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MEXICO EMISSIONS INVENTORY PROGRAM MANUALS

VOLUME VIII – MODELING INVENTORY DEVELOPMENT

FINAL

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and

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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.
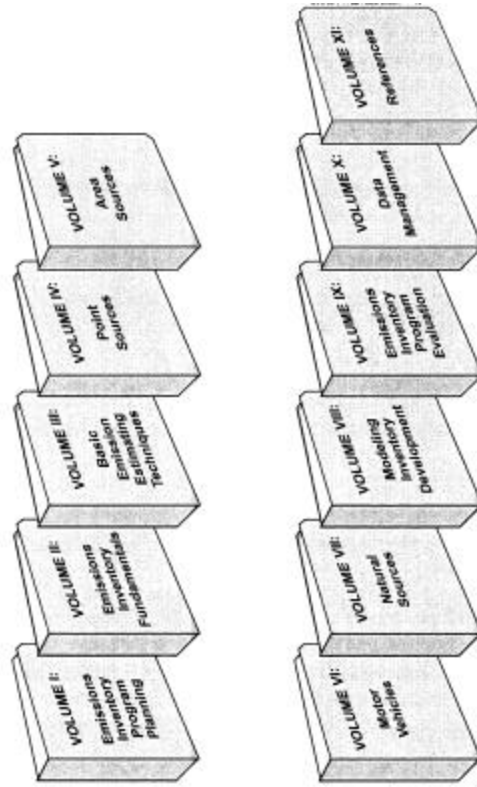
Figure 1. Mexico Emissions Inventory Program Manuals

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., hard-copy documents, electronic documents, and computer models).

CONTENTS

FIGURES AND TABLES

Figures **Page**

Tables   **Page**

ACRONYMS

AMS	Area and Mobile Source
ARB	California Air Resources Board
BAC	Binational Advisory Committee
CAS	Chemical Abstract System
CB-IV	Carbon Bond IV
CC	crankcase emissions
CE	control efficiency
CEIDARS	California Emission Inventory Development and Reporting System
CFC	chlorofluorocarbon
CMAP	Mexican Classification of Activities and Products
CO	carbon monoxide
CST	cold start emissions
DNL	diurnal emissions
EC	elemental carbon
EMS-95	Emissions Modeling System - 95
FIRE	Factor Information Retrieval Data System
g	gram
GEMAP	Geocoded Emissions Modeling and Projections System
GCVTC	Grand Canyon Visibility and Transport Commission
GIS	geographic information system
GPS	global positioning systems
HAP	hazardous air pollutant
HC	hydrocarbon
HCFC	hydrochlorofluorocarbon
HFC	hydrofluorocarbon
hr	hour
HSK	hot soak emissions
HST	hot start emissions

H_2SO_4	sulfuric acid
ID	identification number
IFU	Fraunhofer-Institut für Atmosphärische Umweltforschung (Fraunhoter Institute for Atmospheric Environmental Research)
I/M	inspection and maintenance
INE	Instituto Nacional de Ecología (National Institute of Ecology)
km	kilometer
m	meter
m^2	square meter
MCCM	IFU's regional scale air quality model
Mg	megagram (10^6 grams; 1 metric ton)
MOBILE	U.S. Environmental Protection Agency's motor vehicle emission factor model
N/A	not applicable
NAICS	North American Industry Classification System
NH_3	ammonia
NMHC	non-methane hydrocarbon
NMOG	non-methane organic gas
NO	nitric oxide
NO_x	nitrogen oxides
NO_2	nitrogen dioxide
OC	organic carbon
OH^-	hydroxyl radical
O_3	ozone
PCBEIS	U.S. Environmental Protection Agency's biogenic emissions model
PFC	perfluorocarbon
PM	particulate matter
$PM_{2.5}$	particulate matter less than 2.5 micrometers in aerodynamic diameter
PM_{10}	particulate matter less than 10 micrometers in aerodynamic diameter
QA	quality assurance

QC	quality control
RACM	Regional Atmospheric Chemistry Mechanism
RADM2	Regional Atmospheric Deposition Model Mechanism, Version 2
RE	rule effectiveness
REV	running evaporative emissions
REX	running exhaust emissions
ROG	reactive organic gas
RP	rule penetration
SAPRC	California Statewide Air Pollution Research Center
SCC	Source Classification Code
SIC	Standard Industrial Classification
SNIFF	Sistema Nacional de Información de Fuentes Fijas (National Information System of Point Sources)
SO_x	sulfur oxides
SO_2	sulfur dioxide
SO_3	sulfur trioxide
SO_4^{2-}	sulfate ion
SPECIATE	U.S. Environmental Protection Agency's speciation profile database
TDM	travel demand models
THC	total hydrocarbon
TNRCC	Texas Natural Resource Conservation Commission
TOG	total organic gas
TSP	total suspended particulate
UAM	Urban Airshed Model
U.S.	United States
U.S. EPA	United States Environmental Protection Agency
UTM	Universal Transverse Mercator
VKT	vehicle kilometers traveled
VOC	volatile organic compounds
WGA	Western Governors' Association

yr   year

μg   microgram

1.0   INTRODUCTION

Over the past 25 years, numerous studies have been performed to address air quality problems. More recently, many of these investigations have relied upon the use of advanced air quality models. Air quality modeling is often used to show compliance with ambient air quality standards for criteria pollutants (e.g., ozone [O_3], carbon monoxide [CO], nitrogen oxides [NO_x], etc.) or to analyze the effectiveness of various control strategies. Though photochemical modeling has traditionally been used to demonstrate attainment with ozone standards, regional modeling is expected to also be used in the future as a tool for demonstrating attainment with particulate matter and regional haze standards. Also, regional modeling is sometimes used to examine the health and/or environmental risk associated with hazardous air pollutant (HAP) emissions. Pollutant emission rates are a key input to these models. A modeling emissions inventory is a compilation of these pollutant emission rates, which are then utilized by an air quality model.

The purpose of this manual is to educate the reader on the steps that are involved in developing a modeling inventory. It is intended to be an introductory "bridge" document between Volume IV *(Point Source Inventory Development)*, Volume V *(Area Source Inventory Development)*, and Volume VI *(Motor Vehicle Inventory Development)* of this manual series and the user's guides for specific emissions modeling tools (e.g., Geocoded Emissions Modeling and Projections System [GEMAP] [Radian, 1993], Emissions Modeling System-95 [EMS-95] [U.S. EPA, 1999a], etc.). As such, the content of this document is not model-specific, but presents the general concepts of modeling inventory development and illustrates them through the use of figures and numerical examples.

A number of papers that describe the use of GEMAP and EMS-95 for developing modeling inventories were identified in the technical literature (Beidler et al., 1996; Benjey and Moghari, 1995; Bruckman, 1993; Bruckman and Oliver, 1993; Dickson and Oliver, 1991; Dickson et al., 1992; Dickson et al., 1993; Dickson et al., 1994; Janssen, 1996; Janssen, 1998; Koerber, 1992; Mayenkar et al., 1992; and Oliver et al., 1998); these references are provided in

Section 10.0. It should be noted that GEMAP and EMS-95 are two widely used emissions modeling tools; other useful emissions modeling tools may exist. The specific inventory and modeling objectives should be examined in order to select the appropriate emissions modeling tool. Selection of an emissions model is often made on the basis of:

- Familiarity with existing emissions models; and
- Compatibility of emissions model formats with both existing input data and requirements of the air quality model.

The availability of input data for the emissions model is essential to the success of emissions modeling, but usually does not significantly affect the selection of a particular emissions model. All such models require a great amount of site-specific and source-specific input data.

The technical steps conducted during modeling inventory development to process the inventories for input to air quality models are as follows:

1. Temporal allocation – breaking down the annual emission estimates in the base year inventory into smaller time increments (usually hourly);

2. Spatial allocation – distributing the base year emission estimates into individual grid cells defined over the inventory domain;

3. Speciation – breaking down total organic gas (TOG)/reactive organic gas (ROG) emissions into reactivity groups and/or individual chemical species, total NO_x into nitric oxide (NO) and nitrogen dioxide (NO_2), and total particulate matter (PM) by particle size and/or individual chemical species; and

4. Projections – combining base year emission estimates with growth and control factors to estimate emissions for future years.

To implement these technical steps, many different data sets are required. These data need to be specifically tailored to the geographic modeling region and to the operating conditions of the source types within that region. For example, site-specific data are needed for spatial allocation profiles and seasonal operating rates. Source-specific data are needed for temporal allocation profiles (seasonal, weekly, hourly), emissions chemical speciation, and growth/control factors. Thus, each modeling domain and each source category requires specific data sets for temporal and spatial allocation, speciation, and emission projections.

Many of the required data sets should not be generalized. For example, hourly vehicle traffic patterns in Mexico City are likely to be different than in metropolitan areas along the Mexico-U.S. border (e.g., Ciudad Juárez, Mexicali, etc.). The appropriate data needed for the emissions model are specific, in many cases, to prevailing conditions in each region and for each source type. In such cases, these data cannot simply be assumed without affecting the validity of the emissions model results. Examples include the required spatial allocation profiles, temporal profiles for motor vehicles and airports, and emission projections.

For those data sets in which assumptions or generalizations will not compromise the results, Mexico-specific data are preferred. However, it is expected that U.S.-derived data sets will be used in selected cases until the Mexico- or site-specific information can be developed. Examples of these types of data include emissions, chemical speciation profiles for most source types, and some temporal allocation profiles (e.g., operating patterns for solvent usage, etc.).

Nevertheless, a large amount of data is required to implement the temporal, spatial, speciation, and projection steps in an emissions modeling system. These data sets must be obtained for the modeling domain so that the emissions modeling methods described in this manual can be reliably applied.

In order to clearly explain the four modeling inventory development steps listed above, an easy-to-understand modeling inventory example is used throughout this document and is presented in shaded boxes. The example is based upon the hypothetical modeling inventory community presented in Figure 1-1. The community contains the following six emission sources:

- A point source (i.e., a large factory) with a boiler for seasonal heating and a surface coating process (counted as two separate emission sources);
- On-road motor vehicles (i.e. light-duty passenger automobiles);
- Gasoline stations;
- Residential consumer solvent use; and
- Agricultural pesticide application.
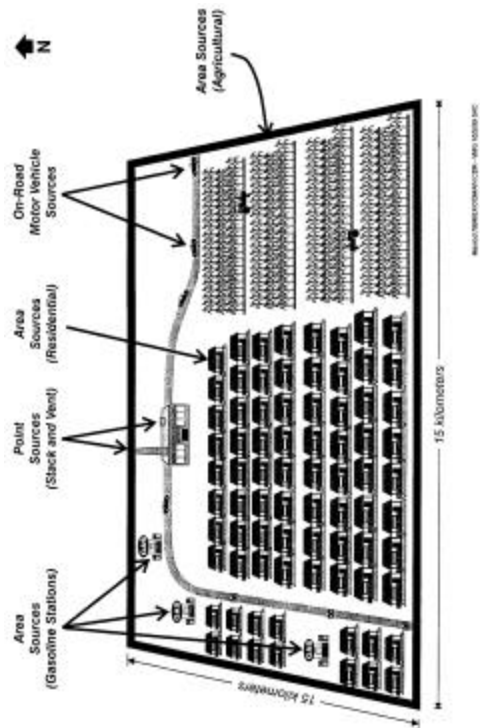
Figure 1-1. Hypothetical Modeling Inventory Community

All six emission sources emit TOG, while CO and NO_x emissions are limited to the two combustion sources (i.e., the factory boiler and light-duty automobiles). Assumed annual emissions for these six emission sources are presented in Table 1-1.

Table 1-1. Assumed Annual Emissions for Emission Sources in Hypothetical Modeling Inventory Community

Emission Source	TOG (Mg/yr)	CO (Mg/yr)	NO_x (Mg/yr)
Factory (Boiler)	200	600	400
Factory (Surface Coating)	300	N/A	N/A
Light-Duty Automobiles	400	800	600
Gasoline Stations	150	N/A	N/A
Residential Consumer Solvent Use	200	N/A	N/A
Agricultural Pesticide Application	100	N/A	N/A

Mg/yr = megagrams (10^6 grams or 1 metric ton) per year
N/A   = not applicable

The number of emission sources has been limited to six, so that the various modeling inventory development steps can be adequately demonstrated without the number of associated calculations becoming too large. An actual modeling inventory will contain many more emission sources and will require more sophisticated data manipulation tools than the simple calculations presented in this manual. In addition, only TOG, CO, and NO_x emissions will be directly addressed in the model. There will be some discussion of PM and other pollutants, but the main focus of the example will be on TOG, CO, and NO_x. Finally, it should be noted that all values used in the hypothetical modeling inventory are for demonstration purposes only and should <u>not</u> be used in actual modeling inventories.

The remainder of this manual is organized as follows:

- Section 2.0 presents the data and computing requirements for a modeling inventory;

- Section 3.0 explains temporal allocation;

- Section 4.0 describes spatial allocation;

- Section 5.0 explains speciation;

- Section 6.0 discusses emission projections;

- Section 7.0 presents the modeling inventory development example for one source category;

- Section 8.0 contains some analyses of the entire hypothetical modeling inventory;

- Section 9.0 presents a conclusion for this manual;

- Section 10.0 contains references used in development of this manual;

- Appendix A contains the calculation spreadsheets used for the hypothetical modeling inventory;

- Appendix B presents the TOG speciation profiles associated with the source categories used in the hypothetical modeling inventory; and

- Appendix C presents the PM speciation profiles associated with the source categories used in the hypothetical modeling inventory.

2.0　MODELING INVENTORY REQUIREMENTS

The starting point for development of a modeling inventory is a database of emissions-related data, often referred to as the *base year inventory*. It is important to understand that a spreadsheet containing only the annual emission estimates for the base year would not be a sufficiently robust enough data set to support modeling inventory development. Examples of other emissions-related data that would need to be included in the base year inventory are facility information, material types and throughputs, stack parameters, etc. An extensive, but not comprehensive, list of needed base year inventory data for point sources is provided in Table 2-1. Similar data for area, motor vehicle, and biogenic sources are presented in Tables 2-2 through 2-4.

Table 2-1.　Typical Base Year Inventory Data – Point Sources

Data Type	Data Element
Facility Data	Facility ID Facility Name Facility Industrial Code – SIC, NAICS, CMAP Facility UTMs (Easting, Northing, Zone)
Stack Data	Stack ID Stack Inside Diameter Stack Height (above ground surface) Stack Exit Temperature Stack Exit Velocity Stack Exit Flow Rate Stack UTM Coordinates (Easting, Northing, Zone) Stack Elevation (of base above sea level)
Device Data	Device ID Operation Schedule Data – Fractional Monthly Throughputs Fractional Seasonal Throughputs Operation Weeks/Year Operation Days/Week Operation Hours/Day
Process Data	Process ID SCC Annual Process Rate/Throughput

Table 2-1. (Continued)

Data Type	Data Element
Emissions Data	Pollutant ID Actual Emission Factors Actual Annual Emissions Primary Control Equipment Code Secondary Control Equipment Code Overall Control Equipment Efficiency

CMAP = Mexican Classification of Activities and Products
ID = identification number
NAICS = North American Industry Classification System
SCC = Source Classification Code
SIC = Standard Industrial Classification
UTM = Universal Transverse Mercator

Table 2-2. Typical Base Year Inventory Data – Area Sources

Data Type	Data Element
Location Data	State Code County/Municipality Code
Source Data	Area Category Code
Emissions Data	Pollutant ID Actual Emission Factor Allowable Emission Factor Actual Emission Estimate Allowable Emission Estimate Primary Control Equipment Secondary Control Equipment Control Efficiency Temporal Basis (Average Annual or Average Day)

ID = identification number

Table 2-3. Typical Base Year Inventory Data – Motor Vehicle Sources

Data Type	Data Element
Location Data	State Code County/Municipality Code
Source Data	Vehicle Class Vehicle Technology Type
Emissions Data	Pollutant ID Motor Vehicle Emission Process Code (i.e., REX, CST, HST, REV, HSK, DNL, CC) Total Daily County-Wide Emission Estimate

CC = crankcase emissions   HST = hot start emissions
CST = cold start emissions   ID = identification
DNL = diurnal emissions   REV = running evaporative emissions
HSK = hot soak emissions   REX = running exhaust emissions

Table 2-4. Typical Base Year Inventory Data – Biogenic Sources

Data Type	Data Element
Location Data	State Code County/Municipality Code
Source Data	Plant Community Code (i.e., Vegetation Type)
Emissions Data	Pollutant ID Canopy Type Biogenic Emission Flux ($\mu g/m^2$-hr)

hr = hour
ID = identification number
m^2 = square meter
μg = microgram

These additional data are needed to support the modeling and its end-uses such as analyzing source impacts and assessing the effectiveness of air pollution control strategies. For example, facility information can help identify which industrial sectors are the major contributors to air pollution in the inventory region and focus the development of control measures. Material types and throughputs may also be used to refine the control strategy (e.g., which fuel types are responsible for most of the combustion emissions). Stack parameters are used together with meteorological data to model the dispersion and transport of the pollutants from their release point. If accurate, inventory-specific data are not available, appropriate assumptions should be made for these missing data.

The base year inventory data also typically include fields for coding the emissions-related data. Coding systems are usually keyed to source types and facilitate the extensive manipulation of modeling inventory data. Without coding systems, data manipulation becomes difficult, if not impossible. Some examples of commonly used coding systems include state and municipality abbreviations, industrial classifications, and emission category codes. Coding systems are used to assign appropriate temporal profiles, spatial surrogates, and/or speciation profiles to emission estimates. An example of this assignment is provided in Table 2-5.

**Table 2-5. Sample Coding System Assignment of Temporal Profiles,
Spatial Surrogates, and Speciation Profiles**

Source Category	SCC	AMS	Temporal Profile ID[a]	Spatial Surrogate ID[b]	Speciation Profile ID[c]
Factory Boiler	10200601	N/A	024	N/A	0002
Gasoline Stations	N/A	25-01-060-000	075	99	1190
Light-Duty Automobiles	N/A	22-01-001-000	051	47	1101

[a] The temporal profile ID is a numerical code that identifies a specific temporal profile; in this table, the temporal profile IDs
     are fictitious.
[b] The spatial surrogate ID is a numerical code that identifies a specific spatial surrogate; in this table the spatial surrogate IDs
     are fictitious.
[c] The speciation profile ID is a numerical code that identifies a specific speciation profile; in this table the speciation profile
     IDs were obtained from U.S. EPA's SPECIATE database (U.S. EPA, 1999c).

ID   =   identification number
N/A =   not applicable
SCC =   Source Classification Code

The existing industrial classification system in Mexico is the 1999 Mexican
Classification of Activities and Products (CMAP), while the 1987 Standard Industrial
Classification (SIC) system (OMB, 1987) is widely used in the United States (U.S.). The CMAP
classification system is somewhat similar to the SIC system. However, the North American
Industry Classification System (OMB, 1997; U.S. Census, 1999), a tri-national industrial
classification system, is starting to be implemented in Mexico, the U.S., and Canada. Another
example of codes are industrial location data codes that are used in the UBICIND database file
within Mexico's National Information System of Point Sources (SNIFF).

The U.S. currently employs Source Classification Codes (SCC) for point sources
and Area and Mobile Source (AMS) category codes for area and mobile sources. Listings of
SCC codes are provided in Appendix E of Volume IV (*Point Source Inventory Development*)
and listings of AMS codes are provided in Appendix A of Volume V (*Area Source Inventory
Development*). Mexico currently does not have a comprehensive system of emission category
codes, but such a coding system is needed before modeling inventories can be developed.

Due to the volume of data involved, an electronic emissions modeling system is a
necessity for modeling inventory development. An emissions modeling system is a group of
emissions models executed in a specific sequence that processes annual emission estimates to

generate speciated, spatially and temporally resolved values for input to photochemical and other regional air quality models. Each emissions model is an integrated collection of calculational procedures, or algorithms, properly encoded for computer-based computation. For example, GEMAP and EMS-95 have distinct emissions models for point, area, motor vehicle, and biogenic sources. Figure 2-1 identifies the distinct emission models within the overall GEMAP structure. Emissions modeling systems also include a geographic information system (GIS) tool to process the various spatial data sets or "coverages" (e.g., the definition of the inventory domain, political boundaries, population, vegetation type, etc.). The GIS tool can be used to visualize various aspects of the modeling inventory that may not be readily apparent by simply looking at the numerical data in the inventory database.

Modeling inventories will have large quantities of data associated with them. This is not surprising given that inventory domains can be on the order of thousands of square kilometers with a required spatial resolution as fine as 500 meters. This is further compounded by the need for hourly estimates of potentially hundreds of chemical species for the large number of source categories that comprise a comprehensive modeling emissions inventory. A Mexico-specific example of the large volume of data generated with modeling inventories is conceptually illustrated in Figure 2-2.

An air toxics inventory was previously performed for Ambos Nogales (i.e., Nogales, Sonora; and Nogales, Arizona) (Radian, 1997). The characteristics of the inventory included:

- Domain evenly divided between Mexico and the U.S.;
- Domain measuring 19 kilometers (km) (north-south) by 12 km (east-west);
- 500-meter grid cells (total number of grid cells – 912);
- Four different seasons (total of 96 different hours);
- 113 individual air toxic species; and
- 103 different area and motor vehicle sources.
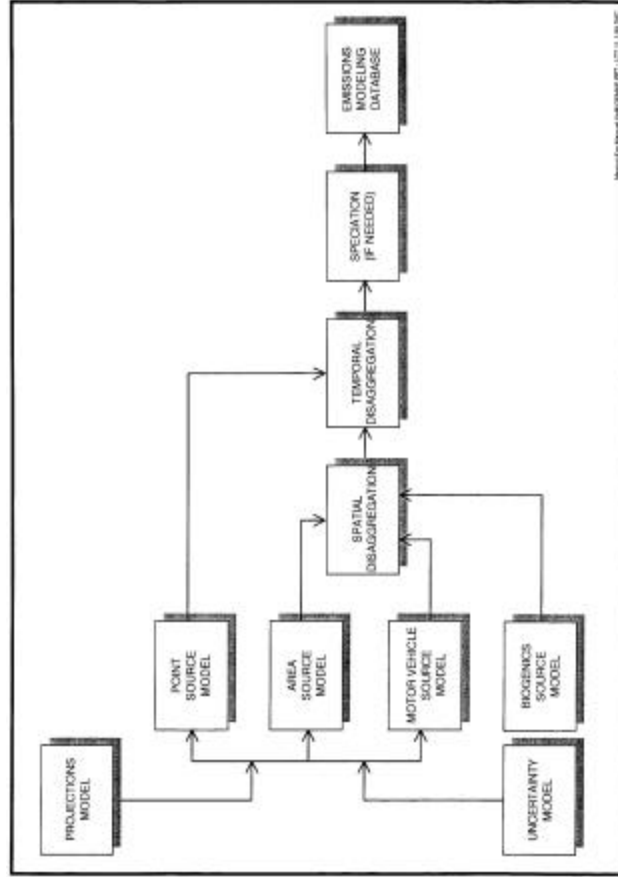
Figure 2-1. GEMAP Structure
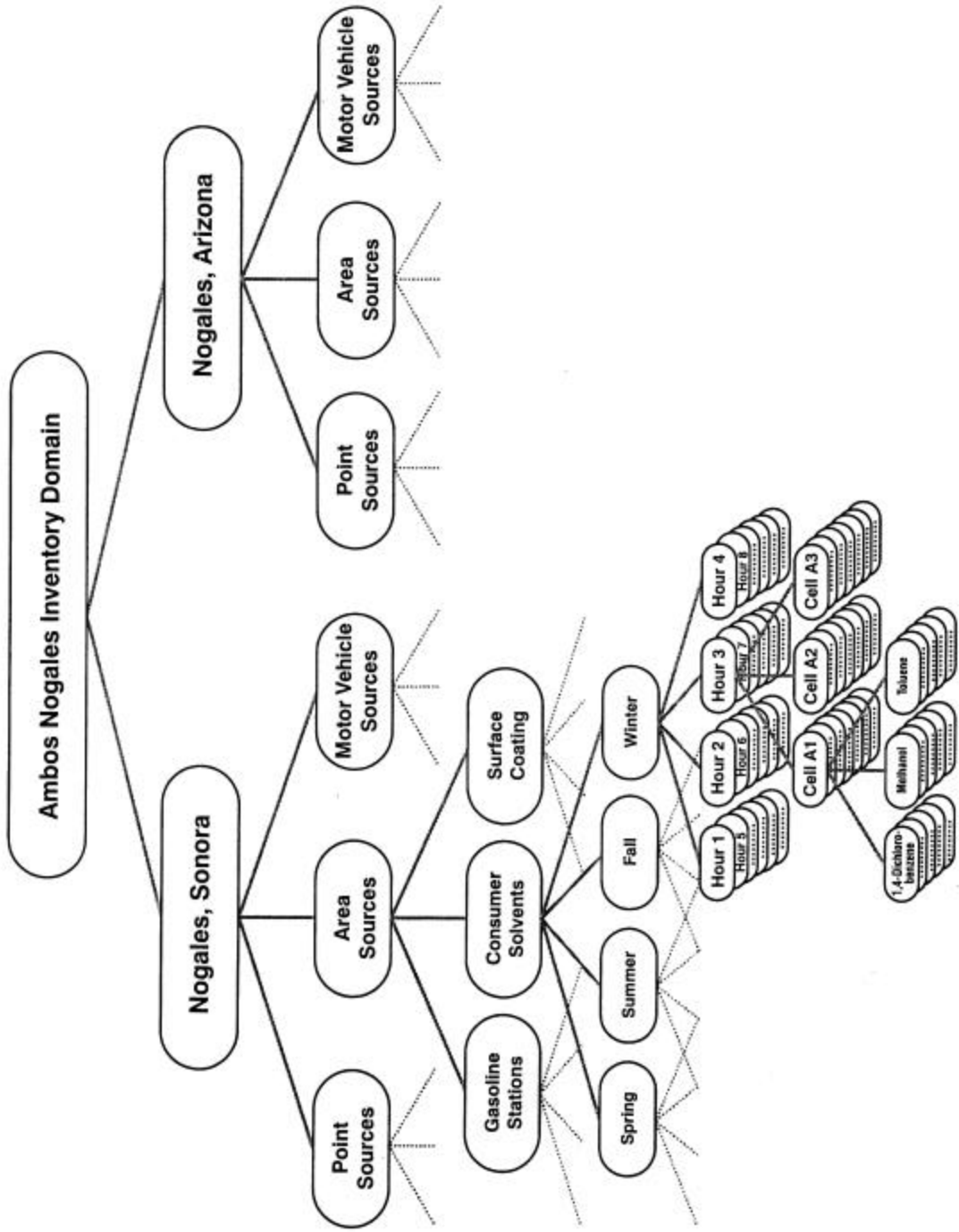
Figure 2-2. Conceptual Diagram of Ambos Nogales Hazardous Air Pollutant Modeling Inventory

Although not all air toxics were emitted from every source category and not all source categories were located in every grid cell for the Ambos Nogales air toxics inventory, the total potential number of speciated, spatially and temporally resolved emission values exceeded one billion (1×10^9). The actual number of emission values was somewhat less. In Figure 2-2, only some of the speciated consumer solvent emissions in Cell A1 for Nogales, Sonora during Hour 3 of an average winter day are represented. The entire inventory was much larger than this, but it could not be clearly represented in one figure; the other emissions were not presented in the figure in order to preserve conceptual clarity.

3.0   TEMPORAL ALLOCATION

The first step of modeling inventory development is the temporal allocation of emissions. Because air quality modeling attempts to represent the actual physical and chemical processes as they occur over a specific duration of time, it is important that the temporal allocation of emissions be as accurate as possible. Temporal allocation can be thought of as an accounting of emissions variation over time. The simplest temporal allocation is for a steady-state emissions source that continually releases emissions at the same rate all the time. Under actual conditions, however, steady-state emission sources are quite rare. Instead, under actual conditions, emission sources may operate only in the winter (e.g., space heating), not operate on Sundays (e.g., many commercial or industrial sources), or their activity may peak during certain hours of the day (e.g., motor vehicle commute traffic). Temporal allocations allow emissions variability to be correctly modeled during the desired modeling periods. The desired modeling periods will vary depending upon the purpose of the inventory. For instance, some inventories will need only average day emissions for each season, while other inventories will require more specific data to reproduce a historical multi-day ozone episode.

In general, the starting point for temporal allocation in modeling inventories is annual emission estimates. Temporal allocation is then performed using *temporal allocation profiles*. Temporal allocation profiles indicate the distribution of emissions over the selected period of disaggregation (e.g., season, week, day). The annual emission estimates are first disaggregated using seasonal (spring/summer/fall/winter) allocation profiles. Weekly allocation profiles are then used to account for differences in typical weekday, Saturday, and Sunday activity levels. Finally, hourly allocation profiles are used to estimate the hour-by-hour differences in emissions.

Default seasonal, weekly, and hourly temporal allocation profiles are often included in electronic emissions modeling systems. However, for each modeling inventory being developed, it should be determined whether or not it is appropriate to use the default allocation profiles. For some source categories, default allocation profiles do not accurately characterize the

actual temporal distribution of emissions. If the use of default allocation profiles is not appropriate, some inventory-specific allocation profiles will need to be developed.

It should also be noted that "day-specific" emission estimates are required for some specialized modeling applications. The use of day-specific emission estimates, however, is not widespread because of typical inventory resource constraints and lack of day-specific data. Instead of estimating hourly emissions using temporal allocations in a "top-down" approach, day-specific emissions are estimated using a "bottom-up" approach that incorporates activity data (e.g., material throughput, hours of operation, etc.) from a specific designated day. Day-specific emissions are typically limited to a few significant point sources. In general, the disperse nature of other source types usually prevents activity data from being collected for a specific day. However, day-specific emissions are sometimes estimated for episodic source categories (e.g., wildfires, prescribed burning, agricultural pesticide application, etc.). Additional discussion of day-specific emissions can be found in Section 3.4.

3.1 <u>Seasonal Allocation Profiles</u>

The first step of temporal allocation is to disaggregate annual emissions into four seasonal emissions subtotals using seasonal temporal profiles. In some cases, seasonal temporal profiles are readily available, but in other situations they must be derived from monthly emissions or activity data. This is done by summing the monthly portion of emissions or activity data for three months into a single season. In general, modeling inventory seasons are conventionally defined as follows:

- Spring (March, April, May);
- Summer (June, July, August);
- Fall (September, October, November); and
- Winter (December, January, February).

However, local circumstances may dictate that different seasonal groupings be used. Monthly temporal allocation is sometimes, but not often, performed as part of modeling inventory development.

Some emission sources release emissions at the same rate throughout the year, while other emission sources have significant seasonal variations. Figure 3-1 shows assumed seasonal allocation profiles for two of the sources in the hypothetical modeling inventory. The first assumed seasonal profile shows an emission source that is constant throughout the year (i.e., the factory coating process); the second assumed seasonal profile shows a seasonally variable emission source (i.e., the factory boiler used for heating). The boiler shows high emissions during the winter, which is a period of high space-heating demand, while no emissions are assigned to the summer because the boiler is not used during that period of time. Other examples of seasonally variable emission sources include motor vehicles (due to possible increased usage during vacation and holiday periods) and agricultural activities (due to seasonal crop requirements). Regardless of the seasonal variability, all seasonal (or monthly) allocations should add to 1.00 (or 100 percent).

3.2   **Weekly Allocation Profiles**

After seasonal allocation has been completed, emissions must be allocated on a weekly basis (i.e., typical weekday, Saturday, and Sunday). For many sources, emissions are not constant throughout the week. For instance, operation of many industrial facilities will be limited to a five- or six-day workweek. Likewise, urban motor vehicle activity and emissions will be somewhat different during the weekend, which is strongly influenced by recreational activities, compared to weekdays, which are dominated by commute traffic. Unlike the seasonal allocation profiles, which sum to 1.00 and are easy to estimate from monthly allocations, the determination of weekly profiles is more complex. The steps for determining weekly profiles are outlined as follows:

- The average daily factor (F_{ad}) for any season is 0.011 of the seasonal emissions (100 percent divided by 91 days in a season).

- The average daily factor is converted to an average weekday factor (F_{wd}) by multiplying the average daily factor by the ratio of the actual weekday fraction of weekly emissions (A_{wd}) divided by the average day fraction of weekly emissions (i.e., 1 day divided by 7 days, or approximately 0.1429).
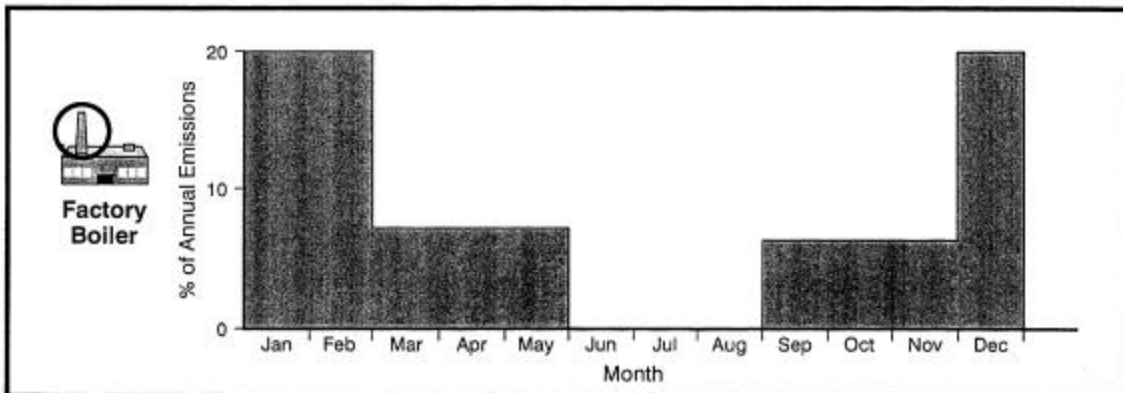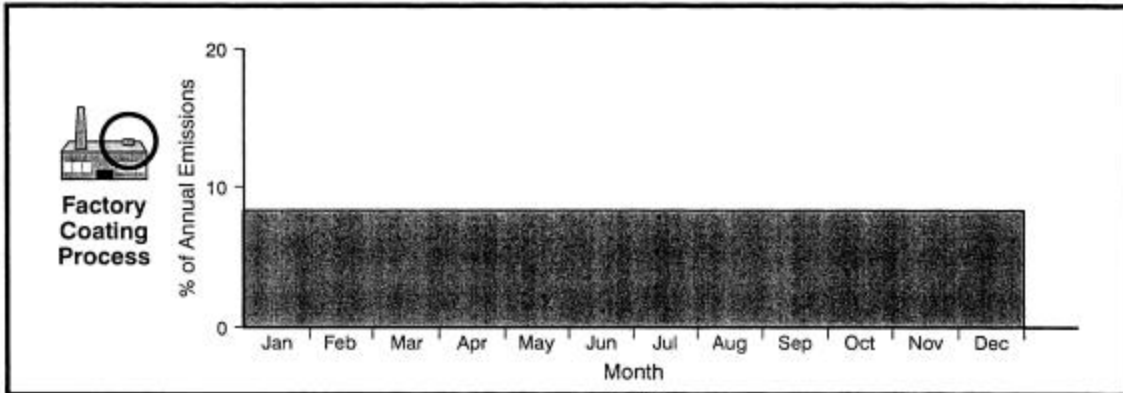
Figure 3-1. Examples of Assumed Constant and Variable Seasonal Allocation Profiles for the Hypothetical Modeling Inventory

- Average Saturday and Sunday factors (F_{sat}; F_{sun}) are estimated in a similar manner; the average daily factor is multiplied by the ratio of the actual Saturday and Sunday fractions of weekly emissions (A_{sat}; A_{sun}) divided by the average day fraction.

For example, assume that a source category operates on Monday through Friday with equal activity on each day and with no operation on Saturday or Sunday. As mentioned above, the average daily emissions are 1.1% of the total seasonal emissions. The actual average weekday fraction of weekly emissions is 0.200 (i.e., 1.00 divided by 5 weekdays), while the actual Saturday and Sunday fractions of weekly emissions are both 0.000. The calculation of the average weekday, Saturday, and Sunday factors is shown as follows:

$$F_{wd} = 1.1\% \times (0.200/0.1429) = 1.54\%$$
$$F_{sat} = 1.1\% \times (0.000/0.1429) = 0.00\%$$
$$F_{sun} = 1.1\% \times (0.000/0.1429) = 0.00\%$$

The weekly allocation factors can be verified by applying the following equation (where 65 is the number of weekdays in a season and 13 is the number of Saturdays or Sundays in a season):

$$(65 \times F_{wd}) + (13 \times F_{sat}) + (13 \times F_{sun}) = 1.00$$
$$(65 \times 0.0154) + (13 \times 0.0000) + (13 \times 0.0000) = 1.001 \approx 1.000$$

If this equation is not correctly satisfied, an error has been made in the calculation of the weekly allocation factors.

3.3 <u>Hourly Allocation Profiles</u>

The final step of temporal allocation is the disaggregation of daily emissions (i.e., average weekday, Saturday, or Sunday) into hourly emissions. Except for some industrial facilities that may operate at the same level "around-the-clock," most emission sources will undergo some sort of operational variation during the day. For instance, motor vehicle emissions will typically have distinct peak values during the morning and evening commutes, but will drop to very low levels in the early morning (i.e., 2 or 3 a.m.). Emissions from some industrial

facilities will be limited to an 8-hour shift. Assumed hourly allocation profiles for both of these examples are shown in Figure 3-2. The hourly allocation profiles indicate the fraction of daily emissions that occur in each hour. Regardless of the hourly variability, the 24 hourly fractions in the hourly allocation profile should add up to 1.00 (or 100 percent).

3.4   <u>Day-specific Emissions</u>

For most modeling inventories, the "top-down" temporal allocation of annual emissions into progressively smaller time periods as described in Section 3.1 through Section 3.3 can be used. However, there may be some situations where day-specific emissions are desired. In particular, day-specific emissions are often used to model high-ozone (or other pollutant) events. Day-specific emissions are used in an effort to approximate a specific day's emissions as closely as possible; day-specific emissions will be more accurate than temporally allocated emissions which often rely on default temporal profiles. Day-specific emissions are generated using activity data collected for a particular day or even a specific hour. In general, day-specific emissions are usually only estimated from point sources with known operating schedules and parameters, but it may be feasible to estimate day-specific emissions from certain types of episodic area sources (e.g., wildfires, prescribed fires, agricultural pesticide application, etc.). Day-specific emissions also can be estimated for sources that are affected by extraordinary events (e.g., air quality alerts, sporting events, etc.). However, it will usually be too resource-intensive to collect day-specific activity data for all sources in an entire inventory.

3.5   <u>Source Type Considerations</u>

In addition to the general temporal allocation process discussed above, there are some issues that should be considered for certain source types. These issues are addressed as follows:

Point Sources

Ideally, temporal profiles will be assigned to the process level for all point sources. However, data availability and/or resource limitations may force temporal profiles to be assigned at a less refined level (i.e., device level or facility level). In order to determine
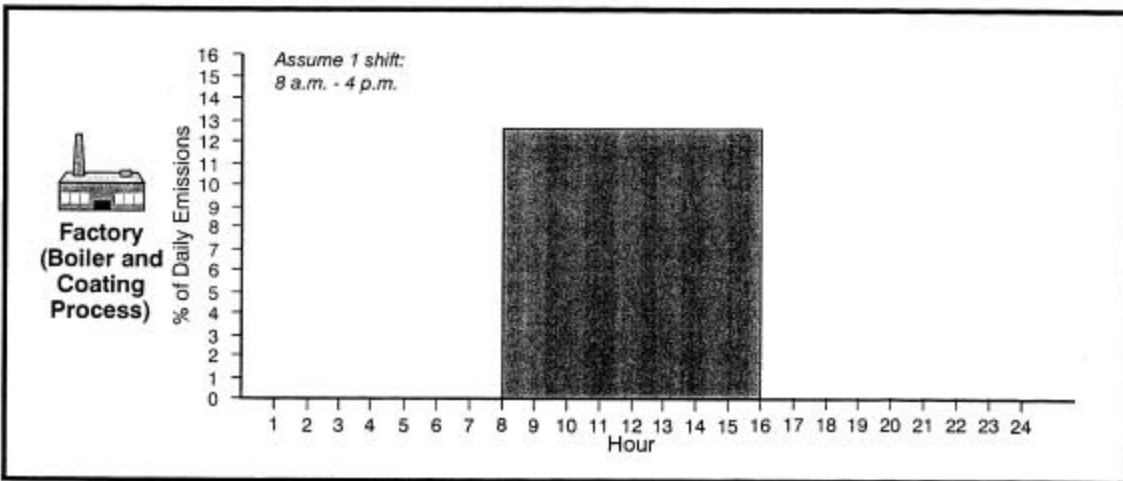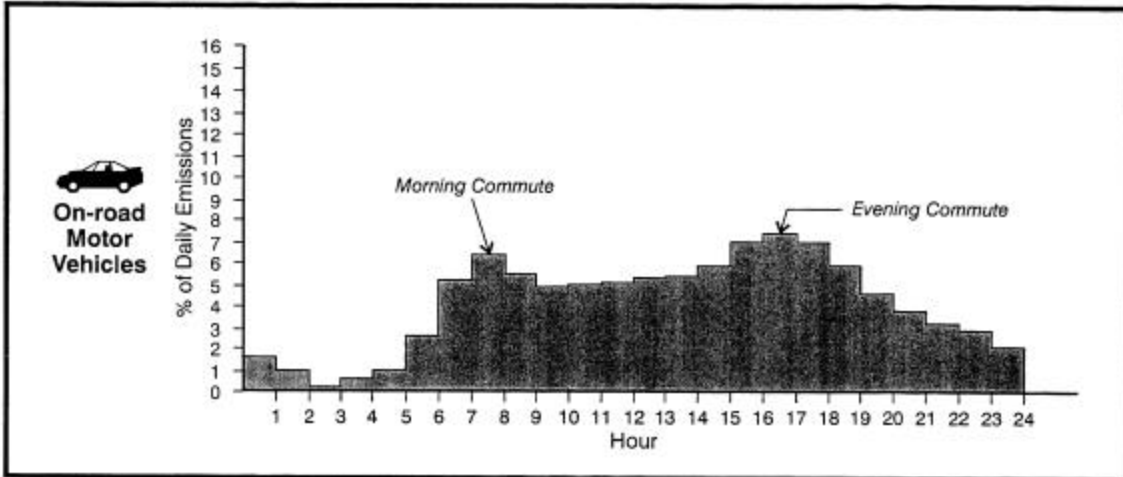
Figure 3-2. Examples of Assumed Hourly Allocation Profiles for the Hypothetical Modeling Inventory

appropriate temporal profiles, actual point source operating schedules should be obtained wherever possible. These schedules will typically be obtained from surveys. Depending upon the selected air quality modeling requirements, temporal profiles for point sources may need to be adjusted for holiday operating schedules. Different temporal profiles should be considered for weekday and weekend activity levels for most sources.

Area Sources

Each area source category typically has a default temporal profile assigned to it by emissions modeling tools. However, the emission processes and temporal distribution for each inventory region varies (e.g., agricultural emissions will vary across different climatic regions due to different crop types and cultivation practices, cutback asphalt paving may be prohibited in summer months in some regions, etc.). Where possible, temporal profiles should be customized for each emissions inventory. If it is necessary to use default temporal profiles, these profiles should be assessed prior to the actual temporal allocation process to determine whether or not they are appropriate for a particular emissions inventory. Accurate temporal profiles will certainly improve the quality of hourly emissions.

Motor Vehicle Sources

Motor vehicles typically have considerable temporal variation. The amount of motor vehicle travel may vary significantly from season-to-season or month-to-month. Also, depending upon the inventory region, weekday travel patterns may be quite dissimilar to weekend travel patterns. Holiday motor vehicle activity levels may also be different from non-holiday activity levels. It is crucial that the temporal allocation profiles for motor vehicles accurately reflect actual motor vehicle activity for the specific time periods of interest.

Natural Sources

If computer models (e.g., PCBEIS [U.S. EPA's biogenic emissions model]) (U.S. EPA, 1998) are used to develop biogenic or other natural source emissions, temporal allocation normally is not needed because the temporal allocation has already been accounted for in the models.

3.6 <u>Temporal Allocation Example</u>

This portion of the example will focus on the temporal allocation of annual emissions to hourly emissions only; other modeling inventory development steps are demonstrated elsewhere in this document. In order to provide a clear example, the calculation of one hourly emission estimate (i.e., hourly emissions for the eighth hour [between 7 a.m. and 8 a.m.] on an average summer weekday) is shown for one emission source (i.e. on-road motor vehicles). A more detailed example sequentially showing all modeling inventory development steps for one source category is presented in Section 7.0; the emission calculations associated with the entire example are presented in Appendix A.

The assumed temporal allocations that are associated with the six sources in the hypothetical inventory grid are graphically shown in Figure 3-3 (monthly profiles), Figure 3-4 (weekly profiles), and Figure 3-5 (daily profiles). The numerical data for these profiles are provided in Appendix A. The temporal profiles shown in these figures are hypothetical and should <u>not</u> be used in the development of actual modeling inventories.
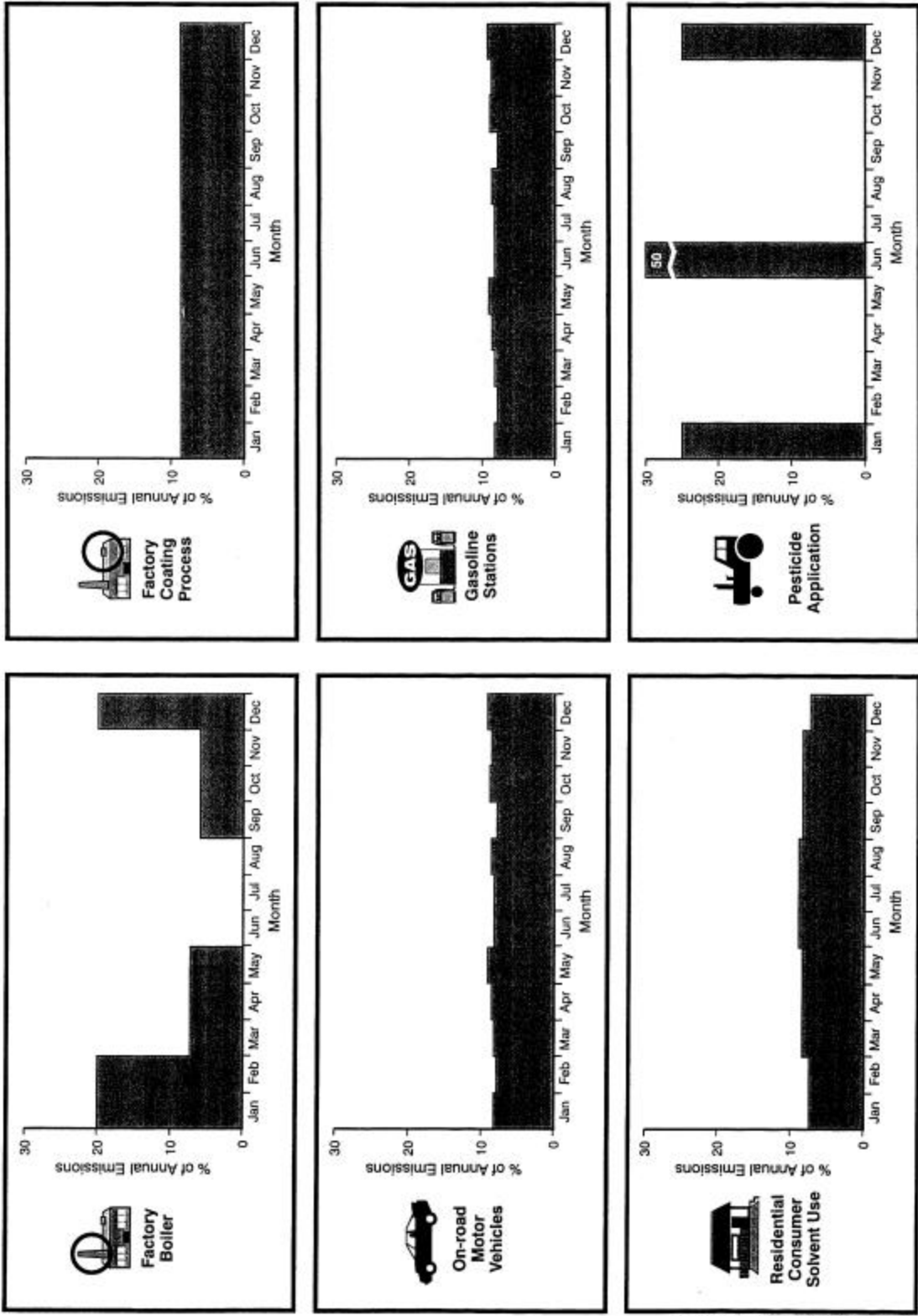
Figure 3–3. Assumed Monthly Temporal Allocation Profiles for the Hypothetical Modeling Inventory

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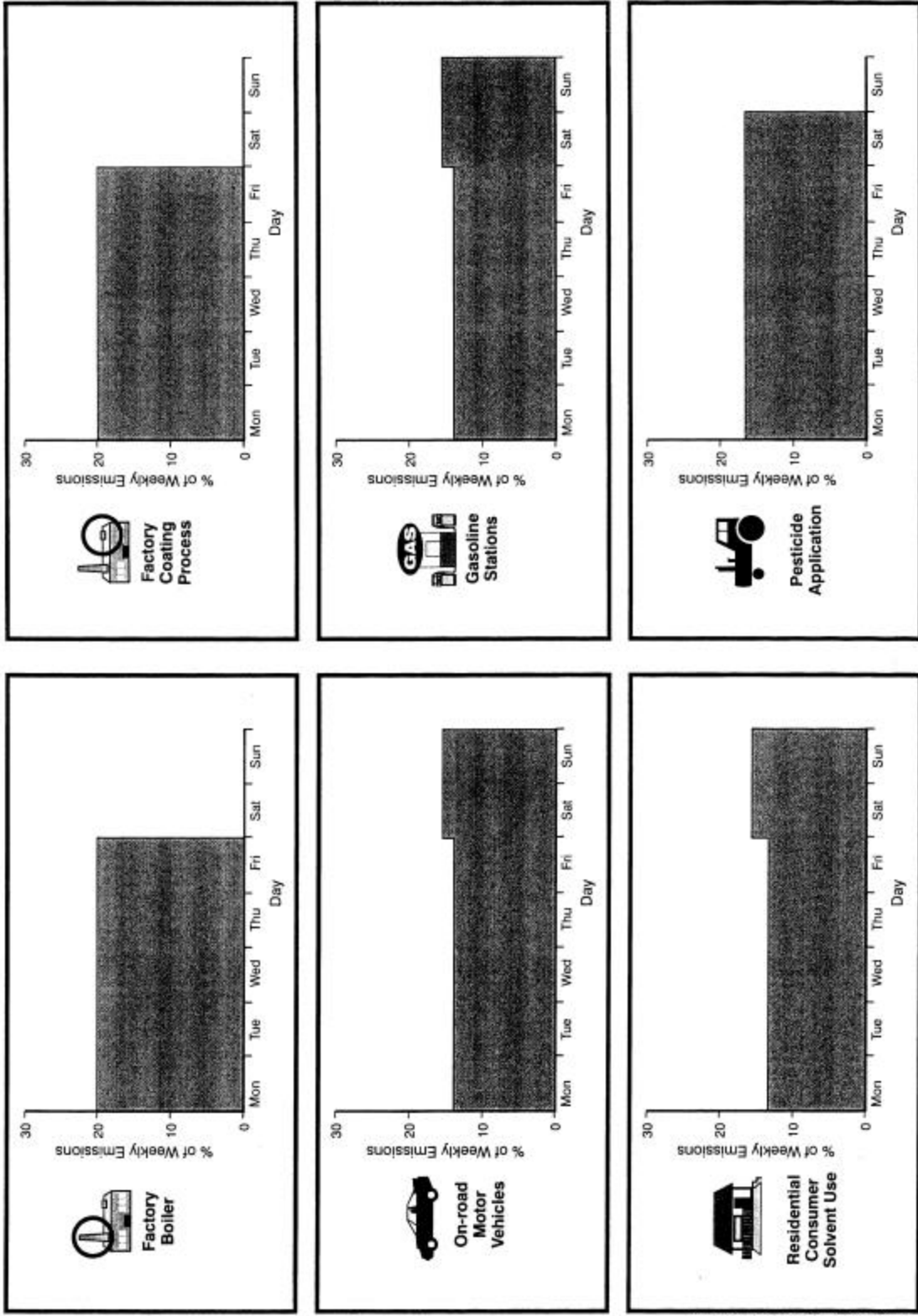
Figure 3-4. Assumed Weekly Temporal Allocation Profiles for the Hypothetical Modeling Inventory
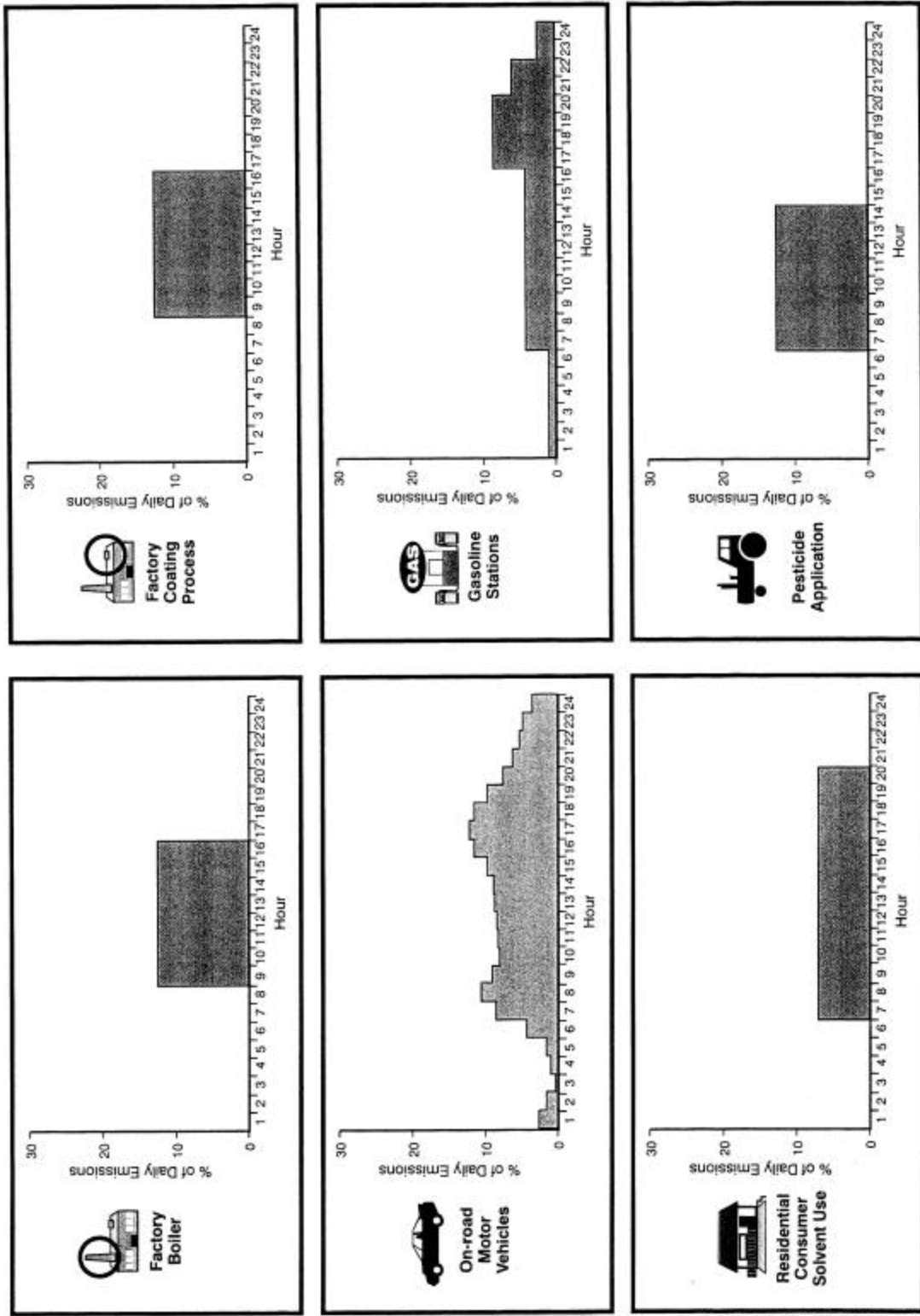
Figure 3-5. Assumed Hourly Temporal Allocation Profiles for the Hypothetical Modeling Inventory

Example Calculation

Although the calculations presented in this example are quite straightforward, it should be pointed out that these calculations were limited to one season, day, hour, and source category. If all seasons, days, hours, and source categories are to be addressed, a large number of calculations will need to be performed. The number of calculations would further expand if the other modeling inventory steps (i.e., spatial allocation, speciation, and projections) are considered. This large volume of calculations will need to be performed with a computer modeling tool, rather than by hand, in order to reduce calculation time and minimize the number of potential errors

Step 1 – Seasonal Temporal Allocation

Motor vehicle activity is distributed throughout the year as shown in Table 3-1.

Table 3-1. Assumed Monthly Motor Vehicle Temporal Allocation Profile for the Hypothetical Modeling Inventory

Month	Fraction of Annual Activity
January	0.081
February	0.078
March	0.080
April	0.084
May	0.089
June	0.081
July	0.082
August	0.083
September	0.079
October	0.088
November	0.084
December	0.091
Total	**1.000**

The equation for converting monthly temporal allocations into seasonal temporal allocations is as follows:

$$TA_s = TA_{m1} + TA_{m2} + TA_{m3}$$

Where TA_s = Seasonal temporal allocation for season "s";

        TA_{m1} = Monthly temporal allocation for month 1 of season "s";

        TA_{m2} = Monthly temporal allocation for month 2 of season "s"; and

        TA_{m3} = Monthly temporal allocation for month 3 of season "s."

The four seasonal temporal allocations are calculated as follows (only the summer seasonal temporal allocation will be used throughout this example):

$$
\begin{aligned}
TA_{win} &= TA_{Dec} + TA_{Jan} + TA_{Feb} &&= 0.091 + 0.081 + 0.078 = 0.250 \\
TA_{spr} &= TA_{Mar} + TA_{Apr} + TA_{May} &&= 0.080 + 0.084 + 0.089 = 0.253 \\
TA_{sum} &= TA_{Jun} + TA_{Jul} + TA_{Aug} &&= 0.081 + 0.082 + 0.083 = 0.246 \\
TA_{fal} &= TA_{Sep} + TA_{Oct} + TA_{Nov} &&= 0.079 + 0.088 + 0.084 = 0.251
\end{aligned}
$$

The calculation of the seasonal temporal allocations also should be checked, as shown below, to make sure it was performed correctly.

$$TA_{win} + TA_{spr} + TA_{sum} + TA_{fal} = 0.250 + 0.253 + 0.246 + 0.251 = 1.000 \;\; �$$

Assuming annual on-road motor vehicle emissions of 400 Mg/yr of TOG, 800 Mg/yr of CO, and 600 Mg/yr of NO_x (as previously defined in Table 1-1), the summer seasonal emissions are calculated as follows:

$$
\begin{aligned}
E_{TOG,sum} &= \text{Annual}_{TOG} \times TA_{sum} &&= 400 \text{ Mg/yr} \times 0.246 = 98.4 \text{ Mg/yr} \\
E_{CO,sum} &= \text{Annual}_{CO} \times TA_{sum} &&= 800 \text{ Mg/yr} \times 0.246 = 196.8 \text{ Mg/yr} \\
E_{NOx,sum} &= \text{Annual}_{NOx} \times TA_{sum} &&= 600 \text{ Mg/yr} \times 0.246 = 147.6 \text{ Mg/yr}
\end{aligned}
$$

STEP 2 – Weekly Temporal Allocation

Weekly motor vehicle activity is distributed as shown in Table 3-2.

Table 3-2. Assumed Weekly Motor Vehicle Temporal Allocation Profile for the Hypothetical Modeling Inventory

Day	Fraction of Weekly Activity
Monday	0.138
Tuesday	0.138
Wednesday	0.138
Thursday	0.138
Friday	0.138
Saturday	0.155
Sunday	0.155
Total	**1.000**

The equations for converting weekly temporal allocation into average weekday, Saturday, and Sunday factors are shown as follows (only the average weekday temporal allocation will be used throughout the example).

$$F_{wd} = F_{ad} \times (A_{wd}/0.1429) = 0.0110 \times (0.138/0.1429) = 0.0106 = 1.06\%$$
$$F_{sat} = F_{ad} \times (A_{sat}/0.1429) = 0.0110 \times (0.155/0.1429) = 0.0119 = 1.19\%$$
$$F_{sun} = F_{ad} \times (A_{sun}/0.1429) = 0.0110 \times (0.155/0.1429) = 0.0119 = 1.19\%$$

Where F_{wd} = weekday factor;
F_{sat} = Saturday factor;
F_{sun} = Sunday factor;
A_{wd} = Average weekday activity;
A_{sat} = Saturday activity;
A_{sun} = Sunday activity;
F_{ad} = average daily factor (1.00/91 days per season); and
0.1429 = average day fraction of weekly emissions (see page 3-3).

The calculation of the weekly temporal allocations also should be checked, as shown below, to make sure it was performed correctly (when 65 is the number of weekdays in a season and 13 is the number of Saturdays or Sundays in a season; see page 3-5).

$$(65 \times F_{wd}) + (13 \times F_{sat}) + (13 \times F_{sun}) = (65 \times 0.0106) + (13 \times 0.0119) + (13 \times 0.0119)$$
$$= 0.689 + 0.1547 + 0.1547 = 0.9984 \approx 1.00$$

Using the calculated summer on-road motor vehicle emissions (98.4 Mg/yr of TOG, 196.8 Mg/yr of CO, and 147.6 Mg/yr of NO_x) and the calculated weekday factor of 0.0106, the average summer weekday emissions are calculated as follows:

$$E_{TOG,sumwd} = E_{TOG,sum} \times F_{wd} = 98.4 \text{ Mg/yr} \times 0.0106 = 1.043 \text{ Mg/day}$$
$$E_{CO,sumwd} = E_{CO,sum} \times F_{wd} = 196.8 \text{ Mg/yr} \times 0.0106 = 2.086 \text{ Mg/day}$$
$$E_{NOx,sumwd} = E_{NOx,sum} \times F_{wd} = 147.6 \text{ Mg/yr} \times 0.0106 = 1.565 \text{ Mg/day}$$

Step 3 – Hourly Temporal Allocation

Assumed hourly motor vehicle activity is distributed as shown in Table 3-3 below. As a convention, Hour 1 refers to the first hour of the day (midnight to 1 a.m.), Hour 2 refers to the second hour of the day (1 a.m. to 2 a.m.), and so on. Therefore, Hour 8 refers to the eighth hour of the day (7 a.m. to 8 a.m.).

**Table 3-3. Assumed Hourly Motor Vehicle Temporal Allocation Profile
for the Hypothetical Modeling Inventory**

Hour	Fraction of Daily Activity
1	0.016
2	0.010
3	0.003
4	0.006
5	0.010
6	0.026
7	0.053
8	0.064
9	0.055
10	0.048
11	0.050
12	0.052
13	0.054
14	0.055
15	0.059
16	0.070
17	0.074
18	0.070
19	0.058
20	0.046
21	0.037
22	0.033
23	0.028
24	0.022
Total	**1.000 ×**

The hourly emissions for Hour 8 of an average summer weekday emissions are given below:

$$E_{TOG,sum,wd,8} = E_{TOG,sum,wd} \times F_8 = 1.043 \text{ Mg/day} \times 0.064 = 0.067 \text{ Mg/hr}$$
$$E_{CO,sum,wd,8} = E_{CO,sum,wd} \times F_8 = 2.086 \text{ Mg/day} \times 0.064 = 0.134 \text{ Mg/hr}$$
$$E_{NOx,sum,wd,8} = E_{NOx,sum,wd} \times F_8 = 1.565 \text{ Mg/day} \times 0.064 = 0.100 \text{ Mg/hr}$$

Hourly emission calculations for the other hours are performed in the same manner.

4.0 SPATIAL ALLOCATION

After performing the temporal allocation of emissions, the second step of modeling inventory development is the spatial allocation of emissions. Because air quality modeling strives to replicate the actual physical and chemical processes that occur in an inventory domain, it is important that the physical location of emissions be determined as accurately as possible. In an ideal situation, the physical location of all emissions would be known exactly. In reality, however, the spatial allocation of emissions in a modeling inventory only approximates the actual location of emissions.

Before any spatial allocation can be performed, several characteristics of the inventory must be identified. First, the modeling grid domain must be established. The grid domain of the hypothetical community is shown in Figure 4-1 as thick black perimeter line. The dimensions of the grid domain measure 15 km by 15 km. A modeling grid domain is a rectangular area that encompasses all the desired emission sources to be modeled. In this manual's hypothetical example, the modeling grid domain corresponds exactly with the community boundaries. In real life, however, rectangular modeling grids will be assigned to irregularly-shaped areas.

The modeling objectives and purposes often will determine the modeling grid domain used. For example, a hazardous air pollutant (HAP) inventory conducted for Ambos Nogales (Nogales, Sonora; and Nogales, Arizona) used a relatively small grid domain (12 km by 19 km) (Radian, 1997). This grid domain size was determined by the actual limits of urban development. In contrast, the emissions inventory developed in support of the Grand Canyon Visibility and Transport Commission (GCVTC) extended from southern Canada to northern Mexico in the north-south direction and from the Mississippi River to the Pacific Ocean in the east-west direction (Radian, 1995). A large domain size was selected to address the issues of long-distance transport and visibility impairment. The choice of modeling grid domain may also be influenced by local topography and/or meteorology. For instance, topography often determines the size and shape of air basins which may affect grid domain selection. In addition,
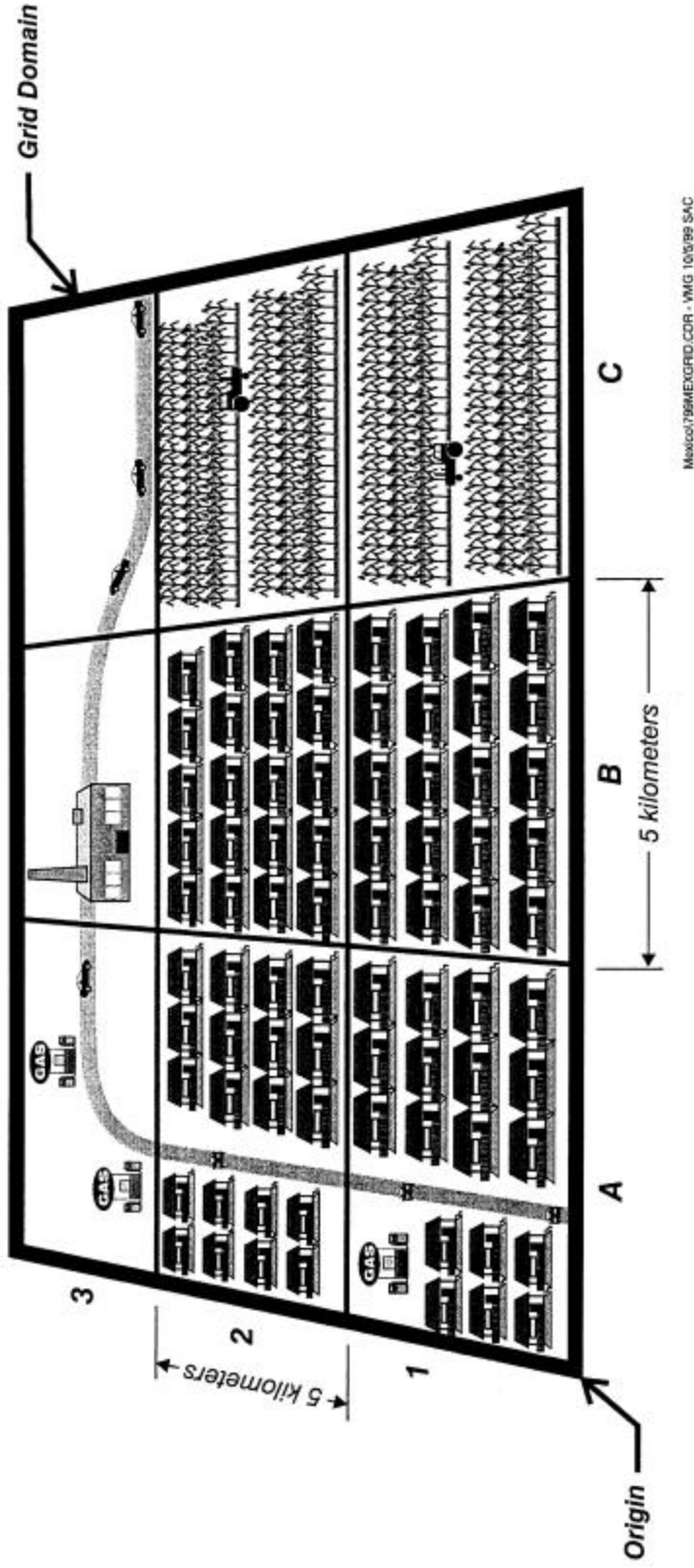
Figure 4-1. Hypothetical Modeling Inventory Community and Modeling Grid

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meteorology (e.g., prevailing wind direction) may cause a particular grid domain to include certain emission sources.

The next step after establishing the extent of the grid domain is to determine the size of the smaller grid cells within the grid domain. The nine grid cells shown in Figure 4-1 each measure 5 km by 5 km. Grid cells always will be square and nearly always will be of equal size. Smaller grid cells are occasionally nested inside other grid cells in order to effectively model local effects, but this is generally not done. Once again, selected modeling objectives and purposes may influence the grid cell size to be used. Large regional inventories may have grid cells 5 km by 5 km or larger; smaller inventories for a single metropolitan area may have grid cells 1 km by 1 km or smaller. The Ambos Nogales inventory mentioned above used grid cells that measured 500 meters (m) by 500 m. In this inventory, several of the ambient air monitors were located very close together. In order to have these monitors located in their own grid cells, a small grid cell size was required. On the other hand, the Grand Canyon inventory used 50 km by 50 km grid cells. Using smaller grid cells for this inventory might have adversely impacted resources needed for data management.

The advantages and disadvantages of specific grid cell sizes should be assessed prior to actual selection. For example, smaller grid cells will reduce modeling uncertainty; however, they may adversely affect inventory resources (e.g., insufficient computer memory, overly long modeling run times, unwieldy data outputs, etc.). Reducing the size of grid cells from 2 km by 2 km to 1 km by 1 km will increase the total number of cells in the grid by a factor of four. Inventory resources will likely be affected in a similar manner. Finally, if three-dimensional grid models are to be employed, cell heights will need to be established. A three-dimensional grid model will have two to five cell layers representing different heights in the atmosphere; however, most emissions will occur in the bottom layer (i.e., ground level).

The final step in establishing grid characteristics is fixing the grid origin and associated cell-naming convention. Without a cell-naming convention, describing a certain cell as "the eighth cell in the sixth row" does not refer to a unique cell (i.e., is this the sixth row from

the top or from the bottom? Is this the eighth cell from the left or from the right?). In the U.S. and elsewhere, the southwest corner of the grid domain conventionally has been designated as the grid origin. In Figure 4-1, the southwest (i.e., bottom left) corner of the grid domain is the origin and all the grid cells are numbered from there. The grid cells are identified from west to east (i.e., left to right) using letters of the alphabet and from south to north (i.e., bottom to top) using numbers. As an example, in Figure 4-1, "the second cell in the third row" uniquely refers to cell B3.

After defining the necessary grid characteristics, the spatial allocation of emissions can be performed. Spatial allocation can refer to both horizontal and vertical allocation. (Most of the discussion in this manual relative to spatial allocation focuses on horizontal allocation because it is applicable for all emission sources. Vertical allocation will be addressed to a lesser degree because it is applicable for only a few types of emission sources.) Horizontal spatial allocation refers to assigning emissions to their proper grid cell prior to modeling activities. The specific method of allocation will vary depending upon the source type emissions being allocated. Vertical spatial allocation refers to assigning emissions to their proper layer in the atmosphere prior to modeling activities.

Vertical allocation is limited to those emissions that are released from an elevated height with a significant upward velocity and/or buoyancy. It is most important for specific air quality episodes that are characterized by low mixing heights. For all practical purposes, vertical allocation is limited to significant point sources with elevated stacks. An example of vertical allocation is shown in Figure 4-2. The emissions from the elevated point source stack are shown rising into Level 2, which indicates a relatively high upward release velocity and/or buoyancy. The emissions from the rooftop vent of the same point source, however, stay within Level 1; these emissions likely have a lower upward release velocity and/or buoyancy than the point source stack emissions. Also, as shown in Figure 4-2, emissions from motor vehicles (and area sources) are assumed to remain within Level 1. In general, vertical spatial allocation is a step performed automatically by the emissions modeling system (or in some cases by the air quality model) based upon the stack parameters listed in Table 2-1.

Level 2

Level 1

Mexico\789-PLUME-HEIGHT.CDR - VMG 10/22/99 SAC
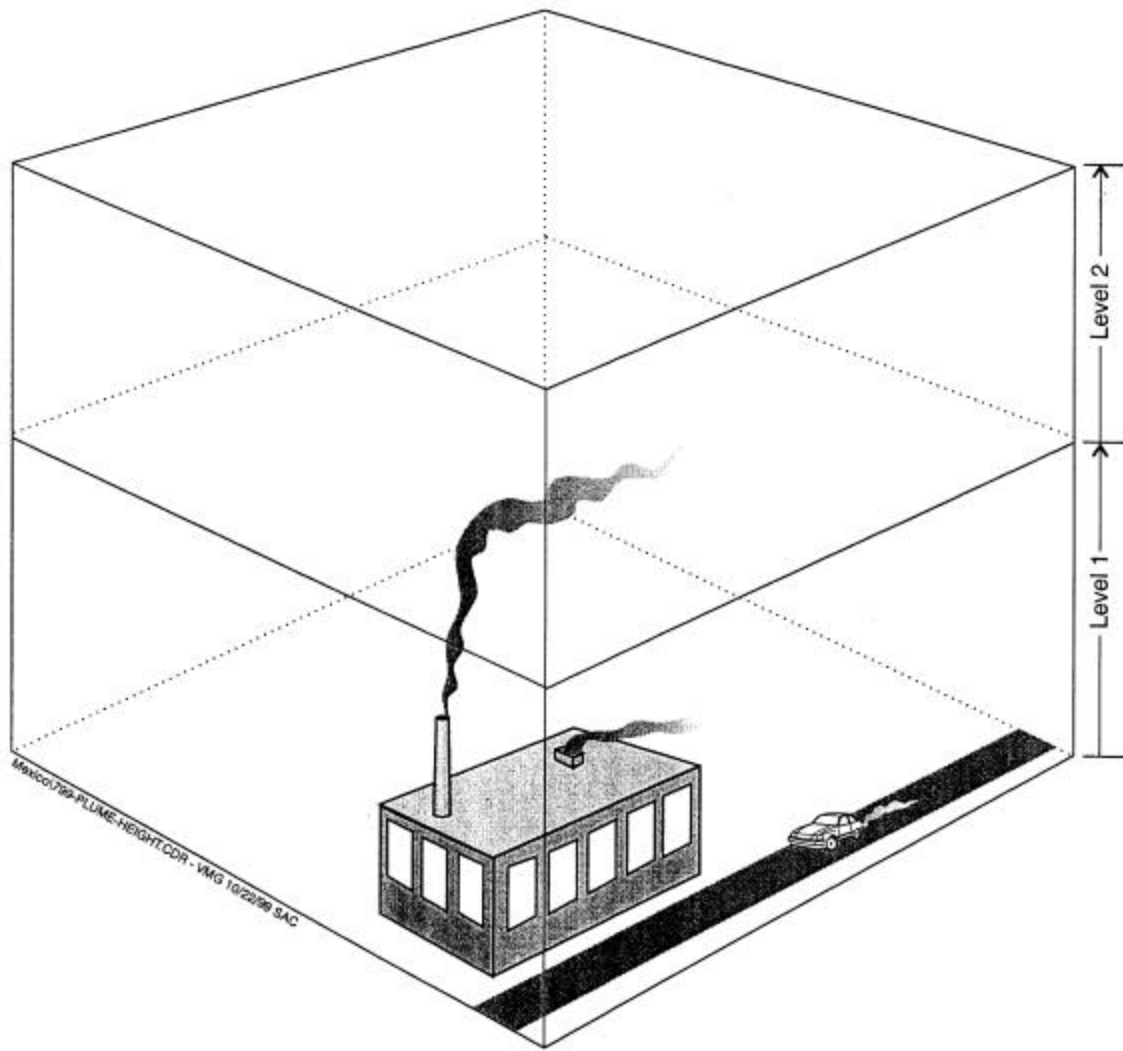
4.1   **Points (Point Sources)**

Point sources are spatially allocated to a modeling grid based upon precise location information and stack parameters. Point sources are, by definition, emission sources that have a specific, identifiable point of release.

Point source emissions are typically spatially allocated to the modeling grid using Universal Transverse Mercator (UTM) projection coordinates. Emission locations identified by latitude-longitude coordinates or other geographic coordinate systems should be transformed into UTM coordinates. The transformation of latitude-longitude coordinates to UTM coordinates is typically performed using a GIS-type application with this built-in capability (e.g., ArcInfo™), rather than by hand. An example of UTM and latitude-longitude coordinates in Lázaro Cárdenas, State of Michoacan, Mexico, is presented in Figure 4-3. Specific geographic coordinate information should be collected for those point sources that are only identified by census tracts, postal codes, or physical addresses; these types of location identifiers are insufficient for use in a modeling inventory. Some maps can provide UTM coordinates. More recently, however, global positioning systems (GPS) have become an economical way to identify UTM coordinates. Ideally, each individual point source (e.g., stacks, vents, etc.) would be precisely identified on a device level and allocated to the modeling grid. However, this level of detail is sometimes not available. In such circumstances, emissions are allocated on a less refined basis (i.e., process level or facility level).

The vertical spatial allocation of point source emissions is determined by the stack parameters associated with each point source. Stack parameters (i.e., stack height, stack diameter, flowrate, exit velocity, and gas exit temperature) are used by air quality models to estimate the plume rise and trajectory of emissions. Emissions from stacks with higher exit velocities and/or gas exit temperatures will tend to rise to a higher altitude than emissions from stacks with lower exit velocities and/or gas exit temperatures.

Latitude

Longitude

1

500

980

0

José Maria Morelos

500

GL HL

GK HK

12

Guacamoyas

ISLA LA PALMA

Zacatula

9

CIUDAD LAZARO CARDENAS

PUNTA CAYACAL

8

79   15'   80   81   102°00'

UTM Eastings   Longitude

201

200

18°00' ← Latitude

199 →

198 →

UTM Northings
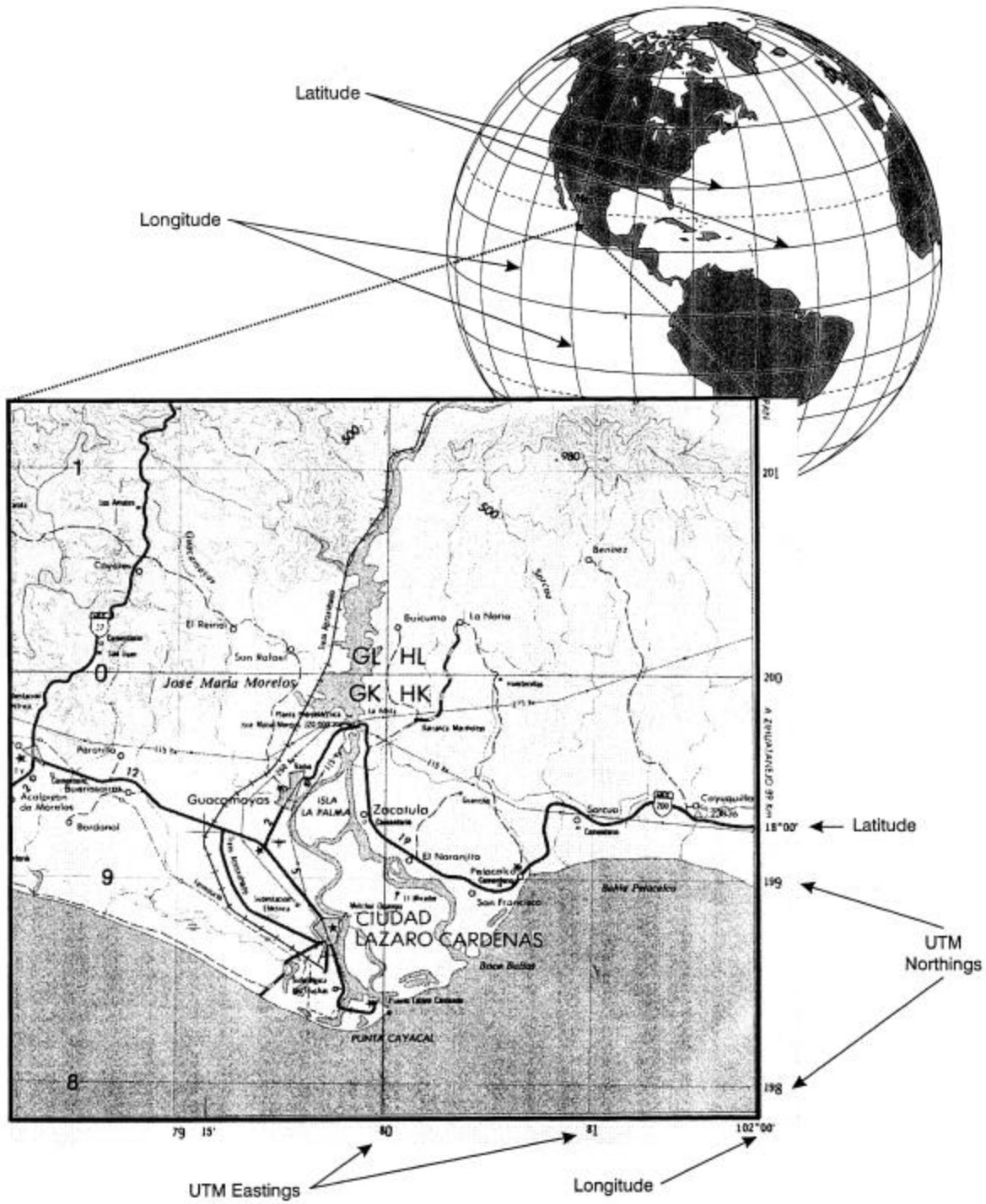
It is important that these stack parameters be collected at the same time that point source emissions are estimated. Also, stack parameters should be screened for "reasonableness"; incorrect stack parameters may lead to suspect air quality modeling results. Experience in the U.S. indicates that approximately 20% to 30% of the stacks have one or more incorrect stack parameters (U.S. EPA, 1999b). Some examples of questionable stack parameters include stack heights greater than 400 meters, supersonic exit velocities, and gas exit temperatures cooler than ambient temperature. Such stack parameters should not automatically be discarded, but further research should be conducted to assess their validity.

4.2   __Areas (Area and Natural Sources)__

The major difference between point source emissions and area and natural source emissions is that point source emissions are released from an individual discrete location while area and natural source emissions are released from a large number of disperse locations. It is impractical, if not impossible, to identify all the release points associated with area and natural source emissions; thus, a more indirect method of spatial allocation is used for area and natural source emissions. This spatial allocation method involves the use of "spatial surrogates." Some examples of spatial surrogates include population, housing, land use, etc. The spatial surrogates are thought to approximately represent the spatial distribution of emissions throughout the grid domain. For example, population is typically thought to be an appropriate spatial surrogate for allocating consumer solvent emissions because consumer solvent users are the population in general. On the other hand, population would probably not be an appropriate spatial surrogate for allocating agricultural emissions because the entire population is not involved in agricultural activities.

A short example demonstrating how spatial surrogates are developed is provided here. There is a hypothetical inventory domain (unrelated to the other hypothetical inventory domain presented in this document) that contains only four grid cells (e.g., A, B, C, and D). It is assumed that consumer solvent emissions are proportionally related to population. The population of the four grid cells is provided in Table 4-1.

Table 4-1. Population for a Hypothetical Four Grid Cell Inventory Domain

Cell	Population
A	103,800
B	26,900
C	57,200
D	71,500
Total	**259,400**

The spatial allocation factor for Cell A is calculated by dividing the population for Cell A by the total population for the four grid cells (103,800/259,400 = 0.4002). The spatial allocation factors for the other three cells are calculated in a similar manner. These spatial allocation factors are presented in Table 4-2.

**Table 4-2. Calculated Consumer Solvent Spatial Surrogates for
a Hypothetical Four Grid Cell Inventory Domain**

Cell	Spatial Surrogates
A	0.4002
B	0.1037
C	0.2205
D	0.2756
Total	**1.0000**

In order to spatially allocate an entire inventory, a unique spatial surrogate will need to be assigned to each area source category which is typically defined using source codes (some recommended source codes are provided in Volume V of this manual series [*Area Source Inventory Development*]). It should be noted that all area and natural source emissions are assumed to be ground-level releases. Thus, spatial allocation for area and natural source emissions is usually limited to horizontal allocation. Some natural source emissions (e.g., biogenic emissions) may often be estimated using an emissions model (e.g., PCBEIS) which often include spatial allocation in the calculation process. Such emissions models typically use land use and vegetative cover information to estimate emissions on an individual county basis.

4.3   Lines (Motor Vehicles, Railroads, and Shipping Lanes)

Although mobile sources (including on-road motor vehicles and nonroad mobile sources) are sometimes grouped with area sources in an inventory, their spatial allocation is somewhat different. Specifically, many mobile sources are limited to operation on linear transportation networks (e.g., on-road motor vehicles to road networks, locomotives to railroad systems, and commercial marine vessels to specific shipping lanes). On-road motor vehicle activity (e.g., vehicle kilometers traveled [VKT], trips, starts, etc.) is often modeled on the road network using travel demand models (TDM) or other transportation models; simpler models may also exist for other types of mobile sources. These transportation models can be used to allocate activity data (e.g., VKT) to individual network segments. Activity data can then be adjusted for any special conditions that exist at the individual network segment level. For example, the effects of higher vehicle speeds or more traffic congestion can be assigned to individual segments.

The modeling inventory ultimately needs to have emissions assigned to either specific UTM coordinates (for point sources) or specific grid cells (all other sources). As a result, motor vehicle emissions are spatially allocated to specific grid cells depending upon the relevant activity occurring within those grid cells. Activity data may be fractionally split into multiple grid cells based upon the fraction of activity within each grid cell. For instance, a road segment that crosses three grid cells and has equally distributed motor vehicle activity along its entire length would have one-third of its emissions assigned to each one of the three relevant grid cells.

4.4   Spatial Allocation Example

This portion of the example focuses on the spatial allocation of annual emissions to individual grid cells only; other modeling inventory development steps are demonstrated elsewhere in this document. In an actual modeling inventory, temporal allocation of annual emissions to hourly emissions would be performed first. However, in order to provide a clear illustration of the spatial allocation process, spatial surrogates are applied directly to annual

emissions. This example is limited to spatial allocation of annual emissions for one source category only. A more detailed example sequentially showing all modeling inventory development steps for one source category is presented in Section 7.0; the emission calculations associated with the entire example are presented in Appendix A.

Figure 4-4 presents the six spatial surrogates that are associated with the hypothetical inventory grid. The fraction of emissions assigned to each grid cell is indicated as a decimal number. If emissions are not present in a particular grid cell, then a zero is indicated in the spatial surrogates. It should be noted that this example does not include UTM coordinates or other geographic coordinates for the factory stack and vent. All the emissions from the factory stack and vent are simply allocated to the cell where the factory is located (i.e., Cell B3). Also, this example does not include vertical allocation of the factory stack emissions; all emissions are assumed to occur at or near ground level.

Example Calculation

One road segment is assumed to pass through the inventory grid as shown in Figure 4-1. The road segment passes through five grid cells (A1, A2, A3, B3, and C3). It is assumed that the fractional road segment distance and motor vehicle activity is equally distributed among these five grid cells. The motor vehicle spatial surrogate, therefore, has 20% of the total emissions assigned to each grid cell. The equation for spatially allocating emissions is as follows:

$$E_{xy} = \text{Annual} \times SS_{x,y}$$

Where E_{xy} = Annual emissions in grid cell x,y (Mg/yr);
Annual = Annual emissions for entire domain (Mg/yr); and
$SS_{x,y}$ = Spatial surrogate fraction for grid cell x,y.

Using this equation, the TOG, CO, and NO_x emissions for motor vehicles in Cell A1 are calculated as follows using the emission values previously defined in Table 1-1.

$$E_{TOG,A1} = \text{Annual}_{TOG} \times SS_{A1} = 400 \text{ Mg/yr} \times 0.200 = 80 \text{ Mg/yr}$$
$$E_{CO,A1} = \text{Annual}_{CO} \times SS_{A1} = 800 \text{ Mg/yr} \times 0.200 = 160 \text{ Mg/yr}$$
$$E_{NOx,A1} = \text{Annual}_{NOx} \times SS_{A1} = 600 \text{ Mg/yr} \times 0.200 = 120 \text{ Mg/yr}$$

Emission calculations for the other four grid cells that contain motor vehicle emissions (i.e., Cells A2, A3, B3, and C3) are identical to these.

Factory Stack (Boiler)

	A	B	C
3	0	1.000	0
2	0	0	0
1	0	0	0

Factory Vent (Coating Process)

	A	B	C
3	0	1.000	0
2	0	0	0
1	0	0	0

Highway Vehicles

	A	B	C
3	0.200	0.200	0.200
2	0.200	0	0
1	0.200	0	0

Gasoline Stations

	A	B	C
3	0.667	0	0
2	0	0	0
1	0.333	0	0

Residential Consumer Solvent Use

	A	B	C
3	0	0	0
2	0.250	0.250	0
1	0.250	0.250	0

Agricultural Pesticide Use

	A	B	C
3	0	0	0
2	0	0	0.500
1	0	0	0.500

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Figure 4-4. Spatial Surrogates for the Hypothetical Modeling Inventory

5.0   SPECIATION

The third step in modeling inventory development is speciation. This is the process of disaggregating inventory pollutants (e.g., TOG, NO$_x$) into individual chemical species components (e.g., toluene, NO$_2$) or groups of species. The need for speciation is determined by the inventory purpose. Inventory applications that require detailed speciation include photochemical modeling, air toxics inventories, chemical mass balance modeling, and visibility modeling. This section describes different speciation procedures for a variety of pollutants and source types.

Depending on the purpose of a particular emissions inventory, the inventory may include TOG, NO$_x$, sulfur oxides (SO$_x$), CO, total suspended particulate matter (TSP), particulate matter less than 10 micrometers in aerodynamic diameter (PM$_{10}$), or ammonia (NH$_3$). However, modeling inventories may require these emissions to be expressed in terms of other pollutants. For example, most photochemical models require that hydrocarbon emissions are expressed in terms of designated reactivity groups or "classes" of compounds. Additionally, for some models, NO$_x$ emissions may need to be specified as NO and NO$_2$. Also, PM may need to be separated into various size fractions, such as PM$_{10}$ and PM less than 2.5 micrometers in aerodynamic diameter (PM$_{2.5}$).

Modeling inventories can be developed using either discrete speciation (e.g., for air toxics) or lumped-model speciation (e.g., for photochemical modeling). The specific required speciation mechanism will typically be specified by the modeling software that is used. The following definitions of these two speciation methods are from the U.S. EPA (U.S. EPA, 1999b):

- **Discrete speciation** – refers to splitting emissions for a pollutant into individual chemical compounds or size classifications. For example, TOG emissions from automobile exhaust may consist of 50 or more identified organic compounds (e.g., benzene, hexane, formaldehyde). Discrete speciation is performed using speciation profiles containing weight fractions for each chemical compound; and

- **Lumped-model speciation –** refers to splitting emissions for a pollutant into groups of components that represent numerous discrete compounds. The groups of components are referred to as lumped-model species. The lumped-model species for TOG are developed using split factors that are specific to the type of chemical mechanism employed by the photochemical model to be used.

5.1 TOG and PM Speciation Profiles

Discrete speciation profiles are available for TOG and PM emissions for many source types. Prior to applying speciation profiles, it may be necessary to adjust emissions to account for any components not included in the emissions inventory. For example, ROG may be adjusted to TOG (ROG-to-TOG conversion). This adjustment is necessary because emission factors for certain source categories exclude methane and formaldehyde, and therefore, represent only the reactive components, or ROG; however, most speciation profiles are applied assuming the emissions represent TOG.

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 nonreactive compounds is updated periodically as U.S. EPA designates new nonreactive compounds.

Chemicals considered to be photochemically reactive are termed 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 VOC. Emission factors published in U.S. EPA's AP-42 (U.S. EPA, 1995) are presented both as TOG and ROG/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 5-1 graphically illustrates the relationship between these various hydrocarbon definitions. The shaded areas in Figure 5-1 indicate the compounds included in each definition. The definitions for NMOG, NMHC, THC, and HC are generally used for combustion processes only.

Chemical speciation and particle size distribution information is available through U.S. EPA's SPECIATE database. SPECIATE contains TOG and PM speciation profiles for more than 300 source types. The most recent release of SPECIATE (Version 3.0) was developed as a Windows® application (U.S. EPA, 1999c). U.S. EPA is also considering development of an interactive Internet application. An Internet application would allow researchers to add new profiles to the system. The speciation profiles attempt to distribute the total TOG or PM emissions from a particular source into the individual compounds (in the case of TOG) or elements and size fractions (for PM). Such a breakdown has been developed for use in some photochemical models and source-receptor models (primarily for PM). These profiles were not developed for, and are not recommended for use in, speciating TOG or PM emissions for air toxics inventories. The Factor Information Retrieval (FIRE) Data System contains U.S. EPA's recommended emission factors for both toxic and criteria pollutants. The most recent version of FIRE (Version 6.22) was also developed as a Windows® application (U.S. EPA, 1999d).

Speciation data may also be developed for site-specific applications or by other regulatory agencies. For example, the California Air Resources Board (ARB) has compiled speciation profiles for TOG and PM (ARB, 1991a; ARB, 1991b) and has an ongoing effort to
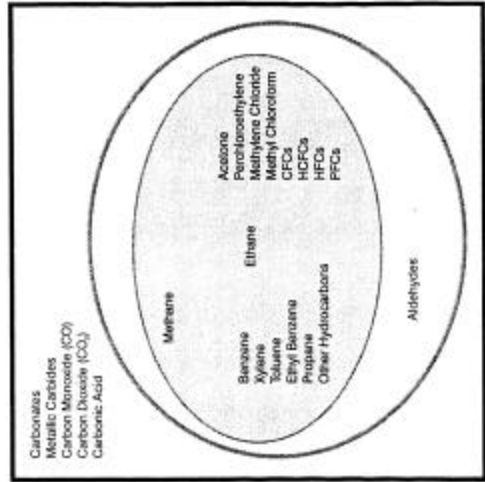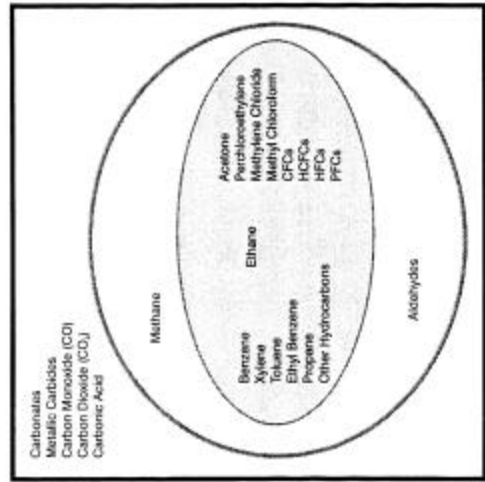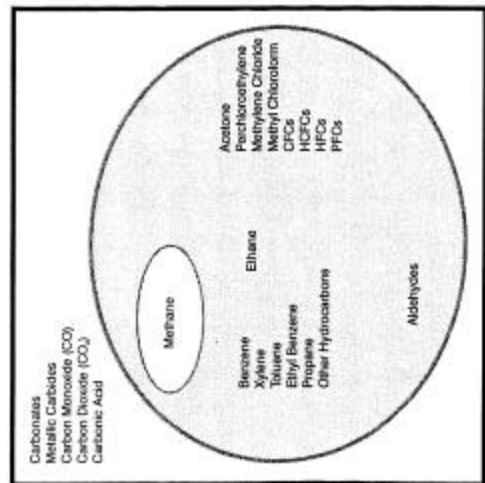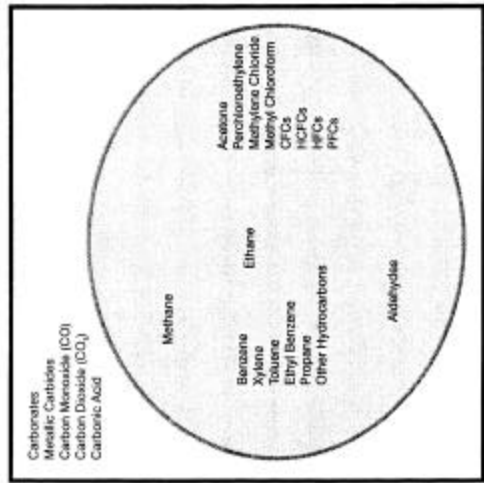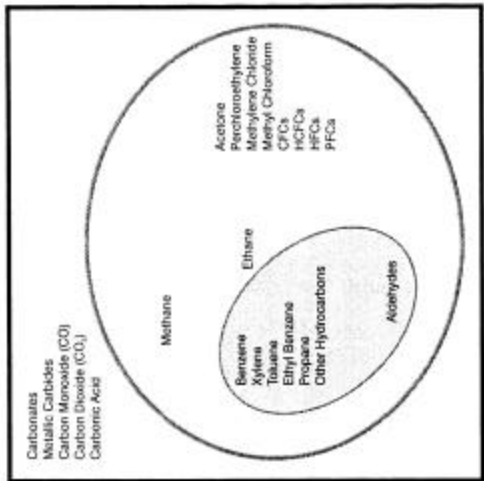
Figure 5-1. Description of Hydrocarbon Definitions

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update estimates of the size fractions and chemical composition of PM profiles for a variety of emission source categories. The ARB has recently proposed new or revised TOG profiles for motor vehicle exhaust and evaporation, utility equipment exhaust, diesel exhaust, and jet engine exhaust. Speciation profiles (both TOG and PM) for the six source categories in the overall example have been provided in Appendix B and Appendix C, respectively. Although PM emissions were not considered in the hypothetical modeling inventory example, the PM speciation profiles in Appendix C are provided for informational purposes.

5.2   **Photochemical Reactivity Groups**

Speciating chemicals into reactivity groups is important for photochemical modeling applications because some species of TOG are far more reactive than others. Researchers have identified differences among TOG species in their contributions to ozone formation in the atmosphere and have developed chemical mechanisms for models that predict transformation of pollutants in the atmosphere. These mechanisms have been evaluated using laboratory experiments. Many chemical mechanisms have been developed, but the following two are most commonly used in photochemical modeling today:

- Carbon Bond IV (CB-IV); and
- California Statewide Air Pollution Research Center (SAPRC).

The CB-IV mechanism requires that TOG emissions be disaggregrated into emissions of lumped species based on the species' carbon bond structure. In the SAPRC mechanism, discrete compounds are lumped together based on their relative reactivity with the hydroxyl radical (OH⁻). The CB-IV and SAPRC lumped species are provided in Table 5-1 and 5-2, respectively

Other mechanisms that may be of interest to Mexico are the Regional Acid Deposition Model Mechanism, Version 2 (RADM2) and the Regional Atmospheric Chemistry Mechanism (RACM). These mechanisms are used within the MCCM regional scale air quality model developed by the Fraunhofer-Institut für Atmosphärische Umweltforschung (Fraunhofer Institute for Atmospheric Environmental Research) (IFU). The RADM2 gas phase mechanism utilizes 61 species, while the RACM gas phase mechanism uses 71 species in their respective

reactivity groups. Mexico's Instituto Nacional de Ecología (INE) has indicated that some of their staff are currently receiving training on the MCCM model in Germany.

Table 5-1. Carbon Bond IV Organic Species

Organic Species	Organic Species ID
Olefins	OLE
Paraffins	PAR
Toluene	TOL
Xylene	XYL
Formaldehyde	FORM
High Molecular Weight Aldehydes	ALD2
Ethene	ETH
Methanol	MEOH
Ethanol	ETOH
Isoprene	ISOP
Nonreactive	Not Applicable

Table 5-2. SAPRC Organic Species

Organic Species	Organic Species ID
Formaldehyde	HCHO
Higher Aldehydes	CCHO
Ketones	MEK
Alkyl Nitrites	RNO3
PAN Analogues	PAN
Phenols	CRES
Glyoxal	GLY
Methyl Glyoxal	MGLY
Uncharacterized Aromatic Fragmentation Product #1	AFG1
Uncharacterized Aromatic Fragmentation Product #2	AFG2

Emissions of lumped-model species are calculated using split factors, which represent the amount (in moles) of lumped-model species per gram of TOG. For each source or

source category emitting TOG, two or more percentages (totaling 100 percent) must be defined, each one corresponding to the fraction of TOG emitted as the lumped-model species.

5.3   NO$_x$ Speciation

Some photochemical models do not require that nitrogen oxides be distinguished as either NO or NO$_2$. Instead, these models assume that all NO$_x$ is NO, which is the predominant form of NO$_x$ emitted from combustion processes (the primary source of NO$_x$ emissions). For models requiring that a distinction between NO or NO$_2$ be made, split factors must be applied. For each source or source category emitting NO$_x$, two percentages (totaling 100 percent) need to be defined: one corresponding to the fraction of NO$_x$ emitted as NO and the other corresponding to the fraction emitted as NO$_2$.

It is important to indicate how NO$_x$ is reported in an inventory. NO$_x$ emissions are commonly expressed "as NO$_2$," which means that a molecular weight of 46 is attributed to NO as well as NO$_2$, even though the true molecular weight of NO is 30. The actual value for NO emissions by weight is 30/46 (or 0.65) times the value of NO reported "as NO$_2$."

At present, few references are available that define split factors for allocating NO$_x$ into NO and NO$_2$ (Milligan et al., 1997). As a rough average, 97% (by weight as NO$_2$) of the NO$_x$ emitted from most boilers will be NO. Default split factors for all sources (including motor vehicles) are often given as 90% by weight of NO (as NO$_2$) and 10% by weight of NO$_2$.

5.4   PM Size Distribution

Size distribution information, which is used for PM$_{10}$, PM$_{2.5}$, or visibility-related modeling inventories, is available through U.S. EPA's SPECIATE database. Size fractions are also available from the California Emission Inventory Development and Reporting System (CEIDARS). PM$_{10}$ and PM$_{2.5}$ emissions are estimated by multiplying total PM emissions by the desired partical size mass fraction.

A potentially significant portion of fine particulate matter (i.e., $PM_{2.5}$) is comprised of elemental carbon (EC) and organic carbon (OC). These two types of particulate matter are especially important for visibility-related modeling inventories because of their light scattering and extinction properties. Information on EC and OC is quite limited; virtually all available information is related to speciation profiles with hardly any emission factor data. Some sources of EC and OC information are U.S. EPA's SPECIATE database, California ARB's VOC and PM speciation profiles, and an EC/OC emissions inventory developed for California's South Coast Air Basin by the California Institute of Technology (Hildemann et al., 1991).

5.5   <u>Other Pollutants</u>

Although speciation is primarily a concern for hydrocarbons, NO_x, and PM, speciation may also be relevant for SO_x in some limited cases. Sulfur oxides are typically released as sulfur dioxide (SO_2). Emitted SO_2 may oxidize to sulfur trioxide (SO_3) and then to sulfuric acid (H_2SO_4) or sulfate (SO_4^{2-}) aerosols. However, SO_x emissions are generally reported on a SO_2 basis. Some photochemical models such as the Urban Airshed Model (UAM) require speciated SO_x emissions, which are disaggregated into SO_2 and SO_4^{2-}.

Finally, speciation is not a relevant issue for the other two commonly inventoried pollutants (CO and NH_3).

5.6   <u>Source Type Considerations</u>

The unique characteristics of each source have to be considered when speciating emissions. The Texas Natural Resource Conservation Commission (TNRCC) has summarized the following considerations for the various source types (TNRCC, 1999):

- **Point sources –** To accurately identify the chemicals in point source emissions, a special study of each specific process is necessary. Since this is not usually economically feasible, a speciation profile is generally used for each SCC. Individual industries emit different VOCs. The SCC-

specific profiles are needed because each process emits different
combinations of chemicals.

- **Area sources –** Similar to point sources, chemical speciation consists of assigning the correct proportion of different chemicals to different activities. For example, the emissions from lawn mowers are mapped to one chemical profile, while emissions from dry cleaners or asphalt road paving are mapped to others.

- **Motor vehicle sources** – Because the chemical composition of vehicular emissions differs among classes of vehicles (e.g., automobiles vs. 18-wheel diesels), separate chemical speciation profiles are used for different vehicle types. Similarly, each type of vehicle can emit hydrocarbons in different ways (e.g., gas tank vapor vs. tailpipe exhaust), so the chemical composition of each loss mode must be addressed as well.

- **Natural sources –** Species composition, or the type of vegetation in the area to be modeled, is significant because different types of vegetation emit different types and vastly different quantities of VOCs.

5.7 <u>Speciation Example</u>

To illustrate the concepts described in this section, the emissions of TOG, NO_x, and PM emissions from the hypothetical boiler introduced in Section 1.0 are speciated using different methods. In modeling inventory development, both temporal allocation and spatial allocation would normally be performed prior to speciation. However, in order to clearly demonstrate the speciation process, speciation is applied in this example directly to ungridded, annual emission estimates. Due to space considerations, speciation was not included in the more detailed example sequentially showing all modeling inventory development steps in Section 7.0 or the emission calculations associated with the entire example in Appendix A.

Example Calculation

This example calculation focuses on lumped–model speciation; an example of discrete speciation can be found in Section 6.4 of Volume II of this manual series (*Emissions Inventory Fundamentals*).

It should also be noted that emissions calculated using lumped–model speciation (i.e., for photochemical modeling) are usually presented on a molar basis, rather than a weight basis. As a result, emission estimates in this example calculation will be shown on a molar basis.

First, SPECIATE is used to determine or identify the species profile and discrete VOC species for the boiler. Assume that the boiler is classified as SCC 10500105 (External Combustion Boilers – Space Heaters – Industrial – Distillate Oil). The profile number assocated with this source category, as given in SPECIATE, is 0002.

Next, TOG emissions are assigned to lumped-species categories of the CB-IV mechanism using split factors from the UAM Emissions Processing System (EPS 2.0) split factors file (Table B-35 in EPS 2.0) and the following equation:

$$Emissions_I = TOG\ emissions \times SF_I / Divisor_I$$

Where

$Emissions_I$	=	Emissions of lumped-model species I (10^6 moles/yr);
TOG	=	TOG emissions (Mg/yr);
SF_I	=	Split factor for lumped-model species I (g-mole/g); and
$Divisor_I$	=	Secondary conversion factor for lumped-model species I.

Total organic gas boiler emissions were presented in Section 1.0 as 200 Mg/yr. Emissions of the Carbon Bond IV lumped-model species were calculated using the above equation and are listed in the Table 5-3. Figure 5-2 shows the discrete species and lumped-model species for the boiler.

TOG emissions are disaggregated into discrete species using SPECIATE.

N-Butane
Propane
Formaldehyde
Isomers of Pentane
Isomers of Heptane
Isomers of Hexane
Isobutane
Hexane
Isomers of Octane
N-Pentane
Heptane
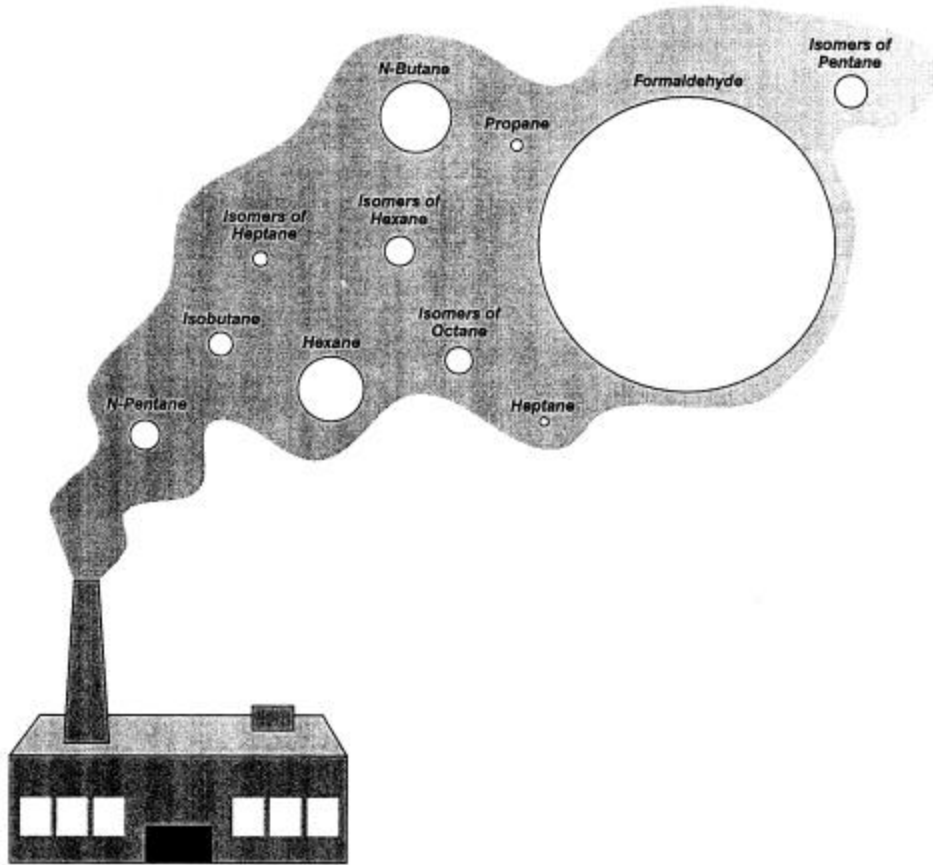
Discrete TOG emissions are aggregated into CB-IV lumped-model species.

PAR
7.07 x 10^6
moles/yr

FORM
3.25 x 10^6
moles/yr

NR
0.11 x 10^6
moles/yr
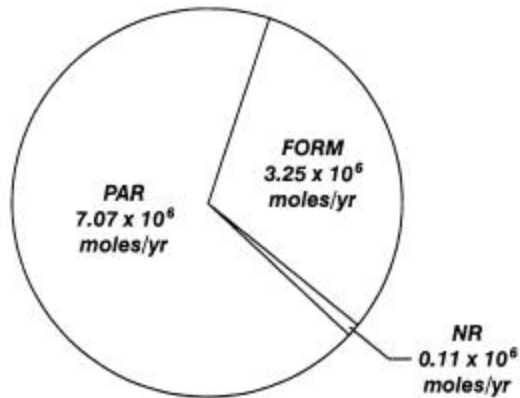
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**Figure 5-2. Carbon Bond IV Speciation for the Hypothetical
Modeling Inventory Point Source**

Table 5-3. Carbon Bond IV Lumped–Model Species Emission Estimates for the Hypothetical Modeling Inventory Boiler

Species I	SF_I (g-mole/g)	$Divisor_I$	$Emissions_I$ (10^6 moles/yr)
FORM	0.0162333333	1	3.25
NR	0.0005454545	1	0.11
PAR	0.0353612035	1	7.07

The hypothetical boiler emits 400 Mg/yr NO_x as NO_2. Given split factors of 90% and 10% by weight for NO and NO_2, respectively, the emissions would be equivalent to 360 Mg NO per year and 40 Mg NO_2 per year; however, the actual emissions of NO would be only 30/46 of 360, or 235 Mg per year. The annual molar NO and NO_2 emissions for the hypothetical boiler are estimated by dividing the annual mass emissions by the molecular weight of NO and NO_2 (30 g/mole and 46 g/mole, respectively). This results in emission estimates of 7.83 x 10^6 moles NO per year and 0.87 x 10^6 moles NO_2 per year.

6.0   PROJECTIONS

Emission projections refers to extrapolating baseline emission estimates to predict future emissions based upon expected future activity levels and emission controls. Projected emission estimates are often used for planning, evaluation of potential control measures, analysis of new source impacts, modeling of future air quality, and assessment of the effectiveness of air pollution control strategies. A baseline emissions inventory is important because it represents a snapshot of emissions for a given baseline year. However, because sources and their associated air emissions are not static over time, baseline emission estimates may not accurately represent emissions for a future year. Emission projections are an attempt to account for the effects of future growth and emission controls. Because projections attempt to quantify the unknown future, there will always be some uncertainty associated with any estimate of projected emissions. This uncertainty can be minimized by using source-specific growth factors and control factors that most nearly approximate future year emissions.

Projections are usually not considered to be a modeling inventory development step. Modeling inventory development steps are typically considered to be limited to temporal allocation, spatial allocation, and speciation. In fact, modeling inventory emissions that have been temporally allocated, gridded, and speciated are usually not projected into the future. Instead, the annual baseline emissions data are projected. These projected emissions can then be temporally allocated, spatially allocated, and speciated to create modeling inventories of the projected emissions.

6.1   Growth Factors

The first component of emission projections is growth. Growth is represented in terms of growth factors, which are expressed either in terms of annual percent change or percent change for a certain number of years. For most areas where air quality is a concern, growth will represent increasing activity and will be expressed as a positive number. However, negative growth rates can exist (e.g., transitioning from primary industries such as farming to industrial or

high-tech industries may cause the agricultural growth rate to be negative). Two equations for projecting growth only are given below.

$$E_{proj} = E_{base} \times (1 + \%_{ann}/100)^y$$

$$OR$$

$$E_{proj} = E_{base} \times (1 + \%_{per}/100)$$

$$\begin{aligned} \text{Where } E_{proj} &= \text{ Projected year emissions (Mg/yr);} \\ E_{base} &= \text{ Base year emissions (Mg/yr);} \\ \%_{ann} &= \text{ Annual growth (\%);} \\ y &= \text{ Number of years between base and projected year; and} \\ \%_{per} &= \text{ Period growth.} \end{aligned}$$

Usually, emission projection growth factors are based upon forecasts of industrial growth, population growth, transportation growth, and land use changes. Air quality agencies generally should not need to develop their own growth forecasts; appropriate forecasts should be available from other agencies. Relying upon growth indicator forecasts from other agencies allows air quality agencies to conserve resources and maintain consistency with the other agencies. However, care should also be exercised to ensure that forecasts from other agencies do not contain inherent biases that misrepresent the growth of emissions.

Industrial growth forecasts are often used to project point source emissions and some area source emissions. There are four primary indicators of industrial economic growth. In descending order of typical data availability, these four indicators are employment, earnings, value added, and product output. The four indicators are discussed below:

- **Employment** — Employment forecasts are usually the most readily available type of forecasts. However, employment forecasts do not account for production efficiencies due to technological improvements.

- **Earnings** — Earnings data incorporate the effects of production efficiencies, which may not be apparent in employment forecasts. For example, a particular industry may have a 15% earnings increase, even though employment rose only by 3%.

- **Value Added** — Value added (i.e., the value of a product sold by a firm less the value of the goods purchased and used by the firm to produce the product; equal to the revenue which can be used for wages, rent, interest,

and profits) is considered to be more accurate than employment or earnings forecasts because it addresses both production efficiencies and production factor substitution. However, value added information is less readily available than employment and earnings statistics.

- **Product Output** — Product output is probably the most direct indicator of future emissions activity. Product output most accurately represents the level of employment, resource availability, capital growth, and technology use. In addition, product output is a direct measure of industrial activity; whereas, employment, earnings, and value added are economic surrogates which may or may not accurately represent the amount of industrial activity. Unfortunately, product output information may not easily be obtained.

These four industrial growth indicators (employment, earnings, value added, and product output) are often used for regional projections of entire industrial sectors. More specific projection information can be obtained from surveying individual facilities. However, extensive surveying for projection information may be too resource-intensive. In addition, many industrial facilities may be unwilling to provide the necessary projection information, which is sometimes considered to be proprietary or confidential. In general, point source projection surveys should be used only for those instances where there is a dominant industry or facility whose emission growth is not likely to be characterized correctly in regional industrial projections.

Population growth is used less widely than industrial growth indicators to project future activity and emissions, but it is still used for some types of very disperse area sources (e.g., architectural surface coating, graphic arts, commercial/consumer solvent use, etc.). These area sources are typically those that are estimated using per capita emission factors. Besides these limited uses, population growth should typically not be used to project emissions. However, in the case of extremely limited forecast data, it may be the only viable alternative.

Ideally, transportation growth indicators should be used to project motor vehicle emissions. In general, as the population of a metropolitan area grows, the motor vehicle activity (i.e., VKT) increases. In fact, it tends to increase at a greater rate than population growth. This is because incremental growth usually occurs at the edge of the metropolitan area, which typically requires more vehicular travel than if the growth occurred in the center of the metropolitan area. Thus, population growth will almost always underestimate transportation growth. Transportation

growth indicators must usually be derived from travel demand models; instructions for using travel demand models are beyond the scope of this manual.

Finally, changes in land use should be considered in the estimation of growth factors. Biogenic sources and a few area sources are the only sources that are directly affected by changes in land use. In general, biogenic sources should be kept constant between the baseline inventory and the project inventory, unless there are land use changes that dramatically alter the biologic nature of an area (e.g., transformation of a heavily wooded forest into a large shopping center or residential development). Even these dramatic changes will tend to be limited to a few grid cells out of the entire inventory.

6.2   Control Factors

In addition to growth, emissions control is the other component of emission projections. Control factors are usually expressed as a percent of controlled emissions relative to uncontrolled emissions. There are several aspects of control factors that are discussed below.

Baseline emissions will include the effects of any control devices that have already been installed, as well as any existing regulations that have already been implemented as of the baseline year. Baseline emissions, however, will <u>not</u> include the effects of current regulations that have not been fully implemented as of the baseline year. These effects will need to be included in the future year projections. Although the emission reductions due to these regulations have not actually occurred, reasonable estimates of the expected reductions can usually be made because the associated regulation has already been established. The future emission reductions due to the adoption of a control strategy in a future year that has not been clearly defined in the base year, however, is much more difficult to quantify. In spite of this, these reductions need to be included in projection control factors. The basic equation for showing control factors only in any given year is given as follows:

$$E_c = E_u \times [1 - (CE/100)]$$

$$\text{Where } E_c = \text{Controlled emissions (Mg/yr);}$$
$$E_u = \text{Uncontrolled emissions (Mg/yr); and}$$
$$CE = \text{Control efficiency (\%).}$$

Although the previous equation demonstrates the general control factor equation, past experience in emissions inventory development has shown that actual levels of control effectiveness fall short of expected levels. As a result, the concepts of rule effectiveness (RE) and rule penetration (RP) need to be incorporated into inventories.

RE attempts to quantify the relative ability of regulations to achieve the full amount of emission reductions expected from complete compliance with regulations. Regulations that have full compliance by all sources at all times would have an RE of 100%. Conversely, owners/operators of sources that ignore relevant regulations would cause the relevant source category to have an RE of 0%. It is often difficult to quantify the actual RE value; this value depends upon many factors, including the nature of the regulation, the nature of the compliance procedures, and the performance of the source in maintaining and assuring compliance over time. In the U.S., a default RE value of 80% has typically been used by U.S. EPA and other agencies responsible for air quality. However, where possible, source-specific RE values should be developed.

RP is a measure of the extent to which a regulation covers emissions from all sources within a source category. In situations where a regulation covers all sources within a source category, an RP value of 100% should be used. However, if a regulation is only applicable for larger facilities, or facilities with certain characteristics (e.g., exceeding certain emissions quantities, operating in excess of a certain number of hours per year, using certain types of fuel, etc.), the RP value would be somewhat less than 100%.

If RE and RP are incorporated into the basic control factor equation shown on page 6-4, the control factor equation becomes:

$$E_c = E_u \times [1 - (CE/100) \times RE \times RP]$$

Where E_c =   Controlled emissions (Mg/yr);
         E_u =   Uncontrolled emissions (Mg/yr);
        CE   =   Control efficiency (%);
        RE   =   Rule effectiveness; and
        RP   =   Rule penetration.

In general, it is desirable that projections incorporate the effects of <u>both</u> growth and control. As a result, the growth factor equation and control factor equations need to be combined into one overall equation. This equation is given below:

$$E_{proj} = E_u \times [1 - (CE/100) \times RE \times RP] \times (1 + \%_{ann}/100)^y$$

Where E_{proj} =   Projected year emissions with controls (Mg/yr);
         E_u =   Uncontrolled base year emissions (Mg/yr);
         CE   =   Control efficiency (%);
         RE   =   Rule effectiveness;
         RP   =   Rule penetration;
         $\%_{ann}$ =   Annual growth (%); and
         y   =   Number of years between base and projected year.

6.3   <u>Source Type Considerations</u>

Since projections are developed from base year emission estimates, several source type-specific considerations should be examined. First, some point sources possess operating permits issued by regulatory agencies. These operating permits often specify daily or annual emission limits as conditions of device operation. When base year emission estimates from this type of permitted point source are projected to a future year, future year emission estimates should be increased only up to the permitted level. To project emissions above the permitted level would represent a permit violation by the facility possessing the permit.

Although not widely used in Mexico at the present time, the possible effects of emission offsets, banking, trading, and other market-based control strategies should be addressed in future year projections. A detailed discussion of these control strategies is beyond the scope of this manual, but it is expected that these types of control strategies will play a greater role in air quality in the future.

For motor vehicles, a significant source type in most emissions inventories, it is important that future control measures be properly incorporated into future year emission estimates. For example, new vehicle emission standards, inspection and maintenance (I/M) programs, and fuel reformulations will have a significant effect on future year emissions. These

controls can be included in emission factor model input files (e.g., MOBILE-type models), but some consideration should be given to which classes of the vehicle fleet will be affected by these controls.

6.4   <u>Projection Example</u>

This portion of the example focuses on the projection of annual emissions to future years. As mentioned earlier, projections may not be considered to be a modeling inventory development step. However, annual base year emissions data are often projected and then temporally allocated, spatially allocated, and speciated to create modeling inventories of the projected emissions. In order to provide a clear illustration of future year projections, growth and control factors will be applied to annual emissions for one source category. A simplified projection calculation is included in the more detailed example showing all modeling inventory development steps presented in Section 7.0. Projected emissions, however, are not included in the Appendix A spreadsheets due to the large number of calculations.

Example Calculation

The emissions from the residential consumer solvent use category are to be projected from a base year of 1999 to the year 2010. The annual base year emissions from this category have been estimated to be 200 Mg/yr. Residential consumer solvent use emissions are typically increased using population forecasts; the local planning agency has estimated that the population in the hypothetical modeling inventory community will grow at an annual rate of 2.3%. A regulation that limits the amount of TOG contained in personal products (a portion of the residential consumer solvent use category) will be implemented in the year 2003. The regulation will reduce the TOG content by 50%. However, due to expected implementation problems, rule effectiveness is expected to be low initially. Rule effectiveness is only expected to be 10% in the first year of the regulation (2003), increasing 10% for each subsequent year until a maximum rule effectiveness of 80% is reached in the eighth year of the regulation (2010). Emissions from personal products use comprise 35% of the total emissions from residential consumer solvent use.

If growth factors alone are considered, the consumer solvent use emissions would increase to 256.8 Mg/yr in the year 2010 as shown by Curve A in Figure 6-1. The calculation for projecting growth only to the year 2005 is provided as follows:

$$E_{proj} = E_{base} \times (1 + \%_{ann}/100)^y$$
$$E_{2005} = E_{1999} \times (1 + 2.3/100)^{(2005-1999)}$$
$$E_{2005} = (200 \text{ Mg/yr}) \times (1.023)^6 = 229.2 \text{ Mg/yr}$$

If control factors alone are considered, the consumer solvent use emissions would decrease to 172.0 Mg/year in the year 2010 as shown by Curve B in Figure 6-1. The calculation for projecting controls only to the year 2005 is provided as follows:

$$E_c = E_u \times [1 - (CE/100) \times RE \times RP]$$
$$E_{c,2005} = E_{u,2005} \times [1 - (50/100) \times 0.3 \times 0.35]$$
$$E_{c,2005} = (200 \text{ Mg/yr}) \times [1 - 0.0525] = 189.5 \text{ Mg/yr}$$

If both growth factors and control factors are considered together, the consumer solvent use emissions would increase to 220.9 Mg/year in the year 2010 as shown by Curve C in Figure 6-1. It should be noted that these emissions are 14% less than if VOC limits had not been implemented. The calculation for projecting both growth and controls to the year 2005 is provided as follows:

$$E_{proj} = E_u \times [1 - (CE/100) \times RE \times RP] \times (1 + \%_{ann}/100)^y$$
$$E_{proj} = (200 \text{ Mg/yr}) \times [1 - (50/100) \times 0.3 \times 0.35] \times (1 + 2.3/100)^6$$
$$E_{proj} = (200 \text{ Mg/yr}) \times (0.9475) \times (1.1462) = 217.2 \text{ Mg/yr}$$

This example illustrates that future year emission projections may be significantly influenced by growth. As shown in this example, the effects of growth may negate any emission reductions brought about by controls. Although the reduction of emissions for personal products due to VOC limits is significant (i.e., 50%), the overall effect of this within the entire consumer solvent use category is much less due to the slow eight-year implementation and somewhat narrow focus (i.e., only 35% of the consumer solvent use category was affected). A real-life example which shows the influence of growth on future year emissions can be seen with motor vehicles in the U.S. Significant technological advances have reduced motor vehicle emissions (on a per-mile basis) by an order of magnitude or more compared to 20 or 30 years ago, but ever-increasing growth of vehicle travel (which typically exceeds population growth) has offset much of the realized emission reductions.
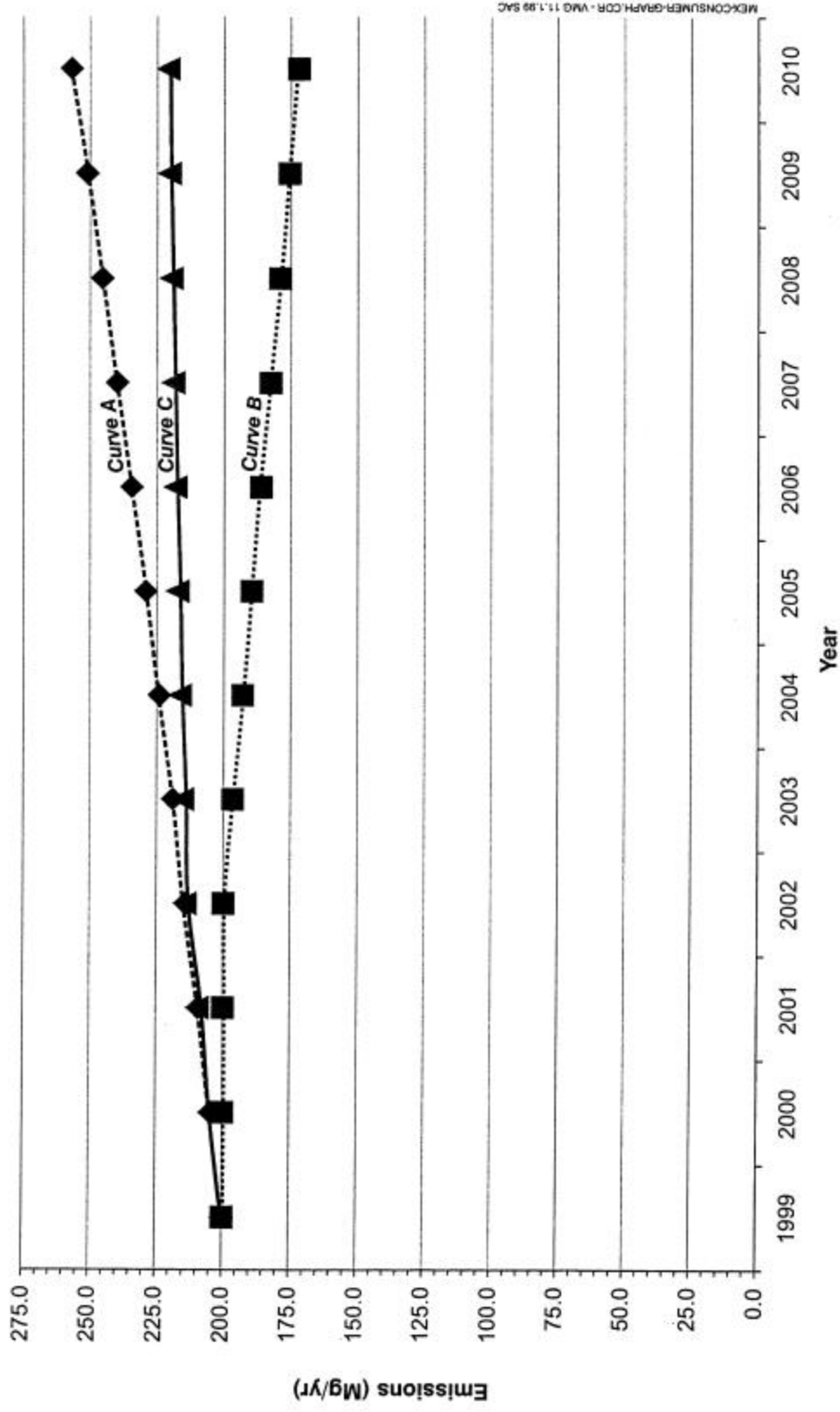
Figure 6-1. Estimated Projections of Consumer Product Use Source Category for Hypothetical Modeling Inventory

7.0 MODELING INVENTORY DEVELOPMENT EXAMPLE

This section presents a comprehensive example for one source category and illustrates temporal allocation, spatial allocation, speciation, and projection performed sequentially. The gasoline station source category was selected for this example. Detailed calculation spreadsheets for this category and the other categories in this hypothetical modeling inventory can be found in Appendix A. The numbers calculated in this example are identified in the Appendix A spreadsheets by a bold font and highlighted cells. For actual modeling inventories, an electronic emissions modeling system will need to be utilized. The calculation spreadsheets presented in this document were included for demonstration purposes only; spreadsheets should <u>not</u> be used for actual modeling inventories.

7.1 Temporal Allocation

The assumed gasoline station temporal profiles were presented in Figure 3-3 (seasonal), Figure 3-4 (weekly), and Figure 3-5 (hourly).

The first step in temporal allocation is to determine seasonal allocation factors. Monthly gasoline station activity assumed for this example is presented in Table 7-1 (this monthly distribution is identical to the assumed motor vehicle activity distribution presented in Section 3.6).

**Table 7-1. Assumed Monthly Gasoline Station Temporal Allocation Profile
for the Hypothetical Modeling Inventory**

Month	Fraction of Annual Activity
January	0.081
February	0.078
March	0.080
April	0.084
May	0.089
June	0.081
July	0.082
August	0.083
September	0.079
October	0.088
November	0.084
December	0.091
Total	**1.000**

Seasonal temporal allocations are estimated as follows:

$$TA_s \quad = \quad TA_{m1} + TA_{m2} + TA_{m3}$$
$$TA_{win} = \quad TA_{Dec} + TA_{Jan} + TA_{Feb} \quad = \quad 0.091 + 0.081 + 0.078 = 0.250$$
$$TA_{spr} = \quad TA_{Mar} + TA_{Apr} + TA_{May} = \quad 0.080 + 0.084 + 0.089 = 0.253$$
$$TA_{sum} = \quad TA_{Jun} + TA_{Jul} + TA_{Aug} \quad = \quad 0.081 + 0.082 + 0.083 = 0.246$$
$$TA_{fal} = \quad TA_{Sep} + TA_{Oct} + TA_{Nov} \quad = \quad 0.079 + 0.088 + 0.084 = 0.251$$

The check of seasonal temporal allocations calculations is also shown.

$$TA_{win} + TA_{spr} + TA_{sum} + TA_{fal} = 0.250 + 0.253 + 0.246 + 0.251 = 1.000$$

Given annual TOG emissions of 150 Mg/yr (previously shown in Table 1-1), the

seasonal emissions are calculated as follows:

$$E_{TOG,win} \quad = \quad Annual_{TOG} \times TA_{win} = 150 \text{ Mg/yr} \times 0.250 = 37.50 \text{ Mg}$$
$$E_{TOG,spr} \quad = \quad Annual_{TOG} \times TA_{spr} \ = 150 \text{ Mg/yr} \times 0.253 = 37.95 \text{ Mg}$$
$$E_{TOG,sum} \quad = \quad Annual_{TOG} \times TA_{sum} = 150 \text{ Mg/yr} \times 0.246 = 36.90 \text{ Mg}$$
$$E_{TOG,fal} \quad = \quad Annual_{TOG} \times TA_{fal} \ = 150 \text{ Mg/yr} \times 0.251 = 37.65 \text{ Mg}$$

After calculating seasonal emissions, the next step is to estimate emissions on a weekly basis. The assumed weekly gasoline station activity is shown in Table 7-2 (this weekly distribution is also identical to the assumed motor vehicle activity distribution presented in Section 3.6).

Table 7-2. Assumed Weekly Gasoline Station Temporal Allocation Profile for the Hypothetical Modeling Inventory

Day	Fraction of Weekly Activity
Monday	0.138
Tuesday	0.138
Wednesday	0.138
Thursday	0.138
Friday	0.138
Saturday	0.155
Sunday	0.155
Total	**1.000**

The equations for converting weekly temporal allocation into average weekday, Saturday, and Sunday factors are shown below.

$$F_{wd} = F_{ad} \times (A_{wd}/0.1429) = 0.0110 \times (0.138/0.1429) = 0.0106 = 1.06\%$$
$$F_{sat} = F_{ad} \times (A_{sat}/0.1429) = 0.0110 \times (0.155/0.1429) = 0.0119 = 1.19\%$$
$$F_{sun} = F_{ad} \times (A_{sun}/0.1429) = 0.0110 \times (0.155/0.1429) = 0.0119 = 1.19\%$$

The check of the weekly temporal allocation calculations is also shown.

$$(65 \times F_{wd}) + (13 \times F_{sat}) + (13 \times F_{sun}) = (65 \times 0.0106) + (13 \times 0.0119) + (13 \times 0.0119)$$
$$= 0.689 + 0.1547 + 0.1547 = 0.9984 \approx 1.00$$

Using the calculated seasonal gasoline station emissions (spring – 37.95 Mg, summer – 36.90 Mg, fall – 37.65 Mg, and winter – 37.50 Mg) and the calculated weekly temporal allocations ($F_{wd} = 0.0106$, $F_{sat} = 0.0119$, and $F_{sun} = 0.0119$), the weekly allocated emissions are calculated as shown below. The calculation shown below is for summer weekdays only; the other allocated emissions are calculated in a similar manner with the results shown in Table 7-3.

$$E_{TOG,sum,wd} = E_{TOG,sum} \times F_{wd} = 36.90 \text{ Mg} \times 0.0106 = 0.392 \text{ Mg/day}$$

**Table 7-3. Estimated Weekly Allocated Gasoline Station Emissions
for the Hypothetical Modeling Inventory**

	Weekday (Mg/day)	Saturday (Mg/day)	Sunday (Mg/day)
Spring	0.403	0.452	0.452
Summer	0.392	0.440	0.440
Fall	0.400	0.449	0.449
Winter	0.398	0.447	0.447

After determining average weekday, Saturday, and Sunday emissions for each of the four seasons, the next step is to distribute daily gasoline station activity to an individual hourly basis. The assumed hourly gasoline station activity is distributed as shown in the Table 7-4; the distribution is assumed to be equally applicable for average weekdays, Saturdays, and Sundays. Note that Hour 1 refers to the first hour of the day (midnight to 1 a.m.), Hour 2 refers to the second hour of the day (1 a.m. to 2 a.m.), and so on. A check to confirm that the daily activity fractions total to 1.000 is also provided.

**Table 7-4. Assumed Hourly Gasoline Station Temporal Allocation Profile
for the Hypothetical Modeling Inventory**

Hour	Fraction of Daily Activity
1	0.009
2	0.009
3	0.009
4	0.009
5	0.009
6	0.009
7	0.043
8	0.043
9	0.043
10	0.043
11	0.043
12	0.043
13	0.043
14	0.043
15	0.043
16	0.043
17	0.086
18	0.086
19	0.086
20	0.086
21	0.060
22	0.060
23	0.026
24	0.026
Total	**1.000 ⌀**

The hourly emissions for Hour 18 on an average summer weekday are given below:

$$E_{TOG,sum,wd,18} = E_{TOG,sum,wd} \times F_{18} = 0.392 \text{ Mg/day} \times 0.086 = 0.034 \text{ Mg/hr}$$

All other hourly emission calculations are performed in an identical manner. The results for average weekday (wd), Saturday (Sat), and Sunday (Sun) in Mg per hour rounded to three decimal places are provided in Table 7-5.

Table 7-5. Estimated Temporally Allocated Gasoline Station Emissions for the Hypothetical Modeling Inventory

	Spring (Mg/hr)			Summer (Mg/hr)			Fall (Mg/hr)			Winter (Mg/hr)		
Hr	Wk	Sat	Sun	Wk	Sat	Sun	Wk	Sat	Sun	Wk	Sat	Sun
1	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
2	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
3	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
4	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
5	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
6	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
7	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
8	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
9	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
10	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
11	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
12	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
13	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
14	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
15	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
16	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019	0.017	0.019	0.019
17	0.035	0.039	0.039	0.034	0.038	0.038	0.034	0.039	0.039	0.034	0.038	0.038
18	0.035	0.039	0.039	0.034	0.038	0.038	0.034	0.039	0.039	0.034	0.038	0.038
19	0.035	0.039	0.039	0.034	0.038	0.038	0.034	0.039	0.039	0.034	0.038	0.038
20	0.035	0.039	0.039	0.034	0.038	0.038	0.034	0.039	0.039	0.034	0.038	0.038
21	0.024	0.027	0.027	0.024	0.026	0.026	0.024	0.027	0.027	0.024	0.027	0.027
22	0.024	0.027	0.027	0.024	0.026	0.026	0.024	0.027	0.027	0.024	0.027	0.027
23	0.010	0.012	0.012	0.010	0.011	0.011	0.010	0.012	0.012	0.010	0.012	0.012
24	0.010	0.012	0.012	0.010	0.011	0.011	0.010	0.012	0.012	0.010	0.012	0.012

7.2   <u>Spatial Allocation</u>

After temporal allocation of emissions has been completed, then spatial allocation is performed. The gasoline station spatial allocation was presented in Figure 4-4. It should be noted that the spatial allocation indicates that one-third of the gasoline station emissions are located in Cell A1 and two-thirds of the gasoline station emissions are located in Cell A3. Gasoline station emissions in the other seven cells (i.e., Cell A2, B1, B2, B3, C1, C2, and C3) will be zero. However, when an emissions modeling system is used, all potential values will be calculated.

Using the calculated hourly emissions shown in Table 7-5 and the spatial allocations shown in Figure 4-4 (Cell A1 = 0.333, Cell A3 = 0.667, and all other cells = 0.000), then the spatially allocated hourly emissions are calculated as follows:

$$E_{TOG,sum,wd,18,A1} = E_{TOG,sum,wd,18} \times SS_{A1} = 0.034 \text{ Mg} \times 0.333 = 0.011 \text{ Mg}$$

This calculation is for Cell A1 and Hour 18 of an average summer weekday, only. Other allocated emissions are calculated in a similar manner, and the results are shown in Table 7-6 and Table 7-7. All emission values are rounded to three decimal places.

Table 7-6. Estimated Spatially Allocated Gasoline Station Emissions (Cell A1)
for the Hypothetical Modeling Inventory

Cell A1	Spring (Mg/hr)			Summer (Mg/hr)			Fall (Mg/hr)			Winter (Mg/hr)		
Hr	**Wk**	**Sat**	**Sun**	**Wk**	**Sat**	**Sun**	**Wk**	**Sat**	**Sun**	**Wk**	**Sat**	**Sun**
1	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
2	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
3	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
4	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
5	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
6	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
7	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
8	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
9	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
10	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
11	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
12	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
13	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
14	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
15	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
16	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006
17	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
18	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
19	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
20	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
21	0.008	0.009	0.009	0.008	0.009	0.009	0.008	0.009	0.009	0.008	0.009	0.009
22	0.008	0.009	0.009	0.008	0.009	0.009	0.008	0.009	0.009	0.008	0.009	0.009
23	0.003	0.004	0.004	0.003	0.004	0.004	0.003	0.004	0.004	0.003	0.004	0.004
24	0.003	0.004	0.004	0.003	0.004	0.004	0.003	0.004	0.004	0.003	0.004	0.004

**Table 7-7. Estimated Spatially Allocated Gasoline Station Emissions (Cell A3)
for the Hypothetical Modeling Inventory**

Cell A3	Spring (Mg/hr)			Summer (Mg/hr)			Fall (Mg/hr)			Winter (Mg/hr)		
Hr	**Wk**	**Sat**	**Sun**	**Wk**	**Sat**	**Sun**	**Wk**	**Sat**	**Sun**	**Wk**	**Sat**	**Sun**
1	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003
2	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003
3	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003
4	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003
5	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003
6	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003	0.002	0.003	0.003
7	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
8	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
9	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
10	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
11	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
12	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
13	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
14	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
15	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
16	0.012	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013	0.011	0.013	0.013
17	0.023	0.026	0.026	0.022	0.025	0.025	0.023	0.026	0.026	0.023	0.026	0.026
18	0.023	0.026	0.026	0.022	0.025	0.025	0.023	0.026	0.026	0.023	0.026	0.026
19	0.023	0.026	0.026	0.022	0.025	0.025	0.023	0.026	0.026	0.023	0.026	0.026
20	0.023	0.026	0.026	0.022	0.025	0.025	0.023	0.026	0.026	0.023	0.026	0.026
21	0.016	0.018	0.018	0.016	0.018	0.018	0.016	0.018	0.018	0.016	0.018	0.018
22	0.016	0.018	0.018	0.016	0.018	0.018	0.016	0.018	0.018	0.016	0.018	0.018
23	0.007	0.008	0.008	0.007	0.008	0.008	0.007	0.008	0.008	0.007	0.008	0.008
24	0.007	0.008	0.008	0.007	0.008	0.008	0.007	0.008	0.008	0.007	0.008	0.008

7.3 <u>**Speciation**</u>

After spatial allocation of emissions has been completed, then speciation is performed. The TOG speciation profile for gasoline stations is presented in Appendix B. Because of the large number of calculations that would be required to speciate each of the hourly, gridded emission estimates, these calculations are not included in this section or in Appendix A. Examples of speciation have been provided in Section 5.0.

7.4 <u>**Projections**</u>

As part of this example, a hypothetical projection factor will be calculated that could be applied to the previously estimated temporally and spatially allocated emissions. In general, projections are needed when an estimate of future emissions which include the effects of growth and controls are desired.

The projection scenario used here is for a projected year 10 years from the base year. The base year emissions from gasoline stations will be used (i.e., 150 Mg/yr). During the 10 years between the base year and the projected year, it is estimated that the population in the inventory domain will increase by an annual growth rate of 1.3%. As a rough estimate, it is assumed that gasoline throughput at the gasoline stations will grow at a similar annual growth rate. Also, various control strategies to be implemented during the 10 years between the base year and the projected year are estimated to provide a 40% control efficiency relative to uncontrolled emissions. Rule effectiveness (RE) and rule penetration (RP) are both assumed to be 90%.

The calculation for estimating the projected emissions is provided as follows:

$$
\begin{aligned}
E_{proj} &= E_u \times [1 - (CE/100) \times RE \times RP] \times (1 + \%_{ann}/100)^y \\
E_{proj} &= (150 \text{ Mg/yr}) \times [1 - (40/100) \times 0.9 \times 0.9)] \times (1 + 1.3/100)^{10} \\
E_{proj} &= (150 \text{ Mg/yr}) \times [0.676] \times (1.1379) = 115.4 \text{ Mg/yr}
\end{aligned}
$$

The projection factor is then calculated by dividing the projected emissions by the base year emissions as shown below:

$$F_{proj} = E_{proj}/E_u = (115.4 \text{ Mg/yr})/(150 \text{ Mg/yr}) = 0.769$$

Assuming that the effects of growth and control are evenly distributed over the entire modeling grid domain and during all time periods, then the temporally and spatially allocated base year emissions can be multiplied by a factor of 0.769 to obtain the temporally and spatially allocated projected year emissions. If the assumption that the effects of growth and control are evenly distributed over the entire modeling grid domain is not valid, then the entire modeling inventory development process should be performed with annual emission estimates from the projected year inventory.

8.0 SUMMARY OF HYPOTHETICAL MODELING INVENTORY

A major benefit of a modeling inventory is that a large body of complex data can be developed for input into air quality models. In addition, this data set can be analyzed to determine if the modeling inventory adequately represents the actual emission processes. A few representative analyses from the complete hypothetical modeling inventory are presented below; similar analyses can be derived from actual modeling inventories.

Figure 8-1 presents the hourly distribution of summer weekday TOG emissions (total and by individual source category) for the hypothetical inventory domain. Table 8-1 shows the source-specific emissions that are allocated to Hour 12.

**Table 8-1. Hour 12 Summer Weekday TOG Emissions
for the Hypothetical Modeling Inventory**

Source Category	Emissions (Mg/hr)
Point – Boiler	0.000
Point – Process	0.144
Highway Vehicles	0.054
Gasoline Stations	0.017
Residential Consumer Solvents	0.041
Pesticides	0.080
Total	**0.336**

As expected, the hourly distribution peaks during the daytime hours. The daytime peak is affected primarily by the emissions from the coating process at the factory and, to a lesser extent, by agricultural pesticide use. Highway vehicle emissions occur throughout the day and are the predominant emission source during nighttime hours. Given the temporal profiles that were assumed for this inventory, these results are reasonable.
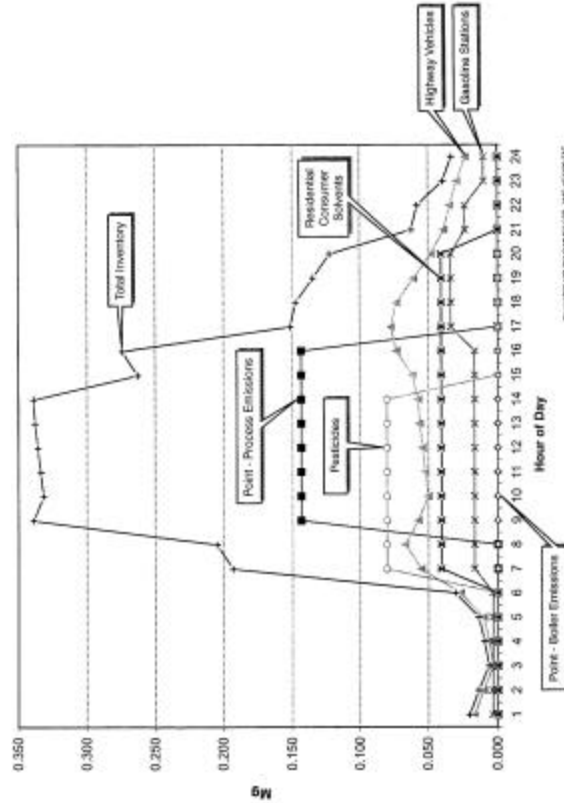
Figure 8-1. Hourly Distribution of Summer Weekday TOG Emissions for the Hypothetical Modelling Inventory

Figure 8-2 presents the hourly distribution of total summer and winter weekday TOG emissions for the entire hypothetical inventory domain. The summer curve is identical to the total curve in Figure 8-1; the scale, however, is different. The summer and winter curves "trace" each other very well from the evening to early morning hours. However, the winter emissions are considerably higher than the summer emissions. The main reason for this difference is that the factory boiler is assumed to be operating at a significant level during the winter and not during the summer. Once again, these results seem to agree with the temporal profiles that were assumed for this inventory.

Figure 8-3 shows the summer weekday TOG emissions for the hypothetical modeling inventory by grid cell. The stacked bar columns show the relative emissions contribution by each source category. The coating process emissions from the factory are the largest source located in Cell B3. Significant emissions from gasoline stations and highway vehicles are also located in Cells A1 and A3. Although pesticides are the only emitting source category in Cells C1 and C2, their contribution could be significant.

The relative distribution of total emissions in Figure 8-3 will be different if specific hours are analyzed. Also, the distribution of emissions would be different if different pollutants, seasons, or days were analyzed. For instance, if the distribution of summer weekday CO emissions was examined, there would be no emissions located in Cells B1, B2, C1, and C2. Only those cells with combustion sources (e.g., highway vehicles) would have any CO emissions. Likewise, the peak value of weekday TOG emissions located in Cell B3 (relative to other grid cells) would be even more pronounced in the winter because the factory boiler would be operating in addition to the coating process, which operates year-round. Finally, if weekend emissions were examined, instead of weekday emissions, there would be no peak value for TOG emissions in Cell B3 (relative to other grid cells) because the factory does not operate on Saturday or Sunday; TOG emissions in that grid cell would be at comparable levels to other grid cells.

The analyses presented in Figures 8-1, 8-2, and 8-3 are more straightforward than those associated with a typical modeling inventory. However, they demonstrate the analytical capabilities that are available through the use of modeling inventories.
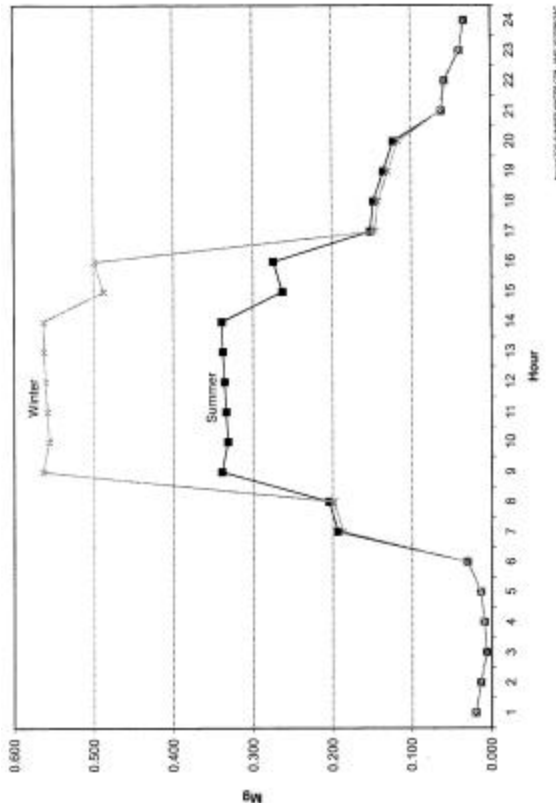
Figure 8-2. Comparison of Hourly Summer and Winter TOG Emissions for the Hypothetical Modeling Inventory
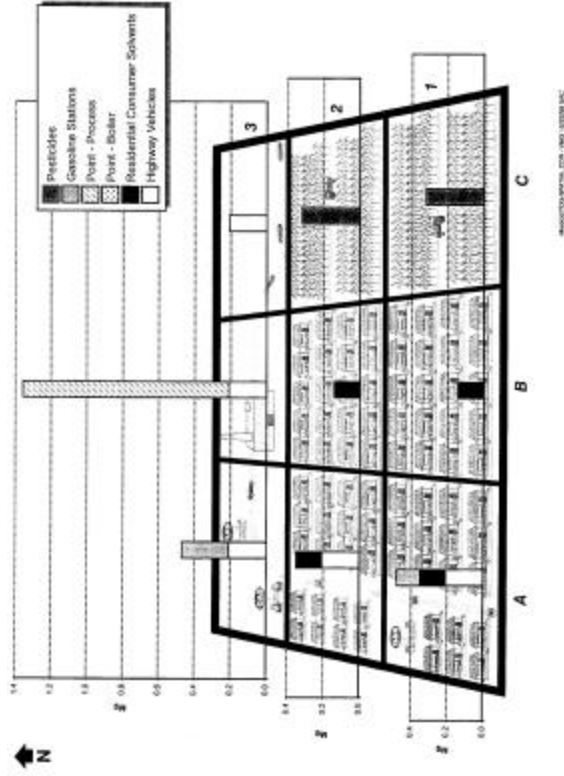
Figure 8-3. Spatial Distribution of Summer Weekday TOG Emissions for the Hypothetical Modeling Inventory

9.0 CONCLUSION

As mentioned previously, the spreadsheets located in Appendix A contain all the calculations used to temporally and spatially distribute emissions in this document's modeling inventory example. Due to the large number of computations, speciation calculations were not included in Appendix A. Likewise, projection calculations were also not included in Appendix A. The 66 pages contained in Appendix A address only temporal and spatial allocation for the six source categories and nine grid cells that were included in the hypothetical modeling inventory example used.

Although the modeling inventory example presented in this document was simplified compared to an actual modeling inventory, the four steps of modeling inventory development (i.e., temporal allocation, spatial allocation, speciation, and projection) are the fundamental methods used in all emissions modeling systems. In general, an electronic emissions modeling system, rather than spreadsheets such as those presented in Appendix A, is needed to develop modeling inventories. Furthermore, this manual should be used along with emissions model user's guides for developing modeling inventories and their required data sets.

10.0 REFERENCES

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APPENDIX A
Hypothetical Modeling Inventory Calculation Spreadsheets

This appendix presents the calculation spreadsheets used for the hypothetical modeling inventory example contained in this manual. The calculation spreadsheets for each of the six emission sources are presented in this appendix as follows:

- Factory boiler – pages A-1 through A-11;

- Factory coating process – pages A-12 through A-22;

- On-road motor vehicles – pages A-23 through A-33;

- Gasoline stations – pages A-34 through A-44;

- Residential consumer solvent use – pages A-45 through A-55; and

- Pesticide application – pages A-56 through A-66.

The format of each 11 page emission source spreadsheet is as follows:

- Page #1 – Presentation of annual emissions; presentation of monthly, weekly, and hourly temporal allocation profiles; calculation of seasonal profiles, weekly activity profiles, and weekly allocation factors; and calculation of seasonal, average weekday, average Saturday, and average Sunday emissions;

- Page #2 – Temporally allocated emissions;

- Page #3 – Gridded and temporally allocated emissions for Cell A1;

- Page #4 – Gridded and temporally allocated emissions for Cell A2;

- Page #5 – Gridded and temporally allocated emissions for Cell A3;

- Page #6 – Gridded and temporally allocated emissions for Cell B1;

- Page #7 – Gridded and temporally allocated emissions for Cell B2;

- Page #8 – Gridded and temporally allocated emissions for Cell B3;

- Page #9 – Gridded and temporally allocated emissions for Cell C1;

- Page #10 – Gridded and temporally allocated emissions for Cell C2; and

- Page #11 – Gridded and temporally allocated emissions for Cell C3.

APPENDIX B
Hypothetical Modeling Inventory TOG Speciation Profiles

This appendix presents TOG speciation profiles that might be used for each of the six emission sources presented in this manual. All of the speciation profiles presented were obtained from U.S. EPA's SPECIATE database (U.S. EPA, 1999c). Each profile is labeled with the SPECIATE database profile number. The five columns for each profile identify the SPECIATE compound number, CAS number, species name, molecular weight, and weight percent for each compound in the speciation profile.

APPENDIX C
Hypothetical Modeling Inventory PM Speciation Profiles

This appendix presents PM speciation profiles that might be used for the two of the six emission sources presented in this manual that would have PM emissions (i.e., factory boiler and on-road motor vehicles). Both speciation profiles presented were obtained from U.S. EPA's SPECIATE database (U.S. EPA, 1999c). Each profile is labeled with the SPECIATE database profile number. The three columns in each profile identify the CAS number, species name, and weight percent for each compound in the speciation profile. It should be noted that these speciation profiles were not actually used in this manual and are presented for informational purposes only.

Factory Boiler

Factory Coating Process

On-road Motor Vehicles

Gasoline Stations

Residential Consumer Solvent Use

Pesticide Application