory include emissions from the same process, the possibility of double-counting emissions exists. In these situations, the area source emission estimate should be adjusted downward, if appropriate. Certain area source categories such as commercial/consumer solvent use and architectural surface coating do not require any point source adjustments. Other categories, such as fuel combustion, and solvent utilization, may share processes with point sources. To avoid double-counting, the point source activity is subtracted from the total activity for the combined point and area source categories. The resulting area source activity is shown in the following equation:

> **Area Source Activity = Total Activity of Source Category - Sum of Point Source Activyty**

If the resulting area source activity is less than zero, the point source data should be reviewed for errors, and any errors found should be corrected. If area source activity is still less than zero, the area source activity is assumed to be equal to zero, with emissions only from point sources.

For example, if the area source emissions are calculated using employment, the number of employees at the point sources must be subtracted from the inventory region employment to give the area source employment. Likewise, if fuel sales statistics are used to estimate fuel use for area industrial fuel combustion, then fuel used at point source facilities should be subtracted from the overall fuel statistics. Another example illustrating graphic arts solvent use is presented in Figure 5-2.

Table 5-1

Emission Mechanisms for Various Area Source Categories

Source Category	Combustion	Evaporation	Mechanical Disturbance	Biological Process
Stationary Source Fuel Use	✓ (Residential Fuel Combustion)			
Non-Road Mobile Sources	✓ (Construction Equipment)	✓ (Recreational Equipment)		
Solvent Use		✓ (Degreasing)		
Petroleum Product Storage and Transport		✓ (Gasoline Distribution, LPG Leaks)		
Light Industrial/Commercial Sources	✓ (Brick Manufacturing)		✓ (Building Construction)	✓ (Bakeries)
Agricultural Sources	✓ (Agricultural Burning)	✓ (Pesticide Application)	✓ (Agricultural Tilling)	✓ (Animal Waste)
Waste Management Sources	✓ (Incineration)	✓ (Publicly Owned Treatment Works [POTWs])		
Miscellaneous Area Sources	✓ (Wildfires)		✓ (Road Dust)	✓ (Livestock Ammonia)

From solvent balance, all sources collectively use 300 Mg of solvent per year

Point Source

Area Source

= 10 Mg/yr

From survey information, point sources use 120 Mg of solvent per year

After reconciliation, area source solvent use is 180 Mg/yr

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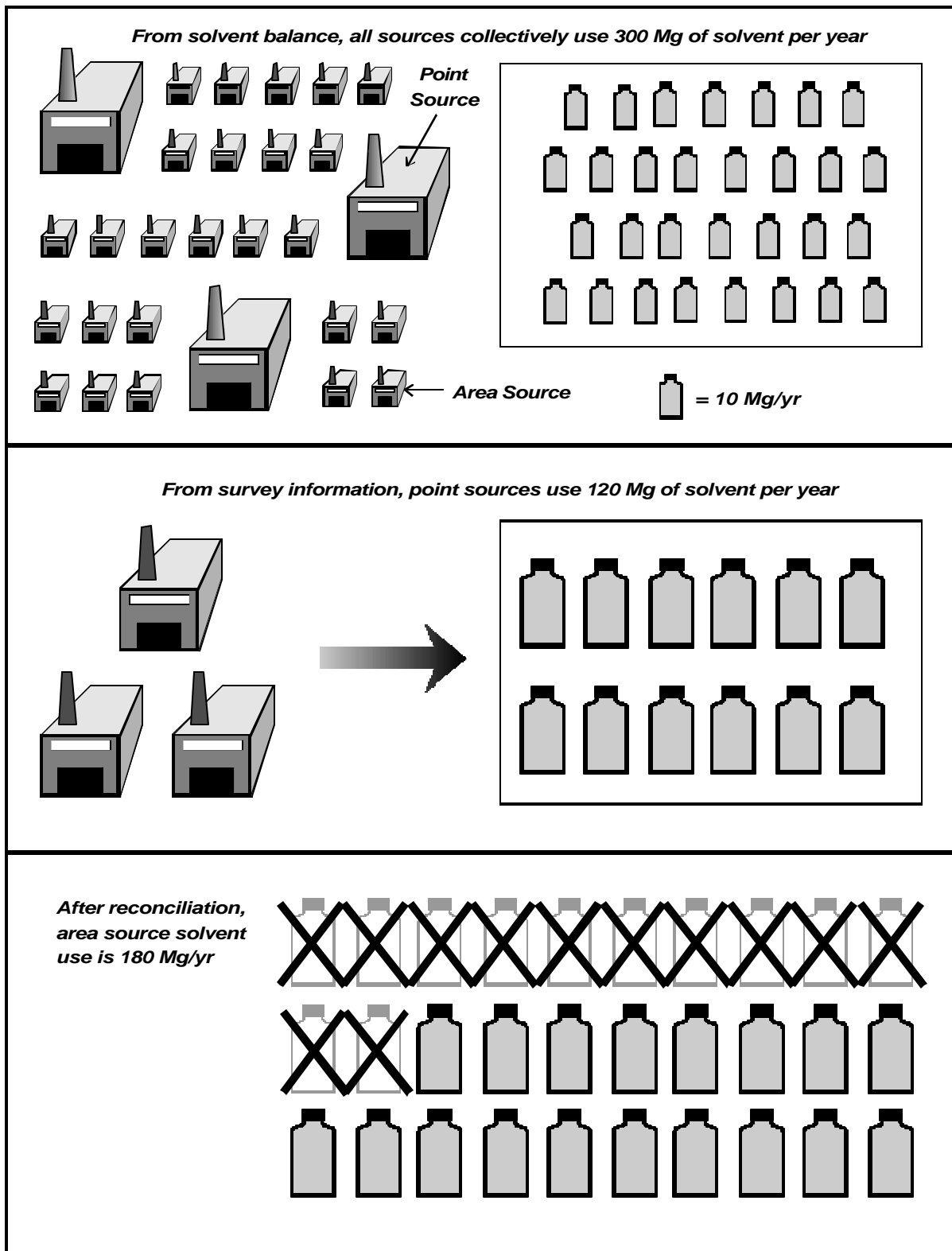
Figure 5-2. Hypothetical Point and Area Source Reconciliation for Graphic Arts Solvents

A point source adjustment is sometimes made by subtracting point source emissions from total source emissions, although this should be the method of last resort. If this method is used, uncontrolled emissions (from total combined sources and point sources) should be used. Any emission control adjustments needed for the area sources should be made after the point source adjustment.

5.4   <u>Motor Vehicle Sources</u>

On-road motor vehicles are those vehicles, such as autos, trucks, and buses, designed to operate on public roads. In most urban areas, on-road motor vehicles are major contributors of emissions of TOG, CO, NO_x, SO_x, PM, air toxics, and visibility-reducing species. Due to their large emissions magnitude and the special considerations required to develop emission estimates, on-road motor vehicles are addressed separately from other area sources. More detailed information about motor vehicle sources may be found in Volume VI of this manual series, *Motor Vehicle Inventory Development.*

Motor vehicle emissions consist of a large number of pollutants resulting from a number of different processes (see Figure 5-3). The most commonly considered are exhaust emissions, which result from fuel combustion and are emitted from the vehicle exhaust tailpipe, and a variety of evaporative emission processes. Evaporative emission processes result in TOG emissions only. These evaporative emissions include:

- **Hot soak emissions** – Emissions occurring due to volatilization of fuel in the fuel delivery system following engine shut-off. Residual engine heat volatilizes the fuel.

- **Running evaporative emissions** – Evaporative emissions from liquid or vapor fuel leaks occurring while the engine is operating.

- **Diurnal emissions** – Emissions from the vehicle fuel tank due to higher bulk liquid temperatures and fuel vapor pressure. These result from rising ambient temperatures, heat input from the vehicle's exhaust system, or heat reflected from the road surface.

Exhaust Emissions

- Hydrocarbons
- Carbon Monoxide
- Nitrogen Oxides
- Particulates
- Sulfates
- Toxics

Evaporative Hydrocarbons

- Refueling
- Diurnal

Evaporative Hydrocarbons

- Hot Soak
- Running Losses
- Resting Losses

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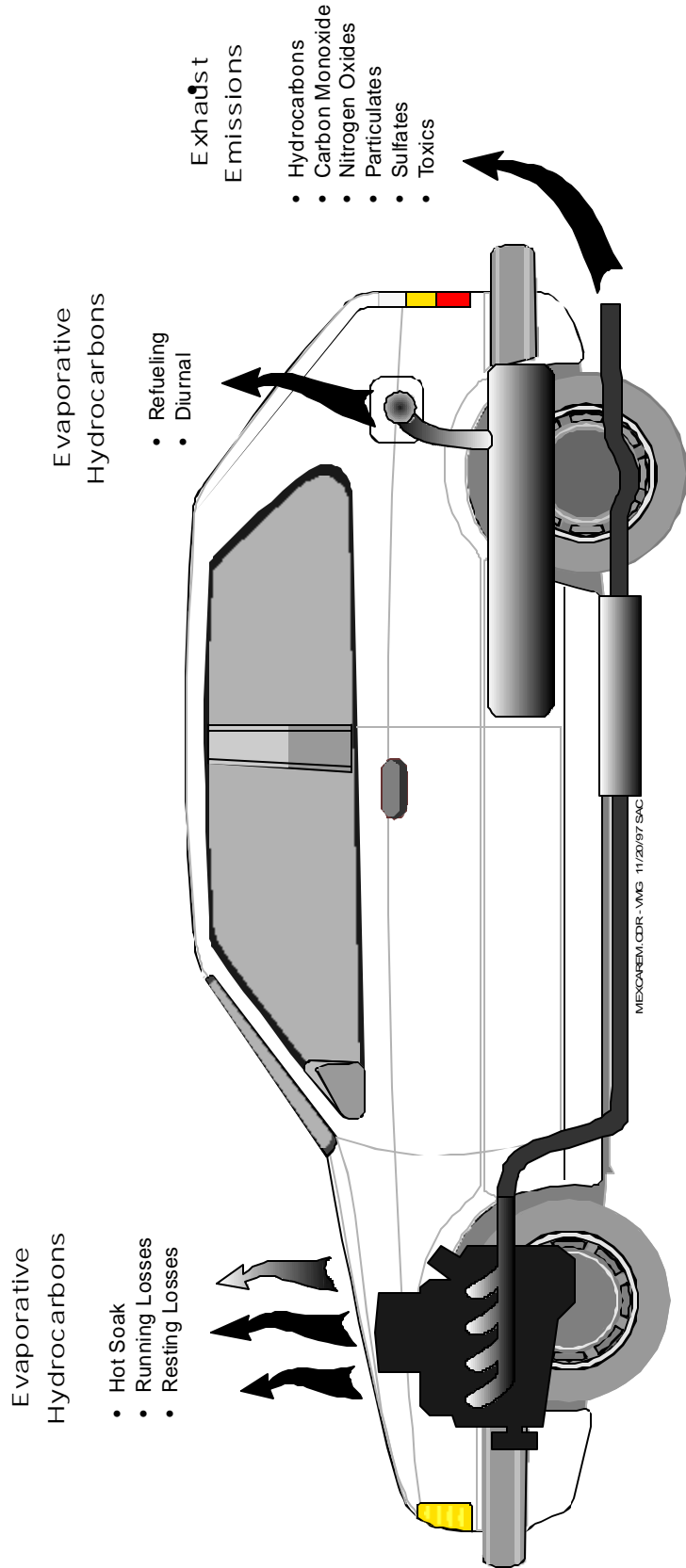
Figure 5-3. Motor Vehicle Emission Processes

Resting evaporative emissions – Evaporative emissions other than hot soak, diurnal, and refueling emissions that occur while the engine is not operating. Resting losses occur primarily from fuel leaks and permeation of vapor through fuel lines.

- **Refueling evaporative emissions** – Evaporative emissions displaced from the vehicle fuel tank during refueling. While the vehicle is the source of the emissions, they occur while the vehicle is stationary and at known locations, such as gasoline stations. Therefore, refueling emissions are typically treated as an area source and discussed in *Volume V: Area Source Inventory Development.* Refueling emission factors can either be estimated using the MOBILE model or obtained from other sources such as AP-42.

Interest in obtaining estimates of the on-road motor vehicle contribution to regional emissions inventories in Mexico has been increasing, leading to the development of motor vehicle emissions inventories for Mexico City, Monterrey, Ciudad Juárez, Guadalajara, and Toluca (Espinosa, et al., 1996). In order to account for potentially different vehicle fleets and driving behavior in Mexico, the U.S.-based MOBILE model has been modified for the Mexico City, Monterrey, and Ciudad Juárez metropolitan areas. The MOBILE model estimates motor vehicle emission factors, which then must be combined with appropriate activity data. Multiple modifications to the MOBILE model have been performed, because it is known that vehicle fleet mix, fuels used, and driving behavior/conditions are not homogeneous throughout Mexico. For example, in the border regions, the Mexican fleet may contain more U.S. vehicles and larger quantities of U.S. fuels may be used. As another example, the high altitude in Mexico City affects the fuel combustion process and, therefore, the emissions from motor vehicles.

5.5   Natural Sources

In addition to human activities, natural phenomena and plant and animal life can play an important role in the air pollution problem. In some areas where natural source emissions may be significant to the overall inventory, it is important to understand the contribution of natural sources, since implementing control strategies generally can not readily reduce these emissions. Two significant natural sources commonly considered in air emissions inventory efforts are described below.

Biogenic emissions. A number of researchers have established that vegetation (e.g., grass, crops, shrubs, forests, etc.) emits significant quantities of hydrocarbons to the atmosphere. Several studies (e.g., Pierce et al., 1990 and Robinson and Robbins, 1968) have shown that biogenic emissions may be comparable to, or exceed, the emissions of nonmethane hydrocarbons (NMHC) from anthropogenic sources in certain areas.

Emissions from soils. As mentioned earlier in the discussion about greenhouse gases in Section 4.9, nitrous oxide (N_2O) is produced naturally in soils by denitrification (i.e., the reduction of nitrite or nitrate to gaseous nitrogen as N_2 or NO_x) and nitrification (i.e., the oxidation of ammonia to nitrate). Commercial nitrogen fertilizers provide an additional nitrogen source, thereby increasing the emissions of N_2O from the soil. The rate of NO_x emissions from soils is also dependent on other variables such as soil type, moisture, temperature, season, crop type, and other agricultural practices. Emissions of NO_x from soils are estimated to be as much as 16 percent of the global amount of NO_x in the troposphere, and as much as 8 percent of the NO_x in North America (U.S. EPA, 1993).

Wind erosion is another natural phenomenon that generates emissions. However, because wind erosion emissions typically are associated with disturbed land, they are sometimes treated as area sources. More detailed information on wind erosion emissions is presented in Section 11.5 of Volume V of this Manual series, *Area Source Inventory Development.*

Some other smaller categories of natural sources include termites (CH_4), lightning (NO_x), and volcanoes and other goethermal activity (SO_x). More detailed information about natural sources may be found in Volume VII of this Manual series, *Natural Source Inventory Development.*

5.6   <u>**Typical Source Category Checklist**</u>

The sources to be included in the inventory should be prioritized based on their importance in the inventory. Resources should be allocated preferentially to the sources that are most important in meeting the end-uses of the inventory. High priority sources include those that are known to be significant contributors of air pollution, are known to be sources of specific targeted pollutants (e.g., PM_{10}), or are most likely to impact air quality.

Table 5-2 is a typical checklist of source categories that might be included in an inventory effort. For each source category, the primary expected emissions are presented by pollutant. **Please note that this checklist should only be used as a tool to begin the process of identifying the source categories to be included in an inventory. Region-specific conditions will likely lead to additions or deletions to this checklist in order to obtain a complete inventory.** For example, bus/truck terminal, small scale brick manufacturing, charbroiling, and street vendors are not source categories that are typically inventoried in the U.S., but they have been added to the checklist as potential source categories for Mexico.

Table 5-2
Example Checklist of Inventory Source Categories and Their Primary Pollutants

Source Category	Inventory Pollutants															
	TOG	ROG	CO	NO$_x$	SO$_x$	PM	PM$_{10}$	PM$_{2.5}$	NH$_3$	EC	OC	HAPs	CO$_2$	N$_2$O	CH$_4$	CFCs
Point Sources																
Electric Utility	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Chemical Manufacturing[a]	✓	✓	✓	✓	✓	✓	✓	✓	✓			✓		✓		✓
Petroleum Refining[a]	✓	✓	✓	✓	✓	✓	✓	✓	✓			✓				
Primary Metal Production[a]	✓	✓			✓	✓	✓	✓				✓				
Secondary Metal Production[a]	✓	✓				✓	✓	✓				✓				
Cement Production[a]	✓	✓	✓	✓	✓	✓	✓	✓				✓				
Miscellaneous Mineral Production[a]						✓	✓	✓		✓	✓	✓				
Automotive Industry[a]	✓	✓										✓				
Wood Pulping Operations[a]	✓	✓			✓	✓	✓	✓		✓	✓	✓				
Oil and Gas Production[a]	✓	✓			✓							✓				
Printing and Publishing	✓	✓										✓				
Surface Coating	✓	✓										✓				
Bulk Terminals	✓	✓										✓				
Mining and Quarrying[a]						✓	✓	✓				✓				
Wood Products Manufacture[a]	✓	✓				✓	✓	✓				✓				
Sugar Production[a]	✓	✓				✓	✓	✓				✓				
Tanning and Finishing[a]	✓	✓										✓				
Glass Production[a]	✓	✓				✓	✓	✓				✓				
Rubber and Plastic Parts Production[a]	✓	✓										✓				
Fabricated Metal Production[a]	✓	✓				✓	✓	✓				✓				
Textile Products[a]	✓	✓				✓	✓	✓				✓				
Landfills	✓	✓	✓	✓								✓	✓		✓	
Municipal Incinerators	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Open Waste Burning	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Asphalt Plants[a]	✓	✓				✓	✓	✓				✓				
Food and Agriculture[a]	✓	✓				✓	✓	✓			✓	✓				
Point Source Fuel Combustion	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Area Sources																

Table 5-2

(Continued)

Source Category	Inventory Pollutants															
	TOG	ROG	CO	NOx	SOx	PM	PM10	PM2.5	NH3	EC	OC	HAPs	CO2	N2O	CH4	CFCs
Industrial and Commercial/Institutional Fuel Combustion	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Residential Fuel Combustion (Commercial Fuels)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Residential Fuel Combustion (Biomass or Waste-derived Fuels)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Locomotives	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Commercial Marine Vessels	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Aircraft	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Other Non-Road Mobile Equipment (Construction, Industrial, Recreational, etc.)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Border Crossings	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Bus/Truck Terminals	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Industrial Surface Coating	✓	✓										✓				
Auto Body Refinishing	✓	✓										✓				
Architectural Surface Coating	✓	✓										✓				
Traffic Paints	✓	✓										✓				
Industrial Surface Cleaning (Degreasing)	✓	✓										✓				
Dry Cleaning	✓	✓										✓				
Graphic Arts	✓	✓										✓				
Asphalt Application	✓	✓										✓				
Commercial/Consumer Solvent Use	✓	✓										✓				
Gasoline Distribution	✓	✓										✓				
Aircraft Refueling	✓	✓										✓				
LPG Distribution	✓	✓										✓				
Bakeries	✓	✓										✓				
Brick Manufacturing	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Construction Activities						✓	✓	✓		✓	✓	✓				
Charbroiling	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Street Vendors	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓	
Pesticide Application	✓	✓										✓				

Table 5-2

(Continued)

Source Category	Inventory Pollutants															
	TOG	ROG	CO	NO$_x$	SO$_x$	PM	PM$_{10}$	PM$_{2.5}$	NH$_3$	EC	OC	HAPs	CO$_2$	N$_2$O	CH$_4$	CFCs
Beef Cattle Feedlots						✓	✓	✓	✓			✓				
Agricultural Burning	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Fertilizer Application									✓			✓		✓		
Animal Waste	✓	✓							✓			✓			✓	
Agricultural Tilling						✓	✓	✓		✓	✓	✓				
On-Site Incineration	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Waste Management— Open Burning	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Wastewater Treatment	✓	✓							✓			✓			✓	
Open Channel Sewage and Wastewater	✓	✓							✓			✓			✓	
Wildfires/Prescribed Fires	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Structure Fires	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Paved Road Dust						✓	✓	✓		✓	✓	✓				
Unpaved Road Dust						✓	✓	✓		✓	✓	✓				
Wind Erosion						✓	✓	✓		✓	✓	✓				
Domestic Ammonia Emissions									✓			✓				
Motor Vehicle Sources																
Light Duty Gas Vehicles (LDGV)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Light Duty Gas Trucks (LDGT)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Heavy Duty Gas Vehicles (HDGV)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Light Duty Diesel Vehicles (LDDV)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Light Duty Diesel Trucks (LDGT)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Heavy Duty Diesel Vehicles (HDDV)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Motorcycles (MC)	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	
Natural Sources																
Biogenic Hydrocarbons	✓	✓														

Table 5-2

(Continued)

Source Category	Inventory Pollutants															
	TOG	ROG	CO	NO$_x$	SO$_x$	PM	PM$_{10}$	PM$_{2.5}$	NH$_3$	EC	OC	HAPs	CO$_2$	N$_2$O	CH$_4$	CFCs
Soil NO$_x$				✓										✓		
Termites															✓	
Lightning				✓												
Volcanoes/Other Geothermal					✓	✓	✓	✓				✓				

[a] Only includes process related emissions; point source fuel combustion is treated as its own subcategory.

6.0 OTHER EMISSIONS INVENTORY CHARACTERISTICS

Two of the ten emissions inventory characteristics (pollutant types and source types) were described in Sections 4.0 and 5.0. The remaining eight characteristics are described below. The definition of these characteristics is determined primarily by the established purpose of the inventory.

6.1 Base Year

The base year of an inventory identifies the year for which emissions are estimated and fixes an inventory's position in time. This provides a benchmark against which previous and subsequent inventories can be compared. It is important to establish a base year, so that all emission estimates have a common basis and represent activities occurring during the same period of time.

Any year can be used as the inventory base year, but it is usually determined by the established purpose of the inventory. For example, if it is desired to see the effects of recently implemented control strategies, then the base year will be some year prior to the implementation of control strategies. A comparison of current emission levels to historic levels might use a base year in the past. The base year of an inventory might also be dictated by various regulatory requirements. The main reason for this is so that emissions inventories from different regions can be easily compared with each other and regulatory standards. In other cases, data availability might determine what the inventory base year is. For example, it might be desired to develop an inventory for 1997, but if statistics to be used as activity data have only been compiled through 1995, then 1995 would probably be a better base year than 1997.

6.2   <u>Time Characteristics</u>

There are two main time characteristics that must be considered for every inventory: time period and temporal variability. Other minor time characteristics may be applicable for some inventories. Time period refers to the length of time represented by the inventory. Inventory emissions will be presented in units of mass of pollutant per inventory time period (e.g., kg CO/yr). For many large-scale inventories, the time period will typically be one year. However, some specialized inventory applications may require shorter periods of time (e.g., one day, one month, the summer ozone season, the heating season, etc.).

Temporal variability describes the variability of emissions over time. If emissions are constant over time, then temporal variability is not of much concern. However, most emissions do change over time. Depending upon the inventory requirements associated with the inventory purpose, the emissions variations might need to be described on a seasonal, monthly, or daily basis. Specialized inventories may even need emissions on an hourly (or shorter time period) basis. For instance, emissions from on-road motor vehicles are variable over different time periods due to different levels of activity. Weekday motor vehicle emissions might be higher than weekend emissions because of high levels of vehicle activity associated with commuting to and from work. Also, as shown in Figure 6-1, emissions in the morning and early evening are likely to be higher than emissions at noon or midnight because those times are characterized by heavy commuting traffic. Because the temporal distribution for motor vehicle activity presented in Figure 6-1 is U.S.-specific, Mexico motor vehicle activity may be distributed differently. Depending upon the purpose of the inventory, one or more of these temporal variabilities may need to be considered.

6.3 <u>Spatial Characteristics</u>

There are two primary spatial characteristics in any inventory: inventory domain and spatial resolution. The inventory domain represents the area for which air pollutant sources will be inventoried. The inventory domain is sometimes determined by the inventory purpose.
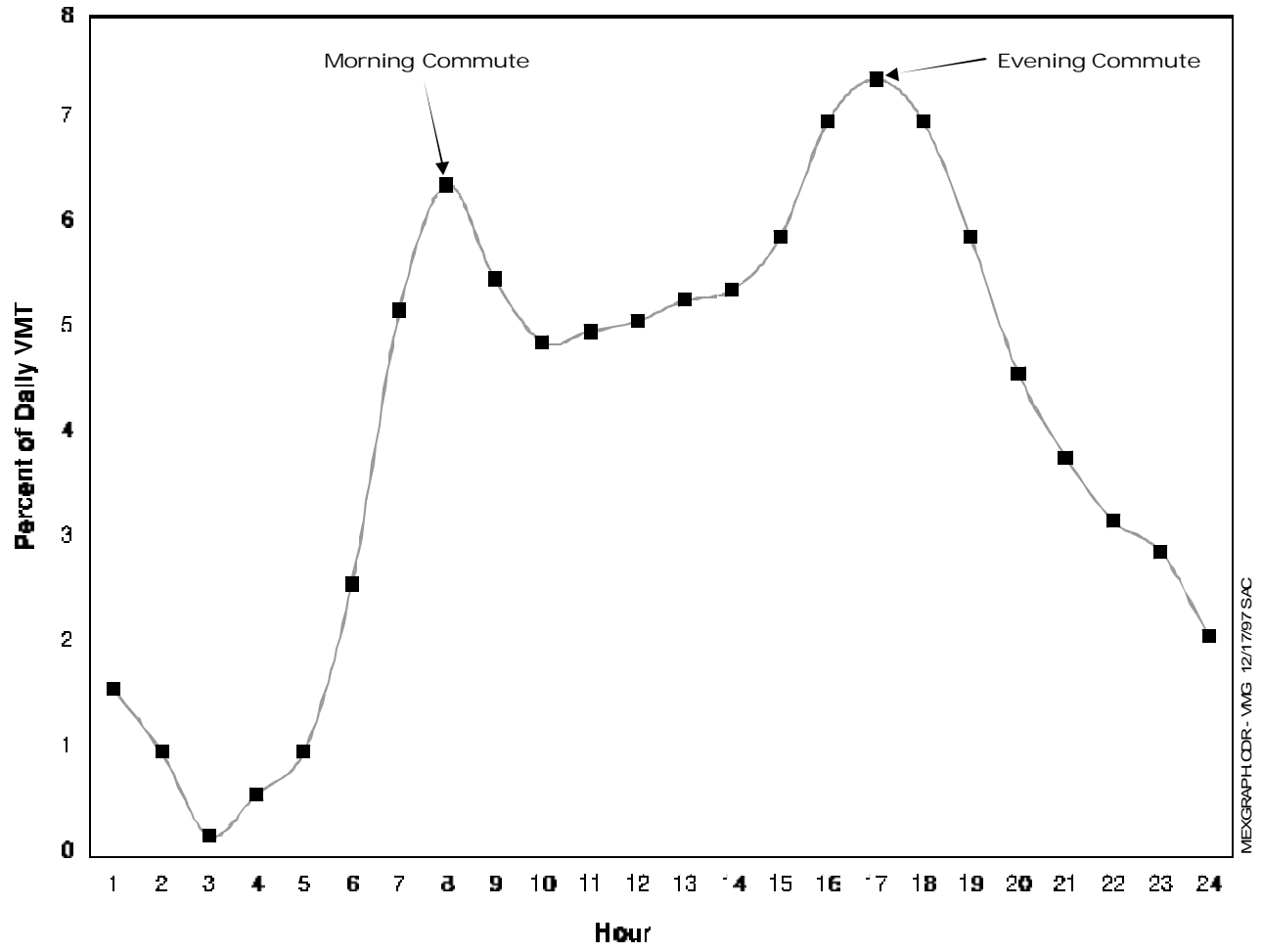
Figure 6-1. Hypothetical U.S. Temporal Distribution of Motor Vehicle Activity

Often, the inventory domain follows political, geographic, or air quality agency boundaries. Depending upon the inventory application, sources external to the defined inventory domain that exert influence upon air quality within the domain due to meteorological transport may also need to be addressed. A square hypothetical inventory domain measuring 25 km on a side is presented in Figure 6-2.

Spatial resolution describes how specifically the geographic location of pollution sources must be defined. Basic inventories will sometimes provide pollutant totals only for the entire inventory domain. More complex inventories, particularly those associated with air quality modeling efforts, will often require a more detailed description of emissions distribution. The resolution of area, motor vehicle, and natural sources within an inventory domain is usually done using grid cells. The inventory domain presented in Figure 6-2 contains 25 grid cells measuring 5 km on a side. Typically, the desired air quality accuracy determines the required grid cell size. However, in general, the required grid cell size is also indicated by the domain size – large inventory domains will have grid cells that typically measure several kilometers on a side, while smaller inventory domains can have grid cells that measure a few hundred meters on a side. From Figure 6-2, the following spatial distribution of emissions can be seen:

- Population/Residential Area Sources: Cells A1 and A2;

- Agricultural Area Sources: Cells B3, B4, C3, C4, D3, and D4;

- Marine Sources: Cells A3, A4, A5, and B5;

- Motor Vehicles: Cells A1, A2, B1, B2, C2, D2, D3, D4, E2, E4, and E5; and

- Natural Biogenic Sources: Cells C5, D5, E1, E2, E3, and E4.

For most types of inventories, point sources will need to be geographically located using either latitude and longitude coordinates or Universal Transverse Mercator (UTM) coordinates. For some complex inventory efforts, the required geographical
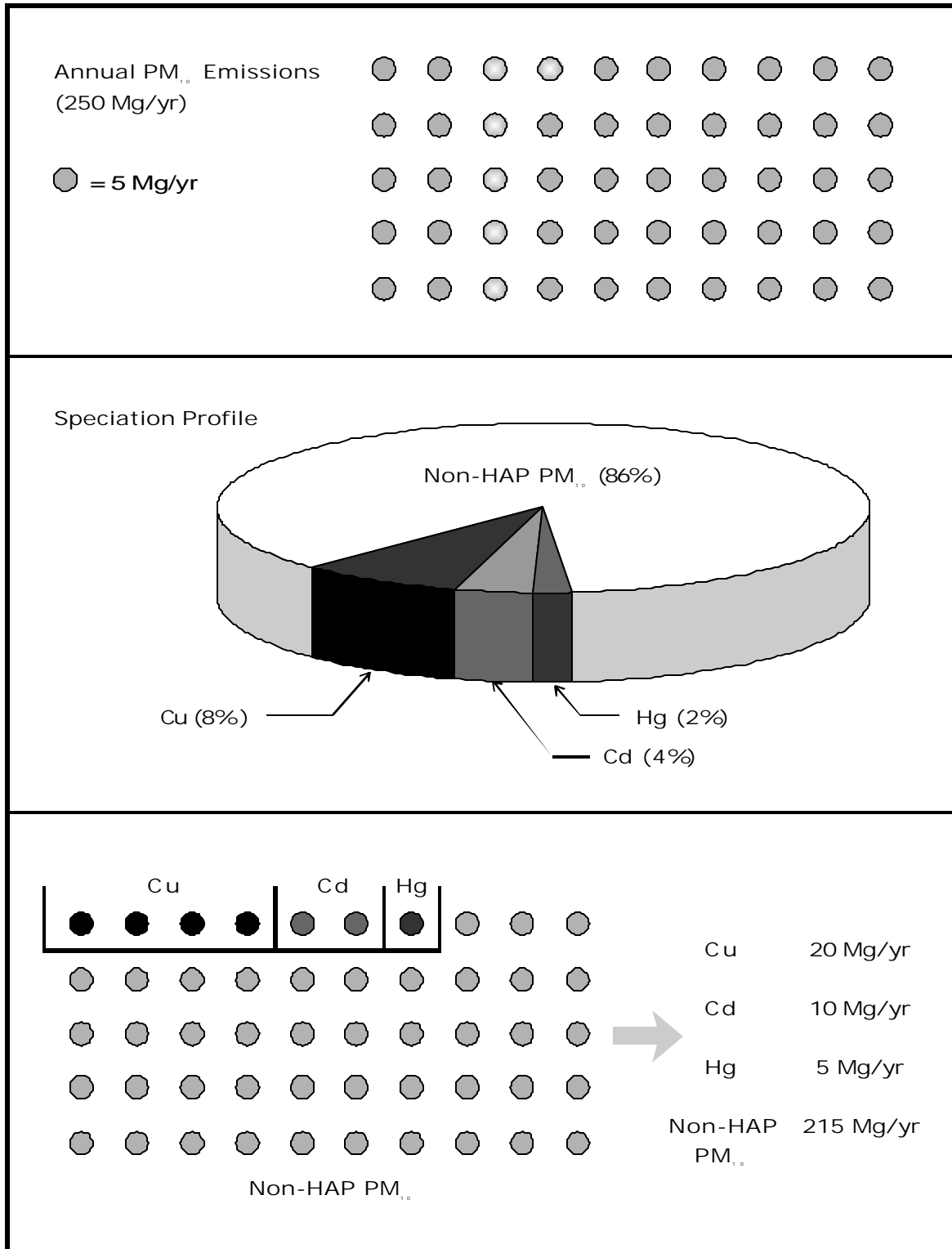
accuracy for point
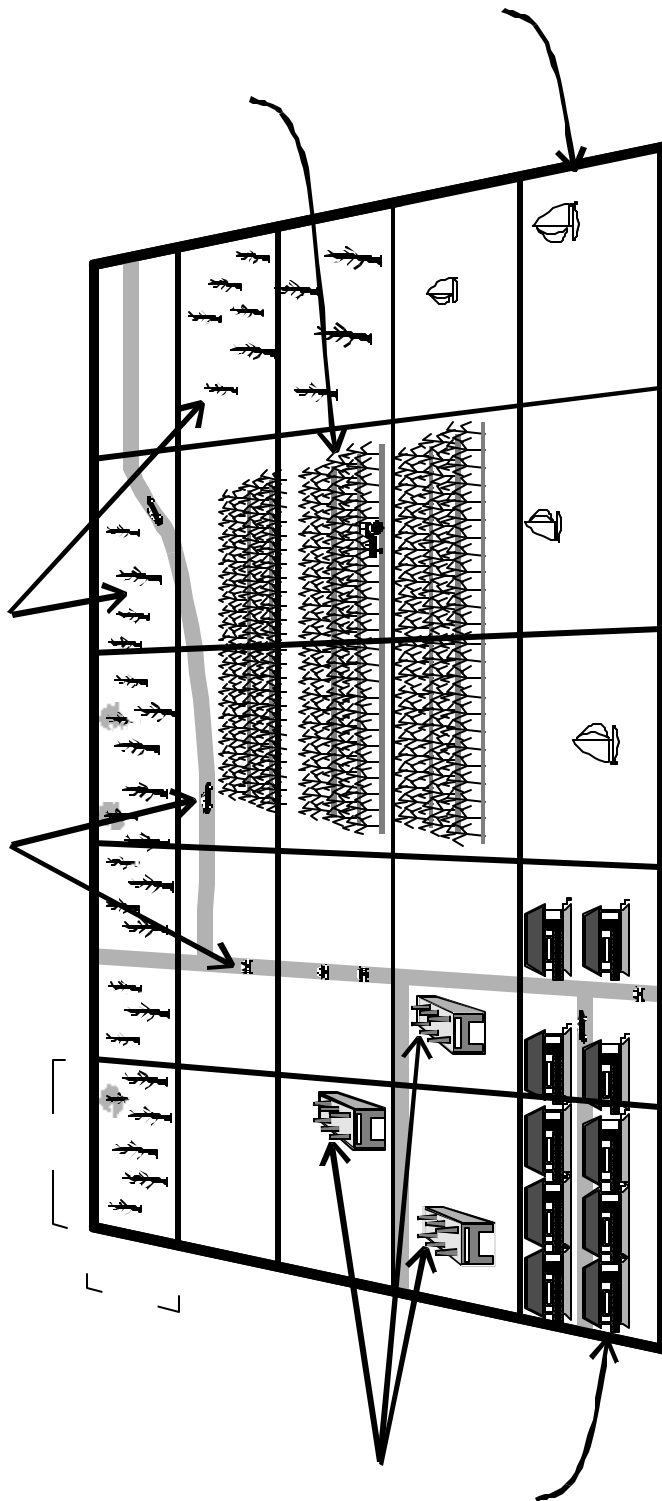
source locations may be as close as ±10 meters. In Figure 6-2, the three point sources located in cells B1, C1, and C2 will require detailed location coordinates.

6.4   **Species Resolution**

Species resolution refers to disaggregating an inventory pollutant (e.g., TOG, PM, etc.) into its individual chemical components (e.g., toluene, lead, EC, OC, etc.) or into specific groups (e.g., paraffins, aromatics, etc.). The need for species resolution, as well as the specific methodology, is determined by the inventory purpose. Species resolution is primarily performed using speciation profiles that describe the fraction of individual chemical species. Many inventories will not include detailed species resolution; other specialized inventory applications will require it. These applications include air toxics inventories, photochemical modeling, and chemical mass balance modeling used for source attribution.

As discussed in Section 4.8, air toxics inventories seek to quantify the amount of hazardous air pollutants (HAPs) that are emitted. Ideally, this would be performed using emission factors for individual HAPs. Although there are some HAP emission factors for combustion and other sources, emission factors often do not exist. As a result, individual HAP species frequently are disaggregated from TOG and PM by using speciation profiles. As mentioned in Section 4.8, this is not the preferred approach for estimating HAPs emissions. If this approach is used, it often results in an overestimation of HAPs. This approach is demonstrated in Figure 6-3.

In photochemical modeling, speciation is needed because emitted hydrocarbon species have different photochemical reactivities. Total hydrocarbon emissions are calculated and then speciated into different hydrocarbon groups. In order to properly represent the chemical reactions occurring in the atmosphere, each species group is assigned an appropriate level of photochemical reactivity.

**Annual PM$_{10}$ Emissions
(250 Mg/yr)**

$\bigcirc$ = 5 Mg/yr

Speciation Profile

Non-HAP PM$_{10}$ (86%)

Cu (8%)

Hg (2%)

Cd (4%)

Cu   **Cd** **Hg**

Cu	20 Mg/yr
Cd	10 Mg/yr
Hg	5 Mg/yr
Non-HAP PM$_{10}$	215 Mg/yr

Non-HAP PM$_{10}$

MEXHAPS.CDR - VMG 11/17/97 SAC

Figure 6-3. Hypothetical HAPs Speciation

Finally, source attribution (or receptor modeling) through the use of a chemical mass balance requires fairly detailed species resolution. Source attribution can be determined working backward from measured TOG and particulate concentrations at a monitoring site using computerized linear algebra matrix calculations. In this instance, species resolution provides the unique chemical content (usually for metals and hydrocarbons) of the emissions for each source type. This chemical content serves as the "fingerprint" for the presence of material from that source in ambient sample data at the receptor. Without species resolution, implementation of this application is impossible. More information on source attribution can be found in some recent source attribution studies (Watson et al., 1984; Chow et al., 1992; and Scheff et al., 1984).

6.5   Quality Assurance

Quality assurance (QA) is an indispensable element of any emissions inventory. Regardless of what type of inventory is being conducted, QA is necessary. The amount and focus of QA, however, will be variable depending upon the specific inventory purpose. For instance, a detailed large-scale modeling inventory will typically require significantly more QA than a facility-level reporting inventory would. Also, if one particular source type had been preliminarily identified as a large pollutant source, then more QA resources could be directed at this source type rather than at some of the more minor source types.

QA should be conducted throughout the development of the inventory rather than as an afterthought conducted at the last minute. Some example QA activities include:

- Using a source category checklist (such as the one presented in Table 5-2), confirm that all necessary source categories have been included in the inventory;

- Check sampling results and activity data for "outliers" prior to emission calculations;

- Confirm that all emission calculations have been performed properly; and

- Compare inventory results with emissions inventories in similar regions.

There are also many other QA activities not listed above that can be devised which will help ensure a high quality emissions inventory.

Although the results of an inventory might affect how QA is conducted later in the inventory effort, QA resources should be identified at the beginning. To the greatest extent possible, the type of QA (e.g., detailed "line-by-line" QA or high-level QA) and areas requiring concentrated QA should be designated at the outset of the inventory effort.

6.6 <u>Data Management</u>

Another essential emissions inventory characteristic is the data management required for the inventory. With the widespread use of computers and increasing inventory data requirements, virtually all inventory data are currently handled electronically. Consideration should be given to whether data management should be performed using a spreadsheet-type application or a database application. Spreadsheets tend to be easier to use, but databases are much more powerful. The method of transfer of inventory-related information and any data confidentiality requirements should also be established early in the inventory development process. The inventory purpose will help determine what type of data management is required. For instance, an inventory used as an air quality model input might require different data management than an inventory designed for regulatory compliance. Also, expected future uses of the inventory might influence the type of data management selected.

6.7   <u>Projections</u>

Projections forecast a base year inventory forward or backward in time. The use of projections is primarily determined by the inventory purpose. Many inventories will not develop projected emissions. Projections are mainly used to track past and future emission trends due to activity growth and implemented control strategies. Projections are also used extensively in theoretical analyses of various control strategies proposed for future implementation. For example, projections could be used to estimate future motor vehicle emissions based upon expected population growth. Likewise, projections could be used to track estimated emission reductions due to the proposed phase-in of reformulated paints that contain lower levels of solvents. Growth projections of emissions are usually based upon growth projections of other surrogates (e.g., population, economic activity). Control projections, on the other hand, are often based on estimated reductions from control strategies. Projection methodologies and required data should be established early in the inventory development process. U.S. EPA has published guidance regarding emissions projection that contains various references and methodologies (U.S. EPA, 1991b).

6.8   <u>Uncertainty Estimation</u>

The final emissions inventory characteristic is uncertainty estimation. Uncertainty estimates are a valuable tool to assess the accuracy of an emissions inventory.

Uncertainty can be estimated quantitatively or qualitatively. Quantitative uncertainty estimates are unusual. There are several reasons for this. First of all, there is no agreed upon method for making quantitative estimates of uncertainty. Also, the derivation of quantitative uncertainty estimates can become very statistically complex. Finally, a large number of assumptions typically are required to make quantitative uncertainty estimates.

In general, when uncertainty estimates are made, they are most commonly qualitative in nature. Qualitative estimates of uncertainty may focus on methodologies, activity data, emission-related data, underlying assumptions, or other components of inventory development. For example, an inventory assumption that emissions from surface coating operations are limited only to solvent contained in the applied surface coating (and not from surface preparation and/or cleanup solvents) will almost certainly lead to an underestimate of TOG emissions in the inventory. In a similar manner, an assumption that all point sources use the same fuel and operate on the same operating schedule will generate uncertainty in the inventory, although it may not be clear if this would result in an overestimate or an underestimate. Although qualitative estimates do not statistically calculate the uncertainty of an emissions inventory, they are valuable because they point out potential weaknesses in the inventory.

7.0 ITERATION OF INVENTORY PROCESS

The technical steps of emissions inventory development were previously shown in Figure 2-1. These steps begin with the identification of the inventory purpose and end with the documentation of the inventory results. It is important to note that even if all of the steps presented in Figure 2-1 are properly implemented during inventory development, it simply represents <u>one</u> iteration of emissions inventory development. Multiple iterations are usually required for the development of high quality emissions inventories. This iteration concept is represented by the puzzles presented in Figure 7-1. Early inventories will be characterized by missing information and other imperfections; subsequent updated inventories will gradually improve in quality.

The end goal is to develop an emissions inventory that is a comprehensive, accurate, and current accounting of air pollutant emissions and associated data from sources within a given geographic area over a specific time interval. However, practical limitations necessitate an iterative approach to accomplish this objective. Systematic, iterative inventory development, over time, will reduce the amount of inventory uncertainty and improve the overall quality of the emissions inventory.

An emissions inventory should be comprehensive, which is to say that all sources of the identified inventory pollutants should be included. Limited resources may reduce the number of inventoried sources to a subset of the total existing sources. Likewise, some emission sources may be unnoticed or overlooked during the initial inventory process. Subsequent inventory revisions are used to fill in missing sources.

To the greatest extent possible, an emissions inventory should also be accurate. Incorrect data or overly simplistic assumptions will introduce inaccuracies into the inventory. These inaccuracies can be corrected in later inventory iterations with more complete or improved information.
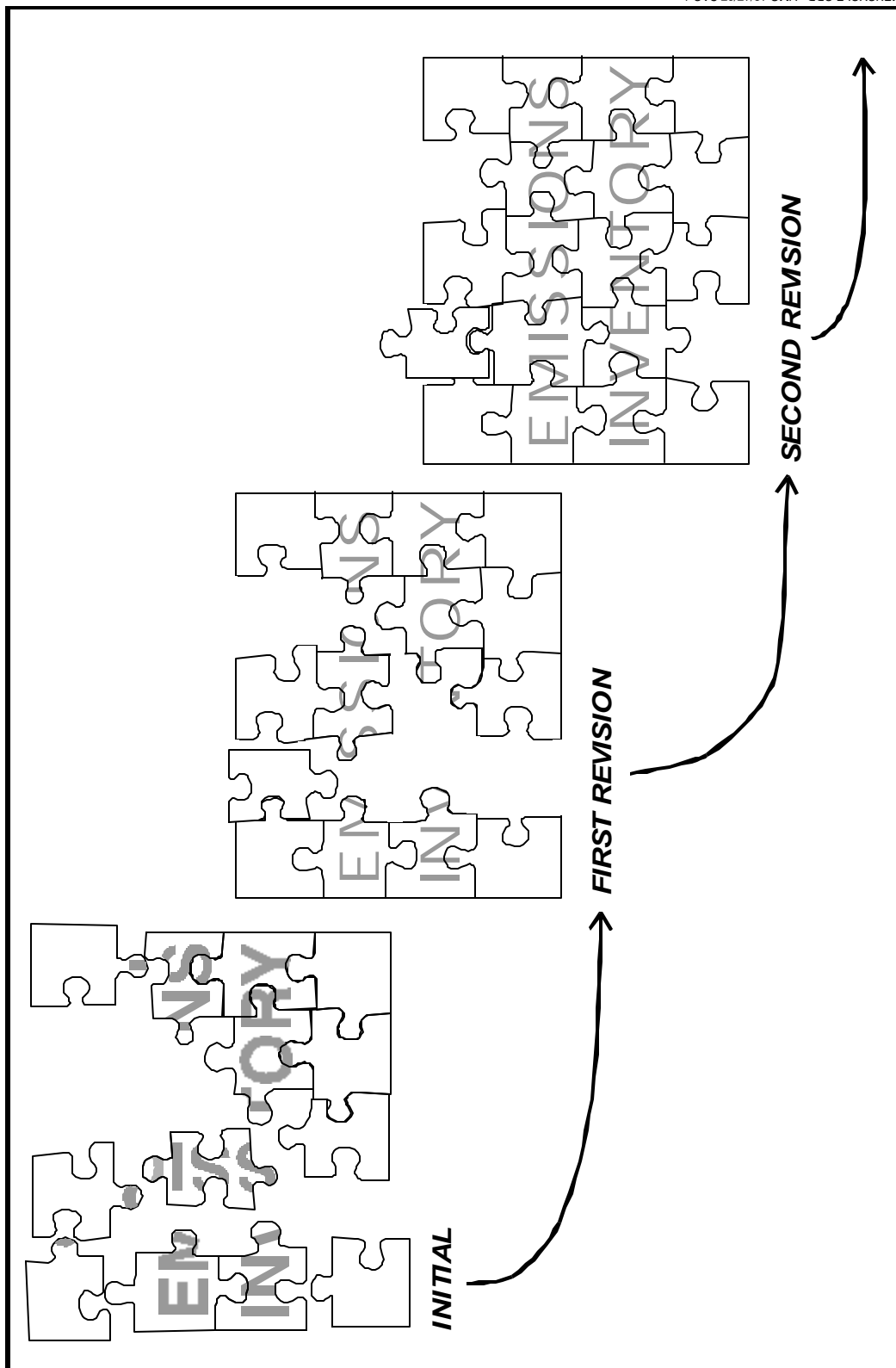
Figure 7-1. Emissions Inventory Iterations

Finally, an emissions inventory should represent current emissions. Some inventory applications will be updated every year and will require current information for that specific year. These inventories will be updated annually to track the increase of emissions due to growth in the emission-producing activity or the decrease of emissions due to the implementation of various emission control strategies. Outdated data and information should be updated in later inventory iterations.

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APPENDIX A

NON-REACTIVE HYDROCARBONS

U.S. EPA Photochemically Non-Reactive Compounds

Chemical	Synonym
methane	
ethane	
methylene chloride	dichloromethane
1,1,1-trichloroethane	methyl chloroform
1,1,2-trichloro 1,2,2-trifluoroethane	CFC–113
trichlorofluoromethane	CFC–11
dichlorodifluoromethane	CFC–12
chlorodifluoromethane	HCFC–22
trifluoromethane	HFC–23
1,2-dichloro 1,1,2,2-tetrafluoroethane	CFC–114
chloropentafluoroethane	CFC–115
1,1,1-trifluoro 2,2-dichloroethane	HCFC–123
1,1,1,2-tetrafluoroethane	HFC–134a
1,1-dichloro 1-fluoroethane	HCFC–141b
1-chloro 1,1-difluoroethane	HCFC–142b
2-chloro 1,1,1,2-tetrafluoroethane	HCFC–124
pentafluoroethane	HFC–125
1,1,2,2-tetrafluoroethane	HFC–134
1,1,1-trifluoroethane	HFC–143a
1,1-difluoroethane	HFC–152a
parachlorobenzotrifluoride	PCBTF
cyclic, branched, or linear completely methylated siloxanes	
acetone	
perchloroethylene	tetrachloroethylene
3,3-dichloro-1,1,1,2,2-pentafluoropropane	HCFC–225ca
1,3-dichloro-1,1,2,2,3-pentafluoropropane	HCFC–225cb
1,1,1,2,3,4,4,5,5,5-decafluoropentane	HFC–43–10mee
difluoromethane	HFC–32
ethylfluoride	HFC–161
1,1,1,3,3,3-hexafluoropropane	HFC–236fa
1,1,2,2,3-pentafluoropropane	HFC–245ca
1,1,2,3,3-pentafluoropropane	HFC–245ea
1,1,1,2,3-pentafluoropropane	HFC–245eb
1,1,1,3,3-pentafluoropropane	HFC–245fa
1,1,1,2,3,3-hexafluoropropane	HFC–236ea
1,1,1,3,3-pentafluorobutane	HFC–365mfc
chlorofluoromethane	HCFC–31

U.S. EPA Photochemically Non-Reactive Compounds (Continued)

Chemical	Synonym
1-chloro 1-fluoroethane	HCFC–151a
1,2-dichloro 1,1,2-trifluoroethane	HCFC–123a
1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-butane	$C_4F_9OCH_3$
2-(difluoromethoxymethyl) 1,1,1,2,3,3,3-heptafluoropropane	$(CF_3)_2CFCF_2OCH_3$
1-ethoxy 1,1,2,2,3,3,4,4,4-nonafluorobutane	$C_4F_9OC_2H_5$
2-(ethoxydifluoromethyl) 1,1,1,2,3,3,3-heptafluoropropane	$(CF_3)_2CFCF_2OC_2H_5$
perfluorocarbon compounds which fall into these classes:	
(i) Cyclic, branched, or linear, completely fluorinated alkanes;	
(ii) Cyclic, branched, or linear, completely fluorinated ethers with no unsaturations;	
(iii) Cyclic, branched, or linear, completely fluorinated tertiary amines with no unsaturations; and	
(iv) Sulfur containing perfluorocarbons with no unsaturations and with sulfur bonds only to carbon and fluorine.	

Source: Federal Register, Vol. 62, No. 164. August 25, 1997. pp. 44900 – 44903.

APPENDIX B

HAZARDOUS AIR POLLUTANTS

United States Federal Hazardous Air Pollutants
(from Clean Air Act – Section 112(b))

CAS Number	Chemical Name
75-07-0	Acetaldehyde
60-35-5	Acetamide
75-05-8	Acetonitrile
98-86-2	Acetophenone
53-96-3	2-Acetylaminofluorene
107-02-8	Acrolein
79-06-1	Acrylamide
79-10-7	Acrylic acid
107-13-1	Acrylonitrile
107-05-1	Allyl chloride
92-67-1	4-Aminobiphenyl
62-53-3	Aniline
90-04-0	o-Anisidine
1332-21-4	Asbestos
71-43-2	Benzene (including benzene from gasoline)
92-87-5	Benzidine
98-07-7	Benzotrichloride
100-44-7	Benzyl chloride
92-52-4	Biphenyl
117-81-7	Bis(2-ethylhexyl)phthalate (DEHP)
542-88-1	Bis(chloromethyl) ether
75-25-2	Bromoform
106-99-0	1,3-Butadiene
156-62-7	Calcium cyanamide
105-60-2	Caprolactam
133-06-2	Captan
63-25-2	Carbaryl
75-15-0	Carbon disulfide
56-23-5	Carbon tetrachloride
463-58-1	Carbonyl sulfide
120-80-9	Catechol
133-90-4	Chloramben
57-74-9	Chlordane
7782-50-5	Chlorine
79-11-8	Chloroacetic acid
532-27-4	2-Chloroacetophenone
108-90-7	Chlorobenzene
510-15-6	Chlorobenzilate

United States Federal Hazardous Air Pollutants (Continued)

CAS Number	Chemical Name
67-66-3	Chloroform
107-30-2	Chloromethyl methyl ether
126-99-8	Chloroprene
1319-77-3	Cresol/Cresylic acid (mixed isomers)
95-48-7	o-Cresol
108-39-4	m-Cresol
106-44-5	p-Cresol
98-82-8	Cumene
94-75-7	2,4-D (including salts and esters)
72-55-9	DDE
334-88-3	Diazomethane
132-64-9	Dibenzofuran
96-12-8	1,2-Dibromo-3-chloropropane
84-74-2	Dibutyl phthalate
106-46-7	1,4-Dichlorobenzene
91-94-1	3,3'-Dichlorobenzidine
111-44-4	Dichloroethyl ether (Bis[2-chloroethyl]ether)
542-75-6	1,3-Dichloropropene
62-73-7	Dichlorvos
111-42-2	Diethanolamine
121-69-7	N,N-Dimethylaniline
64-67-5	Diethyl sulfate
119-90-4	3,3'-Dimethoxybenzidine
60-11-7	4-Dimethylaminoazobenzene
119-93-7	3,3'-Dimethylbenzidine
79-44-7	Dimethylcarbamoyl chloride
68-12-2	Dimethylformamide
57-14-7	1,1-Dimethylhydrazine
131-11-3	Dimethyl phthalate
77-78-1	Dimethyl sulfate
N/A	4,6-Dinitro-o-cresol (including salts)
51-28-5	2,4-Dinitrophenol
121-14-2	2,4-Dinitrotoluene
123-91-1	1,4-Dioxane (1,4-Diethyleneoxide)
122-66-7	1,2-Diphenylhydrazine
106-89-8	Epichlorohydrin (l-Chloro-2,3-epoxypropane)
106-88-7	1,2-Epoxybutane
140-88-5	Ethyl acrylate
100-41-4	Ethyl benzene
51-79-6	Ethyl carbamate (Urethane)

United States Federal Hazardous Air Pollutants (Continued)

CAS Number	Chemical Name
75-00-3	Ethyl chloride (Chloroethane)
106-93-4	Ethylene dibromide (Dibromoethane)
107-06-2	Ethylene dichloride (1,2-Dichloroethane)
107-21-1	Ethylene glycol
151-56-4	Ethylene imine (Aziridine)
75-21-8	Ethylene oxide
96-45-7	Ethylene thiourea
75-34-3	Ethylidene dichloride (1,1-Dichloroethane)
50-00-0	Formaldehyde
76-44-8	Heptachlor
118-74-1	Hexachlorobenzene
87-68-3	Hexachlorobutadiene
77-47-4	Hexachlorocyclopentadiene
67-72-1	Hexachloroethane
822-06-0	Hexamethylene diisocyanate
680-31-9	Hexamethylphosphoramide
110-54-3	Hexane
302-01-2	Hydrazine
7647-01-0	Hydrochloric acid (Hydrogen chloride [gas only])
7664-39-3	Hydrogen fluoride (Hydrofluoric acid)
123-31-9	Hydroquinone
78-59-1	Isophorone
N/A	Lindane (all isomers)
108-31-6	Maleic anhydride
67-56-1	Methanol
72-43-5	Methoxychlor
74-83-9	Methyl bromide (Bromomethane)
74-87-3	Methyl chloride (Chloromethane)
71-55-6	Methyl chloroform (1,1,1-Trichloroethane)
78-93-3	Methyl ethyl ketone (2-Butanone)
60-34-4	Methyl hydrazine
74-88-4	Methyl iodide (Iodomethane)
108-10-1	Methyl isobutyl ketone (Hexone)
624-83-9	Methyl isocyanate
80-62-6	Methyl methacrylate
1634-04-4	Methyl tert-butyl ether
101-14-4	4,4'-Methylenebis(2-chloroaniline)
75-09-2	Methylene chloride (Dichloromethane)
101-68-8	4,4'-Methylenediphenyl diisocyanate (MDI)
101-77-9	4,4'-Methylenedianiline

United States Federal Hazardous Air Pollutants (Continued)

CAS Number	Chemical Name
91-20-3	Naphthalene
98-95-3	Nitrobenzene
92-93-3	4-Nitrobiphenyl
100-02-7	4-Nitrophenol
79-46-9	2-Nitropropane
684-93-5	N-Nitroso-N-methylurea
62-75-9	N-Nitrosodimethylamine
59-89-2	N-Nitrosomorpholine
56-38-2	Parathion
82-68-8	Pentachloronitrobenzene (Quintobenzene)
87-86-5	Pentachlorophenol
108-95-2	Phenol
106-50-3	p-Phenylenediamine
75-44-5	Phosgene
7803-51-2	Phosphine
7723-14-0	Phosphorus
85-44-9	Phthalic anhydride
1336-36-3	Polychlorinated biphenyls (Aroclors)
1120-71-4	1,3-Propane sultone
57-57-8	beta-Propiolactone
123-38-6	Propionaldehyde
114-26-1	Propoxur (Baygon)
78-87-5	Propylene dichloride (1,2-Dichloropropane)
75-56-9	Propylene oxide
75-55-8	1,2-Propylenimine (2-Methylaziridine)
91-22-5	Quinoline
106-51-4	Quinone (p-Benzoquinone)
100-42-5	Styrene
96-09-3	Styrene oxide
1746-01-6	2,3,7,8-Tetrachlorodibenzo-p-dioxin
79-34-5	1,1,2,2-Tetrachloroethane
127-18-4	Tetrachloroethylene (Perchloroethylene)
7550-45-0	Titanium tetrachloride
108-88-3	Toluene
95-80-7	Toluene-2,4-diamine
584-84-9	2,4-Toluene diisocyanate
95-53-4	o-Toluidine
8001-35-2	Toxaphene (chlorinated camphene)
120-82-1	1,2,4-Trichlorobenzene
79-00-5	1,1,2-Trichloroethane

CAS Number	Chemical Name
79-01-6	Trichloroethylene
95-95-4	2,4,5-Trichlorophenol
88-06-2	2,4,6-Trichlorophenol
121-44-8	Triethylamine
1582-09-8	Trifluralin
540-84-1	2,2,4-Trimethylpentane
108-05-4	Vinyl acetate
593-60-2	Vinyl bromide
75-01-4	Vinyl chloride
75-35-4	Vinylidene chloride (1,1-Dichloroethylene)
1330-20-7	Xylene (mixed isomers)
95-47-6	o-Xylene
108-38-3	m-Xylene
106-42-3	p-Xylene
N/A	Antimony Compounds[a]
N/A	Arsenic Compounds[a] (inorganic including arsine)
N/A	Beryllium Compounds[a]
N/A	Cadmium Compounds[a]
N/A	Chromium Compounds[a]
N/A	Cobalt Compounds[a]
N/A	Coke Oven Emissions
N/A	Cyanide Compounds[a,b]
N/A	Glycol ethers[c]
N/A	Lead Compounds[a]
N/A	**Manganese Compounds[a]**
N/A	Mercury Compounds[a]
N/A	Fine mineral fibers[d]
N/A	Nickel Compounds[a]
N/A	Polycyclic Organic Matter[e]
N/A	Radionuclides (including radon)[f]
N/A	Selenium Compounds[a]

[a] For all listings above which contain the word "compounds" and for glycol ethers, the following applies: Unless otherwise specified, these listings are defined as including any unique chemical substance that contains the named chemical (i.e., antimony, arsenic, etc.) as part of that chemical's infrastructure.

[b] X'CN where X = H' or any other group where a formal dissociation may occur. For example, KCN or Ca(CN)$_2$.

[c] Includes mono- and di- ethers of ethylene glycol, diethylene glycol, and triethylene glycol R-(OCH$_2$CH$_2$)$_n$-OR'
where:

        n = 1, 2, or 3
        R = alkyl or aryl groups
        R' = R, H, or groups which, when removed, yield glycol ethers with the structure: R-(OCH$_2$CH$_2$)$_n$-OH.
        Polymers are excluded from the glycol category.

United States Federal Hazardous Air Pollutants (Continued)

[d] Includes mineral fiber emissions from facilities manufacturing or processing glass, rock, or slag fibers (or other mineral derived fibers) of average diameter 1 micrometer or less.

[e] Includes substituted and/or unsubstituted polycyclic aromatic hydrocarbons and aromatic heterocycle compounds, with two or more fused rings, at least one of which is benzenoid in structure. Polycyclic Organic Matter is a mixture of organic compounds containing one or more of these polycyclic aromatic chemicals. Polycyclic Organic Matter is generally formed or emitted during thermal processes including (1) incomplete combustion, (2) pyrolysis, (3) the volatilization, distillation or processing of fossil fuels or bitumens, or (4) the distillation or thermal processing of non-fossil fuels.

[f] A type of atom which spontaneously undergoes radioactive decay.