FUTURE DIRECTIONS OF ATMOSPHERIC DISPERSION MODELING FOR REGULATORY USE IN THE UNITED STATES

D. Eli Sherman
Department of Civil Engineering
Colorado State University
Fort Collins, CO 80523

Advisor: Dr. Sonia M. Kreidenweis
Department of Atmospheric Science
Colorado State University
Fort Collins, CO 80523

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Environmental Engineering Program Within the Civil Engineering Department,
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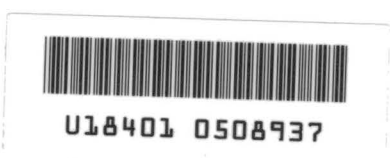

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ABSTRACT

Computer aided mathematical air pollution models are an important tool in the development of successful air pollution control strategies. Today air pollution models are used to determine the impact of anthropogenic activities, where a proposed source may be built, source emission limits, and source control technology requirements.

This paper determines future directions of atmospheric dispersion modeling for regulatory use in the United States. It develops a comprehensive overview of the United States air pollution regulations, reviews the available mathematical modeling theories, presents current model evaluation and validation methods, and examines future advances in air pollution modeling.

Future uses of air pollution modeling are dependent upon environmental regulations, current air pollution research, and advances in computer architecture and programming. In the past, air pollution regulations contained only implicit air pollution modeling requirements. The current regulations contain explicit requirements for the use of air pollution modeling as will future regulations due to the high costs of implementing air pollution control strategies.

Current research efforts are aimed at improving air pollution modeling dispersion, transport, and removal processes. The development and use of advanced model evaluation methods are important in identifying model weaknesses and areas for model improvements. As model become more complex, greater computer power is required. Therefore, current air pollution research, the development of advanced model evaluation methods, and future advances in computer capabilities are limiting factors in the implementation of advanced computer aided air pollution modeling for regulatory use.

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1.0 INTRODUCTION

Today many areas throughout the world are experiencing extensive air pollution problems such as smog, acid deposition, air toxins, climate modifications, and stratospheric ozone depletion. Problems range from the small scale, such as indoor air quality and urban airshed problems, to the large scale, such as regional and global problems. Air pollution problems are becoming increasingly predominant with the continuing growth of the world's population and its increased industrialization. The difficulties that many of the major world cities face in setting air pollution standards and goals have led most countries to develop comprehensive air pollution control strategies to protect public health and the quality of life. One of the most important tools in developing a successful strategy is the use of computer aided mathematical air pollution models to estimate and predict the impact of anthropogenic activities.

This paper develops a comprehensive overview of the United States air pollution regulations, reviews the available mathematical modeling theories, presents current model evaluation and validation methods, and examines future advances in air pollution modeling. The United States air pollution regulations are reviewed to illustrate how air pollution regulations have been the driving force in the continued growth of air pollution modeling. The mathematical modeling theories are reviewed to develop an understanding of the fundamental methods for air pollution modeling. Model evaluation and validation methods are presented to illustrate air pollution modeling uncertainties and methods for determining model weaknesses so future improvements can be made. Recent advances in air pollution modeling are examined to demonstrate where improvements are being made and to illustrate current and future trends in air pollution modeling for regulatory use.

2.0 REGULATIONS

In order to better understand the current air pollution control strategies and their importance to the modeling and permitting processes, it is necessary to look at passed air quality legislation and regulations. This section will briefly discuss the historic regulatory efforts to control air pollution with an in-depth look at the Clean Air Act Amendments of 1990.

2.1. Historic Legislation

Common Law initiatives were the first efforts at controlling the growing air pollution problems of United States. Tort cases involving nuisance, negligence and trespass violations were used to curb local air pollution problems. The first air quality management program in the United States used nuisance law to establish an antismoke ordinance issued in 1881 by Chicago (Davis and Cornwell, 1991).

However, these local initiatives were not sufficient and in 1955, the federal government entered the picture when Congress passed the Air Pollution Control Act. This act provided research opportunities to better understand air pollution problems and the means to control it. However, it did not provide regulatory authority. In 1963, the first Clean Air Act was passed to grant federal regulatory authority to force control of emissions in targeted areas.

2.1.1. Air Quality Act of 1967

The lack of success of past efforts to control air pollution problems led to the Air Quality Act of 1967. This act extended research and development efforts by the federal government. The act was the first legislation to grant the federal government authority to enforce the use of air pollution control equipment on industries. It required states to develop State Implementation Plans (SIPs) and develop ambient air quality standards (Davis and Cornwell, 1991). The enforcing agency was the Secretary of Health, Education, and Welfare (HEW). HEW was required to designate air quality

control regions (AQCR) and promulgate air quality criteria. In addition HEW had to issue documents showing the availability, cost, and the effectiveness of control techniques to prevent further pollution. This act was the first to use the concept of "technology-forcing legislation" to achieve its air quality goals.

2.1.2. Clean Air Act of 1970

The failure of the Air Quality Act to produce noticeable gains resulted in the Clean Air Act (CAA) of 1970. The objective of this act was to attain clean air within five years. It was established "to protect and enhance the quality of the Nation's air resources to promote the public health and welfare and the productive capacity of its population," (Corbitt, 1990). It gave the newly created Environmental Protection Agency (EPA) the responsibility and authority to establish a nationwide air pollution abatement and air quality enhancement strategy. Under the Act the EPA had to establish both primary and secondary National Ambient Air Quality Standards (NAAQS) for the criteria pollutants. The primary standard protected the public health, while the secondary standard protected the public welfare from adverse effects of air pollution.

The Act called for the combination of state and federal stationary source emission standards to achieve the NAAQS goals. It gave the EPA the responsibility to supervise the implementation of these programs by state. Each state developed EPA approved State Implementation Plans (SIP) which explained the state's strategy for attaining the NAAQS goals.

The EPA Administrator was required to write the New Source Performance Standards (NSPS) to ensure that states would not weaken their standards to compete unfairly for new industrial sites. The act required each industrial site to monitor and store its emissions data for the reviewing state control agencies or the EPA to determine compliance with emission standards.

In Title II of the 1970 act, Congress imposed "technology forcing" legislation to achieve at least a 90 percent reduction of carbon monoxide and hydrocarbon emissions from motor vehicles over

the next 5 years. This marked a major shift in federal policy by stressing improvements in available technology (Plater et al., 1992).

2.1.3. Clean Air Act of 1977

The Clean Air Act Amendments of 1977 substantially broadened the federal program with an intent to resolve many of the controversial issues that were not cover or vaguely discussed in the 1970 Act. The most significant provisions of this act were the new requirements for areas that failed to attain the NAAQS by the 1975 deadline for primary pollutants and the new provision for "preventing significant deterioration" (PSD) of air quality in designated areas were the air is cleaner than the NAAQS.

Other issues addressed by the 1977 Amendments dealt with federal facilities, acceptability of pollution dispersion techniques, new enforcement strategies, federal regulations on previously unregulated pollutants and pollution sources, provisions dealing with increase coal utilization, interstate air pollution prohibitions, volatile organic compound (VOC) emission standards, national emission standards for hazardous air pollutants (NESHAP), and more specific but relaxed emission standards for vehicles (Calvert and Englund, 1984).

The failure of 160 of the nation's 247 Air Quality Control Regions (AQCR) to comply with the primary NAAQS by the July 1975 deadline, forced the EPA to develop a strategy to control the air pollution problem but still allow economic growth in those areas (Calvert and Englund, 1984). The EPA's strategy for dealing with nonattainment areas was to develop a nonattainment emissions offsets program and have the ability to inflict stricter emissions limits. This program allowed new sources to be constructed if they arranged for legally enforceable emissions reductions from existing sources in the same nonattainment area.

To determine the degree of offset required in a particular nonattainment area, atmospheric dispersion models were used to calculate the impact of new sources on that particular area. For

example, if the emissions offset ratio for a new source to old source was found to be a 1:1 ratio, then the new source had to find an equal amount of offset between the new and existing sources. If a new source was to emit 20 lbs/hr of SOx then the existing SOx source(s) would have to reduce their emissions by 20 lbs/hr.

To prevent existing sources from leaving nonattainment areas or new sources locating in areas with air quality better than the NAAQSs, the Prevention of Significant Deterioration (PSD) legislation was added to the 1977 CAA. This portion of the act designated areas of the nation into three classes of incremental air quality standards, as shown in Table 2.1 and modified later to those listed in Table 2.6. These increments are based on the level of air pollution permitted to cause significant deterioration in an area. The chief purpose of this program was to make sure new or modified sources would not cause violations of the NAAQS and PSD increment thresholds.

Table 2.1: PSD Area Classification.

Area Classification	Area Description
Class I	Pristine areas including international parks, wilderness areas, and national memorial parks which exceed 5,000 acres in size and national parks which exceed 6,000 acres in size.
Class II	All other areas assumed to be in attainment or unclassified for the NAAQSs.
Class III	Generally Urban areas that are classified as nonattainment for the NAAQSs.

(Source: Arbuckle, 1993.)

The PSD legislation required that a preconstruction review and permit be assembled before construction of any new source. The preconstruction review required that an air quality analysis be conducted. It also required that an analysis for the Best Available Control Technology (BACT) be conducted on the proposed source.

Before a PSD permit may be issued the proposed source must provide a detailed impact assessment, which must be made available to the public. This impact assessment must measure the

source's impact on air quality, visibility, soils and vegetation, and describe the climate and meteorology of the area effected. To determine the air quality impacts of the source an approved EPA models must be used. The models must measure the impact of the new source in the immediate area and in distant areas. The EPA allows the use of preliminary screening techniques to decide whether a full scale model must be used for the review. These screening techniques are a simple conservative way of assessing and estimating a source's impact on the air quality.

This law requires that an approved major source must conduct post-construction ambient air monitoring to determine the source's actual impact on the air quality and the available or unused pollution increment. However, due to the inaccuracies of the measurement devices at that time, and the unavailability of reliable baseline air quality data, atmospheric models were used to account for the available air pollution increment (Calvert and Englund, 1984).

2.2. The Current Clean Air Legislation and Regulations

As President Bush signed the Clean Air Act Amendments of 1990 he said, "It is simply the most significant air pollution legislation in our nation's history." This marked the end of a decade-long debate in Congress over the issue of air pollution. The act offers a significantly new approach to air quality by incorporating a "market-based" approach to environmental problems. The Act addresses problems associated with motor vehicles and their fuels, acid rain, urban air quality, air toxins, and stratospheric ozone. It employs a new federally mandated air pollution permit program similar to the Clean Water Act's (CWA) National Pollution Discharge Elimination System (NPDES) which will be administered by the states through their State Implementation Plans (SIP's). The act provides for continued research opportunities to improve air pollution monitoring, analysis, modeling, and inventory techniques, along with continued research to quantify the environmental stresses associated with several different types of air pollution, clean fuels research, and pollution prevention research.

The 1990 Clean Air Act implications for atmospheric dispersion modeling are significant. Titles I, III, VIII, and IX contain provisions that require the use of air quality dispersion and/or

photochemical modeling to satisfy their requirements. In addition, many sources may be required to perform air quality models under various state-implemented Title V operating permit programs. This will be done to demonstrate compliance with NAAQSs and PSD increment standards along with evaluating concerns about hazardous air pollutant releases and the impact that permit modifications may have on the air quality.

2.2.1. National Ambient Air Quality Standards (NAAQS)

The National Ambient Air Quality standard (NAAQS) program is designed to regulate those pollutants that are emitted from a variety of sources in relatively large quantities (criteria pollutants) that threaten human health (primary standards) and human welfare (secondary standards) across broad regions of the country (Durenberger, 1991). The NAAQS's are to be reviewed and revised as appropriate every five years (CAA section 109). The NAAQS's are to be implemented by the states through State Implementation Plans (SIPs) by placing source specific emission limitations. The criteria for how stringent a SIP is depends upon whether an area is in attainment or the severity of nonattainment for the NAAQS's. The NAAQS's are listed as concentrations that cannot be exceeded over a certain time period more than once per year or it is listed as an annual arithmetic mean concentration. The 1993 NAAQS are listed in Table 2.2.

Table 2.2. National Ambient Air Quality Standards.

Pollutant	Average Time	Primary Standard	Secondary Standard
PM - 10	24-hour	150 $\mu g/m^3$	
	Annual Arithmetic Mean	50 $\mu g/m^3$	
SO_2	3-hour		1300 $\mu g/m^3$
	24-hour	365 $\mu g/m^3$ (0.14 ppm)	
	Annual Arithmetic Mean	80 $\mu g/m^3$	
CO	1-hour	35 ppm	None
	8-hour	9 ppm	None
NO_2	Annual Arithmetic Mean	0.053 ppm	
O_3	Maximum Daily 1-hour Average	0.12 ppm	
Pb	Maximum Quarterly Average	1.5 $\mu g/m^3$	

(Source 40 CFR 50, 1993.)

2.2.2. State Implementation Plans (SIPs)

State Implementation Plans (SIPs) give states the authority and responsibility to assure that the NAAQS's are met and maintained within its borders. States must continually develop SIPs that are up-to-date with federal requirements. States have three years to revise SIPs after any new or modified NAAQS are issued. The EPA must issue written guidelines, interpretations, and information to states and the public to facilitate adequate submittal of SIPs (CAA section 172). Once a complete SIP is submitted, the administrator has one year to approve or disapprove of all or of part of the SIP. If a SIP fails to meet the requirements, the state then has one year to revise the SIP to meet the requirements. If the revised submission is not approved, the administrator must promulgate a Federal Implementation Plan (FIP) for the state. In addition the administrator may either cut off federal highway funds or require additional offsets of at least 2:1 for new or modified sources until the state corrects the deficiency (CAA 179). In addition the EPA administrator must publicly notify a state

and establish deadlines for SIP revisions if the SIP is "substantially inadequate" to maintain or attain the NAAQS's, prevent interstate air pollution, or other requirements of the act are not in compliance (CAA section 110).

Section 110 of the CAA requires SIPs to include provisions for:

i. enforceable emissions limitations and control measures;

ii. development of ambient air quality data;

iii. enforcement under the Title V permit program;

iv. prohibiting emissions that interfere with NAAQS attainment and requirements under the prevention of significant deterioration in another state;

v. adequate personnel, funding, and authority to carry out SIP;

vi. monitoring and periodically reporting emissions data from stationary sources;

vii. adequate contingency plans to restrict emissions of pollutants that present a danger to the public;

viii. revision of the SIP as necessary;

ix. nonattainment area requirements as discussed in the following section;

x. preconstruction review and notification requirements relating to the prevention of significant deterioration program;

xi. air quality modeling to predict the effects on emissions of any regulated pollutant on the ambient air quality;

xii. adequate permit fees for stationary sources for the Title V permit program.

For nonattainment areas, SIPs must provide provisions that require existing major sources to apply Reasonable Available Control Technology (RACT). In addition, new or modified major sources must apply Lowest Achievable Emission Rate (LAER) technology. Table 2.8 outlines these technology requirements for major stationary sources. SIPs must provide a plan to attain reasonable further progress in accomplishing the NAAQS goals. They should include provisions for obtaining

a current inventory of actual emissions from all sources of the nonattainment pollutant(s). Provisions for more restrictive requirements and permits for new and modified major stationary sources must be included in SIPs, along with a quantification of new allowable emissions in accordance with all new source requirements and reasonable further progress goals.

In addition to the requirements on major stationary sources for nonattainment areas, SIPs must include plans to reduce mobile source emissions. For areas in nonattainment for ozone and carbon monoxide, Table 2.3 illustrates the requirements placed on mobile source activities.

Table 2.3. SIPs Mobile Source Requirements for Ozone Nonattainment.

Pollutant	Classification	Requirement
Ozone	Nonattainment	Vehicle inspection and maintenance programs
	Moderate or worse	Gasoline vapor recovery rules
	Serious or worse	Enhanced vehicle inspection and maintenance programs
		Clean fuel vehicle programs and transportation control plans
	Severe or worse	Work related vehicle trip reduction programs
Carbon Monoxide	Moderate or serious	Enhance vehicle inspection and maintenance programs
	Serious	Transportation control plans
		Oxygenated gasoline requirements

(Source: Arbuckle, 1993.)

2.2.3. Addressed Pollution Problems

2.2.3.1. Nonattainment Areas. When the 1990 CAA Amendments passed, 96 of U.S. cities were in nonattainment for ozone (O_3), 41 for carbon monoxide (CO), and 72 for particulate matter (PM-10) (Reilly, 1991). Figure 2.1a and b show the areas of nonattainment for ozone and carbon monoxide respecitively.

Figure 2-1a:

Areas Violating Ozone Standards

Source: Reilly, 1991.

Figure 2-1b:

Areas Violating Carbon Monoxide Standards

Source: Reilly, 1991.

In Colorado, the 1993-1994 Air Quality Control Commission Report to the Public, reported that 73% of Coloradoans lived in nonattainment areas for one or more of the criteria pollutants. Title I of the 1990 CAA amendment addressed these issues by including an incremental approach to meeting the NAAQS's for these criteria pollutants. Table 2.4 illustrates these increments, the stationary sources that are considered major in these areas, along with the time goal for meeting the NAAQS's. Other requirements for major stationary sources are listed in Table 2.8.

Table 2.4. Nonattainment Classifications.

Pollutant	Area Classification	Pollutant Concentrations	Major Source Classification	Time Schedule for Meeting the NAAQS
Ozone	Marginal	0.121 - 0.138	≥ 100 tpy VOC or NO_x	3 years
	Moderate	0.138 - 0.160	≥ 100 tpy VOC or NO_x	6 years
	Serious	0.160 - 0.180	≥ 50 tpy VOC or NO_x	9 years
	Severe	0.180 - 0.280	≥ 25 tpy VOC or NO_x	15 years
	Extreme	0.280 and above	≥ 10 tpy VOC or NO_x	20 years
	Transport regions not classified as severe or extreme		≥ 50 tpy VOC or NO_x	
Carbon Monoxide	Moderate	?	≥	5 years
	Serious	?	≥ 50 tpy CO	20 years
PM-10[1]	Moderate[2]	?	≥	4 years
	Serious	?	≥ 70 tpy PM-10	21 years

1. Particulate matter with a median aerodynamic diameter ≤10 μm.
2. Initially all PM-10 nonattainment areas are classified as moderate and are reclassified as serious if not met by December 31, 1994.

Note: All time periods for meeting the NAAQS's start on November 15, 1990.
(Sources: Arbuckle, 1993, Hosford, 1993, and Kane, 1992.)

In addition, Title I of the 1990 amendments require that air quality modeling be used to demonstrate SIPs for showing reasonable further progress in nonattainment areas. Photochemical grid models must be used in ozone nonattainment areas that are serious to extreme within a state and moderate to extreme if the ozone nonattainment area contains more than one state. The best available

air quality monitoring and modeling must be used in determining source contributions of ozone nonattainment. States containing PM-10 nonattainment areas must use air quality modeling to demonstrate how their plan will provide for attainment of the NAAQS.

2.2.3.2. Mobile Sources.

Prior to the 1990 amendments, Title II of both the 1970 and 1977 CAAs imposed technology forcing legislation with the intent to encourage the development of alternatives to the internal combustion engine. Instead this prompted automakers to develop more advanced add-on pollution control equipment such as the catalytic converter. This resulted in a 96 percent decrease in hydrocarbon and carbon monoxide and a 76 percent decrease in nitrogen oxide (NOx) emissions from cars between 1970 and 1987. In addition the use of a catalytic converter resulted in the development of unleaded fuels which in turn resulted in a 94 percent decrease in lead emissions (Plater et al., 1992). However, the growing number of vehicles traveling on the nation's roadways has offset these technology improvements.

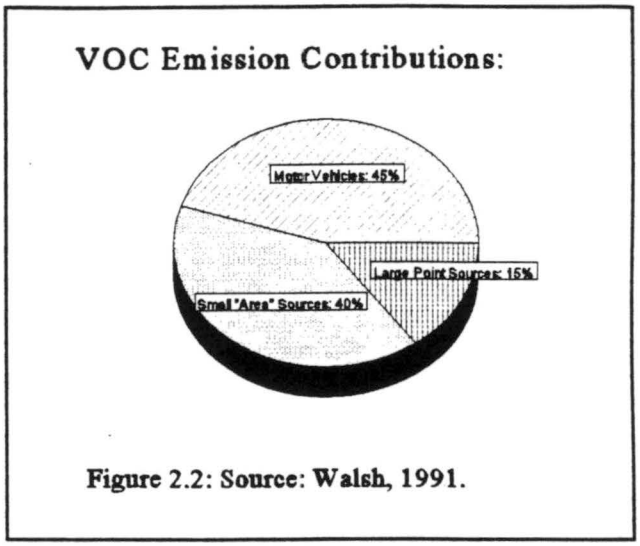


Figure 2.2: Source: Walsh, 1991.

Figures 2.2 and 2.3 demonstrate that motor vehicles still contribute 45 percent of the VOC emissions and 84 percent of the carbon monoxide emissions in the United States. In addition, motor vehicles account for nearly 50 percent of the NOx emissions (Walsh, 1991). The 1990 amendments substantially tighten mobile source emissions by reducing the tailpipe emissions of hydrocarbons by 35 percent and NOx by 60 percent starting with

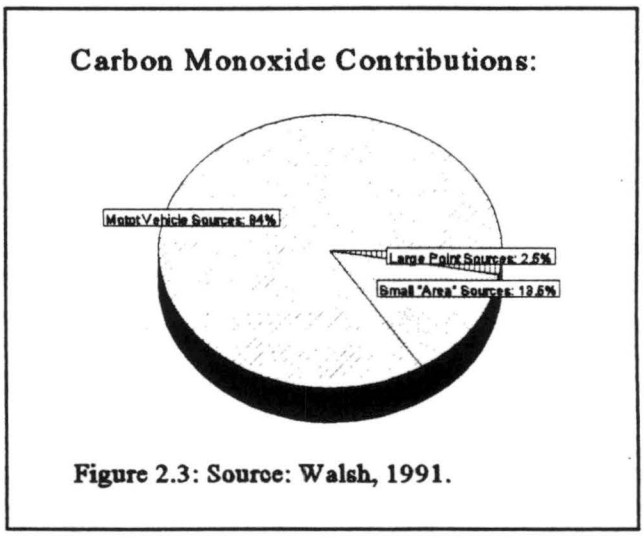


Figure 2.3: Source: Walsh, 1991.

40 percent of the vehicles sold in 1994 and increasing to 100 percent of the vehicles by 1996 (Arbuckle, 1993). The Act also establishes a reformulated fuel program and a clean alternative fuel program. The reformulated fuel program is intended to be used in areas of nonattainment according to Table 2.3.

The clean alternative fuel program is a pilot program that will be tested in California. Some of the clean fuels to be studied are methanol, ethanol, natural gas, and reformulated gasoline (Arbuckle, 1993). It requires the phase in of 150,000 clean fuel vehicles by 1996 and 300,000 clean fuel vehicles by 1999. In 1998, the purchase of clean fuel vehicles is required by operators of centrally fueled fleets of 10 or more vehicles in certain CO and ozone nonattainment areas (Arbuckle, 1993). Other states may volunteer into the pilot program through the "opt in" program. However, these states can only give economic incentives and not sales or production mandates. The success or failure of this program will determine the future of vehicle emission control programs through out the country.

2.2.3.3. Hazardous Air Pollutants. The adverse effects that hazardous air pollutants have on human health and the environment caused Congress to include legislation to control hazardous air pollutants in the 1977 amendments. However, prior to the 1990 amendments, the EPA had regulated only 8 hazardous air pollutants (HAPs) listed in Table 2.5 while the Occupational Safety and Health Administration (OSHA) regulated 500 toxins. The 1987 South Coast Air Basin study found that the cancer risk in humans to be one-in-one thousand due to the mixture of industrial, highway fuel, and small business emissions of air pollutant. As a reference, the EPA standard on cancer risk in humans is one-in-one million. It is also estimated that in Lake Superior 80 percent of the toxic substances found in the lake are deposited from the air (Durenberger, 1991). The lack of EPA success to promulgate more HAPs to provide for an "ample margin of safety to protect public health" lead Congress to change the air toxic regulations from health-based to technology-based regulations.

Table 2.5. Hazardous Air Pollutants Regulated Prior to the 1990 Amendments.

Air Toxin	Health Concern
Asbestos	A variety of lung diseases, particularly lung cancer.
Beryllium	Primary lung disease, although also affects liver, spleen, kidney, and lymph glands.
Mercury	Several areas of the brain as well as the kidneys and bowels affected.
Vinyl Chloride	Lung and liver cancer.
Arsenic	Causes cancer.
Radionuclides	Causes cancer
Benzene	Leukemia.
Coke Oven Emissions	Respiratory cancer.

(Source: Durenberger, 1991.)

In Title III Section 112 Part b of the 1990 Amendment, Congress listed 189 HAPs to be regulated by the EPA. The EPA was given the responsibility to identify all major source categories of these pollutants and develop maximum achievable control technology (MACT) standards by 2000. A major stationary source of a HAP, is one that emits more that 10 tons per year of any one HAP or 25 tons per year of any combination of HAPs. In setting these standards, the EPA must look at pollution control equipment along with pollution prevention methods and list these standards in the National Emission Standards for Hazardous Air Pollutants (NESHAPS) which are found in 40 CFR 61.

The Act provides incentives for early emissions reductions. If a source reduces its emissions by 90 percent before the MACT standards go into effect, then the source will have an additional six years to comply with the MACT standard.

The Act includes a second phase of regulatory control which is a health based regulation. The second phase, is triggered eight years after a MACT standard is published on a source category. In the second phase the EPA is then required to examine the residual risk levels remaining around a

source location to determine if health-based standards are necessary. Examination of the residual risk levels involves the use of dispersion models in determining if the risk level has more than a one-in-one million chance of causing reduced life time (cancer) in humans. If the risk level is more than a one-in-one million chance, then a health-based standard must be implemented to reduce the risk to an acceptable level.

Title III mandates that owners and operators of plants which use substances that have the potential to be emitted in quantities greater than threshold levels prepare risk management plans and hazard assessments for each substance. In preparing these plans and assessments it is essential that the source conduct dispersion models of air toxic releases to determine accidental release responses. The act also establishes a Chemical Safety Board to investigate accidental releases of air toxins (Wegman, 1991). In addition, Title III Section 112 requires the EPA to include the use of emissions models and ambient monitoring in urban areas to comply with the national strategy of reducing public health risks associated with hazardous air pollutant release.

2.2.3.4. Acid Deposition Control. The ability of acid rain to decrease visibility, damage lakes, streams, forests, and soils, corrode monuments and buildings, and threaten human health and welfare brought about the Title IV of the 1990 CAAAs. This is the first legislation to directly address this issue. The purpose of Title IV is to reduce acid deposition by reducing sulfur dioxide (SO_2) emissions by ten million tons annually and nitrogen oxide emissions by two million tons annually from the 1980 emission levels (CAA section 401 part b). The Act also places a national ceiling on sulfur dioxide emissions to 8.9 million tons per year by January 1, 2000.

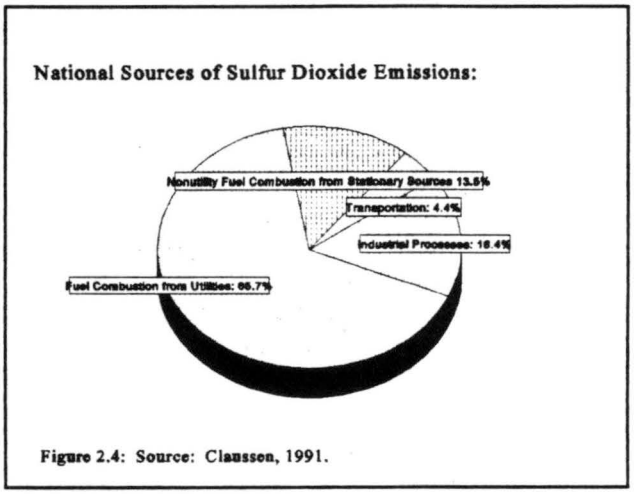


Figure 2.4: Source: Claussen, 1991.

The new program heavily targets utilities due to their large contribution in SO_2 emissions as seen in Figure 2.4. To achieve the reductions in sulfur dioxide emissions, a two phase, market based approach is being implemented. Each year utilities are allotted a budget of SO_2 allowances based on past fuel consumption and the national SO_2 emissions ceiling. Each allowance gives the utility the right to emit one ton of SO_2 emissions in the year they are assigned. If a utility exceeds their SO_2 allowance, it will be charged $2000 per ton and then the utility must offset the excess emissions in the following year.

In the first phase, effective January 1, 1995, 110 Midwest and Eastern coal-burning electric utility plants, listed under Title IV, Section 404, Table A, will be assigned SO_2 allowances that limit their emissions to below 2.5 lbs SO_2 per million Btu times the plants average 1985-1987 fuel use. However, plants may get a two year extension for phase one compliance if certain control technologies are used, such as SO_2 scrubbers.

In the second phase, effective January 1, 2000, all remaining utilities greater than 25 MW in size will have to limit emissions to 1.2 lbs SO_2 per million Btu times the source's average 1985-1987 fuel use. However, plants may receive a four year extension to the phase two compliance date if they repower with clean coal technologies.

In both phases, utilities can buy, trade, sell, or bank from year to year, unused allowances within their systems. This allows utilities flexibility in choosing the most cost-effective way to comply with the new regulations. For example, Illinois Power and Wisconsin Electric Power Company (WEPCo) have entered into a contract with each other to sell allowances back and forth. Illinois Power is purchasing credits for $170 a credit from WEPCo before the 1995 deadline while implementing scrubbers to their units. Between 1995 and 2000 Illinois Power is to sell credits back to WEPCo so they can be in compliance with the regulations (Roethler, 1993). This emissions allowance trading system is expected to save utilities $500 million dollars in phase two implementation (Torrens, et al., 1992).

The reduction in nitrogen oxides is to be achieved through performance standards in a two phase process. The phase one NO_x rules were applied in mid 1992 and established emissions limitations for tangentially fired and dry bottom boilers along with wall fired boilers. The phase two NO_x rules will be applied in 1997 and will contain regulations for all other boiler types. There is no allowance system for NO_x, however, individual utilities can average their NO_x emissions between multiple units.

In addition to the implementation of new control technologies, utilities must install equipment that continuously monitors emissions to ensure compliance with SO_2, NO_x, and other gas regulations. These continuous emission monitors (CEMs) must have an accuracy of within ±10% and must measure concentrations of emissions along with velocity or flow rates of the gases. The phase one monitors must have been operational by November 1993 while phase two monitors must have been operational by January 1, 1995 (Torrens, et al., 1992).

2.2.3.5. Stratospheric Ozone Protection. Title VI of the 1990 Amendments, addresses the issue of stratospheric ozone depletion and global warming by requiring the phase out of ozone depleting substances. In Section 602 Parts a and b, the Class I (chloroflurocarbons, halons, carbon tetrachloride, and methyl chloroform) and Class II (hydrochloroflurocarbons) substances are listed. Starting in 1991, it is unlawful to produce Class I substances in quantities greater than specified in Table 2 of Section 604 of the 1990 Amendments (Section 604 part a). The production of all Class I substances are to be prohibited by January 1, 2000, except methyl chloroform which will be prohibited after January 1, 2002 (Section 604 part b), while the production of all Class II substances will be eliminated by January 1, 2030 (Section 605 part b).

2.2.3.6. Miscellaneous Provisions. Title VIII of the 1990 CAAAs establishes a program to deal with outer continental shelf sources and it requires the EPA to establish a program to monitor and improve the air quality in regions along the United States and Mexican borders. Section 815 of the CAAA requires that the air quality monitoring along the USA and Mexican border

must be sufficient to be used in a state-of-the-art mathematical air quality model to predict emission reductions necessary to achieve compliance with the NAAQSs in both the USA and Mexico.

In addition to the border program, Title VIII, Section 816, requires the EPA to conduct visibility studies in Class I PSD areas. These studies include the use of visibility-adapted regional air quality models to identify and evaluate sources and source regions that contribute to visibility impairment and poor air quality.

Title IX includes provisions for:

i. improving air pollution monitoring, analysis, modeling, and inventory with an intent to improve the modeling of ozone reaction behavior;

ii. research to improve evaluation and quantification techniques that dispersion models use in predicting environmental exposure and stresses caused by air pollution;

iii. research to improve the modeling of accidentally released liquefied gaseous fuels and their atmospheric behavior;

iv. continued acid deposition research by creating an Acid Precipitation Task Force to coordinate air quality modeling with other federal agencies, and maintain and upgrade air quality models that predict atmospheric and ecosystem interactions with acid rain.

2.2.4. New Source Standards

The new source standards range from being performance based standards that are applied to new, modified, or reconstructed sources to a preconstruction review and permitting process that are applied to new or modified major sources. A modified source is one that undergoes a "physical or operational change," a change resulting in an "increase in emissions" of any regulated pollutant, and a modification that is not listed as a specific maintenance activity. A reconstructed source is one that extends the useful life of the facility and is triggered when the reconstruction project expenditures are 50 percent or more the capital cost of a new facility. The type of review and permit process depends on whether the new or modified major source is in an attainment or nonattainment area. A

Prevention of Significant Deterioration (PSD) review is required for attainment areas, while in nonattainment areas, a New Source Review (NSR) and permit is required before construction of the facility. Atmospheric dispersion modeling is required for both review and permitting processes in performing the air quality analysis and demonstrating reasonable further progress. Table 2.8 helps to illustrate the requirements placed on new or modified stationary sources in areas of attainment and nonattainment.

In addition, a new source in either a nonattainment or attainment area must demonstrate that they do not have an adverse impact on air quality related values (including visibility). Federal Land Managers (FLMs) have the ability to disapprove a new source permit if the FLM finds that the source has an adverse impact on the air quality in any Class I area. In addition, the FLM can request that a new source obtain emission offsets in areas where the proposed new source is not normally required to purchase emissions offsets (Arbuckle, 1993).

2.2.4.1. New Source Performance Standards (NSPS). The new source performance standards were first implemented in the 1970 CAAA because Congress concluded that it was less costly to require the implementation of high level technologies at new sources than at existing sources. The NSPS identify source categories and establish emissions standards for them. Examples of these NSPS can be found in 40 CFR 60. These standards are promulgated as design, equipment, work practice, or operational standards.

2.2.4.2. Prevention of Significant Deterioration (PSD) Review Process. A new or modified major source in an attainment area is one that has the potential to emit over 250 tons per year (tpy) of any regulated pollutant or 100 tpy of any regulated pollutant if the source falls within one of 28 sources listed in 40 CFR 52.21 part b.1. A major source in an attainment area must undergo a Prevention of Significant Deterioration (PSD) review. This review process includes an air quality analysis to demonstrate compliance with the NAAQS and the PSD increments listed in Table 2.6.

Table 2.6. Federal Allowable PSD Increments ($\mu g/m^3$).

Pollutant	Class I	Class II	Class III
Sulfur Dioxide			
Annual Average	2	20	40
24-hour Maximum	5	91	182
3-hour Maximum	25	512	700
Nitrogen Oxides			
Particulates (PM-10)			
Annual Geometric	5	19	37
Mean	10	37	75
24-hour Maximum			

(Source: 40 CFR 51, 1993.)

This analysis often requires the use of dispersion models for the criteria and hazardous air pollutants. Individual criteria pollutants must be modeled if the major source's net increase exceeds the limits outlined in Table 2.7. In addition the source must also confirm that it is employing the best available control technology (BACT) for each pollutant emitted in significant amounts and that the BACT is at least as stringent as the NSPS for that source category (Arbuckle, 1993).

Table 2.7. Criteria Pollutant Increase Limits.

Pollutants	Threshold in tpy
Sulfur dioxide	40
Nitrogen dioxide	40
Volatile organic compounds	40
Particulate matter (TSP)	25
Particulate matter (PM-10)	15
Carbon monoxide	100
Lead	0.6

Note: TSP is Total Suspended Particles.
(Source: Martin, Spring 1993.)

2.2.4.3. Nonattainment Review Process. A major new or modified source in a nonattainment area is one that has the potential to emit any of the pollutants in concentrations greater than those listed in Table 2.4. This type of source is subject to a nonattainment review process and permit prior to construction.

The proposed new or modified major sources must demonstrate the implementation of Lowest Achievable Emission Rate (LAER) technologies and it must obtain offsets from nearby facilities at a greater than one to one ratio depending on how severely the area is in nonattainment. This is to ensure compliance with all applicable air quality requirements, like reasonable further progress (Arbuckle, 1993).

Table 2.8. Options and Requirements for Major Stationary Sources.

Source Type	Area Classification	Emissions Trading Options	Applicable Emissions Technology Limit	Can Technology Limit be avoided by Trading?	New Source Review
New	Attainment	Optional Offset	BACT	No	PSD Review
	Non-Attainment	Mandatory Offset	LAER	No	Non-Attainment Review
Modified	Attainment	Optional Netting	BACT	Yes	PSD Review
	Non-Attainment	Optional Netting	LAER	Yes	Non-Attainment Review
	or	Mandatory Offsets	LAER	No	Non-Attainment Review
Existing	Attainment	Optional Bubbles	State Limits	Yes	Not Applicable
	or	Optional Offsets	State Limits	Not Applicable	Not Applicable
	Non-Attainment	Optional Bubbles	RACT	Yes	Not Applicable
	or	Optional Banking	RACT	Not Applicable	Not Applicable

(Source: Plater et al., 1992 and Arbuckle, 1993.)

2.2.5. Title V Operating Permit Program

On July 21, 1992, the EPA promulgated the minimum elements of the operating permit program that states must implement on all major stationary sources, as defined in Titles I, III, and IV of the 1990 Clean Air Act Amendments, along with sources subject to all the new source

requirements discussed above and in 40 CFR 70. Prior to this Amendment, the only federally mandated permit program was the NSR and PSD permit programs on new or modified sources. The goal of this new permit program is to consolidate all the federal and state regulations for a source in a single document.

The Title V permit program is modeled after the National Pollution Discharge Elimination System (NPDES) permits and is expected to increase source compliance with all federal and state regulations by providing greater enforcement capabilities. These enforcement capabilities require sources to self report violations and annually certify compliance with all applicable air pollution regulations and permit limitations. Other enforcement capabilities that the Title V Amendments established are: the establishment of an administrative order system, enhancement of criminal provisions, allowing citizen suits to be brought against sources that are suspected of operating in noncompliance, and the development of a permit fee system. In addition to the permit requirements Title V requires that major stationary sources install enhanced monitoring devices to demonstrate compliance along with satisfying the Title V reporting requirements (Harsch and Mihelic, 1994).

The Title V operating permit program does not contain any provisions pertaining to the use of atmospheric dispersion models. However, it does allow states to require modeling in their state implemented permit programs. Some states are requiring dispersion modeling while others are not or are requiring them on a case-by-case scenario. Maryland and New York have long required modeling in their own permit programs. EPA's 1992 Final Rule on the operating permit program requires that operating permits contain all the information needed to assess ambient air quality impact by a source. In many cases this impact will have to be assessed through modeling.

The issues faced by states in implementing modeling requirements in their operating permit programs vary widely. Some common state concerns are:

i. Should the modeling requirements be implemented initially or later?

ii. Should the modeling guidelines be consistent with the federal guidelines or should the state develop their own protocols?

iii. What types of sources or pollutants should be modeled and if so what levels of modeling should be mandated for these sources?

iv. What should be done if the model demonstrates that the source contributes to a NAAQS violation?

(Source: Martin, Autumn 1993.)

This illustrates some of the many struggles that states are going through in meeting the specific needs and concerns of that state. Another primary concerns in developing modeling requirements are those associated with risk assessment of hazardous air pollutants and the protection of air quality.

2.2.5.1. Permitting Process. Title V gives states the authority to administer the permit program if they develop and submit an operating permit program to the EPA for approval by November 15, 1993. After that time, EPA has one year to approve, disapprove, or partially approve the program. If the state's plan is disapproved or partially disapproved of then the state has 180 days or up to 2 years to make the necessary revisions for approval. If the state fails to develop an approved permit program then, the EPA must adopt, administer, and enforce a federal permit program by November 15, 1997 (Harsch and Mihelic, 1994).

Once a state permit plan is approved, then all applicable sources have an additional year to submit completed permit applications to the state. When a state obtains a permit application, the state permitting authority has sixty days to determine if it is complete. If the permit application is complete, the permitting authority has up to 18 months from the date of receiving the application to approve or disapprove of the permit. However, for the initial implementation of the Title V permit program the state permit authorities must act on one third of the permit applications received in the first year and in each of the three years following, due to the staggering 34,000 estimated sources affected (Martin, 1993).

In addition, the state permit authority must provide to the EPA copies of each permit application, draft permit, and issued final permit. The EPA then has 45 days from receiving the copies of the issued permit to approve or disapprove of the permit. The EPA can disapprove of an

issued permit if it deems that their is a violation of any CAA requirements. If the EPA disapproves of the permit, then the state permit authority must revise the permit within 90 days or the permit will be denied by the EPA. If the EPA approves the permit, then any person may object to the decision within 60 days of the EPA's decision. If an objection is issued, then the EPA is required to review its decision, or a judicial review may occur in the Federal Court of Appeals on behalf of the citizen. Note that when a deadline is not met by the state permit authority or the EPA, the permit is assumed to be approved of for that stage of the decision process. For further information, 40 CFR 70.4 contains all the information on the permitting process.

2.2.5.2. Permit Content. Each state must provide for a standard application form and each permit must be issued for a fixed period of time that does not exceed five years. The contents and requirements for each state varies depending on the regulations the state adopts. Each permit application must contain the following elements:

i. General facility information.

ii. Description of process and products by Standard Industrial Classification (SIC) code (including alternative operating scenarios).

iii. List of regulated air pollutants and all pollutants for which a facility is classified as a major source, and rates in tpy for determining test methods.

iv. Description and location of all emission points.

v. Description of fuels, raw materials, production rates and operating schedules.

vi. Description of any limitations on source operations affecting emissions or work practice standards for all regulated sources.

vii. Information on stack height limitations.

viii. Supporting calculations for all emissions data.

ix. Citation and description of all requirements applicable to the facility.

x. A source compliance plan including current status and statement of continued compliance for complying facilities and schedule of compliance for sources not currently in compliance.

(Source: 40 CFR 70.5(c) and Hosford, 1993.)

Since the objective of the operating permit system is to ensure compliance with all applicable requirements listed in the CAA, an issued permit must contain the following information:

i. Applicable emission limitations and standards

ii. Monitoring and related record keeping and recording requirements.

iii. A permit condition prohibiting the emissions of sulfur dioxide in excess of the utilities allowances under Title IV.

iv. A severability clause to ensure continued validity of remaining permit requirements if any provisions are challenged.

v. A statement that the permit maybe modified, revoked, reopened, and reissued or terminated for cause.

vi. A provision to ensure that a source pays fees consistent with an approved state permitting fee schedule.

vii. Compliance certification, testing, monitoring, reporting, and record keeping requirements to assure compliance with the permit.

viii. Inspection and entry requirements for permitting authorities.

ix. A schedule of compliance and regular progress reports consistent with that schedule.

x. The permit must specify that it is not federally enforceable under any terms or conditions included in the permit that are not required under the act or any of its applicable requirements.

(Source: 40 CFR 70.4 (a)(c) and Arbuckle, 1993.)

2.2.5.3. Permit Shields. Section 504(f) of the 1990 CAAA granted state permitting authorities the ability to include a permit shield within an issued permit. This provision is intended to protect sources from enforcement actions for a violation of the Act when the source is in operational compliance with its permit, and all applicable standards set forth within the permit. 40 CFR 70.6(f) allows permitting authority to include a permit shield within an issued permit if it expressly states in the permit that compliance with the conditions of the permit shall be deemed in compliance with any applicable requirements "as of the date of issuance" if:

i. the permit specifically identifies the applicable requirements that do not apply to the source, or;

ii. the permit includes a written statement by the permitting authority that other specifically identified requirements do not apply to the source.

If the permit does not include a definitive statement that a permit shield applies, then there is no shield for that source.

2.2.5.4. Permit Revisions. Permit revisions constitute administrative permit amendments and permit modifications. An administrative permit amendment is one that allows for clerical changes to facility information, corrections in typographical errors, more frequent monitoring or record keeping, incorporation of requirements from preconstruction permits, or ownership changes. An administrative permit amendment may be implemented as soon as they are filled for application. The permit authority then has 60 days to act on the amendment and no public notice is required (40 CFR 70.7 (d)).

A permit modification includes both minor permit modifications and significant modifications. A minor permit modification is one that does not violate any applicable requirements, involve significant changes to existing monitoring, reporting or record keeping requirements in the permit, require or change a case-by-case determination of an emission limitation or other standard, or seek to establish or change a permit term or condition for which there is no corresponding underlying

application requirement. A minor modification does not require public notice and may be implemented immediately at the source's risk. Once the permitting authority has been informed of a minor modification it is required to notify the EPA within 5 days of receiving the application. The EPA then has 45 days to review the application for approval and the permitting authority has up to 90 days to issue or deny the application (40 CFR 70.7 (e)).

A significant modification is one that does not qualify as an administrative amendment or a minor modification. It requires both the state permit authority and EPA to review the application along with allowing all procedural requirements applicable to permit issuance and renewal (40 CFR 70.7 (e)).

2.2.5.5. Operational Flexibility. In order for affected sources to maintain operational flexibility and not have to produce permit revisions, Title V requires applicants to describe all operating scenarios at the facility. The allowable changes that a source can make if a seven day written notice is given to the permit authority and the EPA are:

i. Operational changes within the facility that do not exceed any emissions allowed under the permit.

ii. Emissions trades within the permitted facility if it meets SIP limits if it is allowed by SIPs. (Optional)

iii. Emissions trading for the purpose of complying with source specific emission caps that is at a value lower than a fully permitted emission limit.

(Source: 40 CFR 70.4 (b).)

2.2.5.6. Permit Fees. Title V requires states to develop an annual permit fee system to ensure that all direct or indirect reasonable costs listed in section 502 (b)(3)(A) of the 1990 CAAA are met. The EPA will assume that the fee structure is adequate if they are not less than $25 per year times the total tons of regulated pollutant emissions up to a maximum of 4000 tpy. A

regulated pollutant, as defined for the purpose of calculating the emissions fee, does not include carbon monoxide, Class I and II pollutants as defined by Title VI, and air pollutants that are regulated under the accidental release program.

2.2.6. Enforcement Actions

Broad enforcement authority has been given to the EPA and the courts in the administration of the CAA requirements under Title VII of the 1990 Amendments. Title VII grants the administrator of the CAA the ability to assess civil and criminal relief for violations of the CAA. It also required the EPA to hire more criminal investigators to enforce these new laws and it allows the EPA to administer "administrative subpoenas" against regulated sources to enhance information gathering and compliance of the CAA.

2.2.6.1. Civil Authority. Civil authority granted to the administrator is similar to the administrative enforcement authority that is granted by the Clean Water Act. It allows the administrator to bring administrative enforcement actions against a violator without filing a court case. The administrator can fine a violator up to $200,000 and require correction of the violation to ensure compliance. In addition, an agency inspector can issue a field citation to a facility of up to $5,000 per day per violation. In both cases, the violator can request an administrative hearing to present their side of the case or just pay the fine.

The Title V enforcement provisions allow permitting authorities to seek civil penalties of not less than $10,000 per day per violation as well as incarceration to violators who knowingly violate permit limitations, miss implementation or fee deadlines, make false statements in any permit required report or notice, and violate HAPs standards.

The new Act allows the EPA to respond to both human health threats and environmental threats in emergency situations. Fines from $5,000 to $25,000 per day of violation and up to five years in jail for known violations of an emergency order can be assessed. The Amendments also

encourage greater citizen enforcement action by allowing citizens to sue a violator. This may force the violator to comply with the Act and pay a cash penalty to the EPA, which must be used for compliance and enforcement activities. The EPA has also been authorized to pay awards to any citizen who provides information that leads to a criminal conviction or civil penalty.

2.2.6.2. Criminal Sanctions. Criminal sanctions can be imposed on "any person" who knowingly violates the act. This includes individuals, management personnel, corporate officers, corporations, and partnerships if they are knowingly involved in the violations. Individuals making false statements and failing to file or maintain records and reports required under the act, can be subject to fines up to $250,000 and two years in jail, while corporations can be fined up to $500,000.

Any person who knowingly releases an air toxin which places another individual in "imminent danger of death or serious bodily injury" can be required to pay fines up to $250,000 per day and receive up to 15 years in prison, while corporations can be fined up to $1 million per day. A fine of up to $100,000 and up to one year in jail can be assessed to persons who negligently release air toxins, while a fine of up to $200,000 can be assessed to corporations.

3.0 MODELING

3.1. Introduction

Atmospheric dispersion modeling is an excellent tool for regulatory authorities to use in the evaluation of activities that affect air quality, such as:

i. Establishing emissions limits to assure protection and maintenance of the NAAQSs and PSD increments in affected areas.

ii. Choosing locations of new air pollution sources to ensure the minimization of environmental impacts.

iii. Conducting health risk assessments for source emissions of HAPs whether before or after application of MACT.

iv. Assuring protection of air quality values by re-modeling old sources or modeling sources not previously modeled by new source reviews.

v. Assuring protection of air quality values that might be threatened by emissions trading or significant modifications to a source.

vi. Evaluating interstate transport of pollutants form sources near a state border.

vii. Assuring protection from adverse health effects caused by severe air pollution episodes in regions through the development of intervention strategies like warning systems and real-time short-term emissions reduction strategies.

viii. Evaluating a source's contribution to existing air pollution levels.

ix. Evaluating the impact that emission control techniques and strategies have on air quality values.

(Source: Martin, 1993 and Zannetti, 1990.)

This list illustrates some of the possible applications for atmospheric dispersion modeling and why it is (or will become in the future) a part of many state implementation plans. The last listed item is currently one of the most important uses of air pollution models for regulatory use. This is due to air pollution models being the only to link between emission limits and the regulatory standards which

are set for observed atmospheric concentrations. The Title V permitting process increases the pressure placed on states in establishing emissions limits on sources that will be acceptable to the EPA. This increases the need for modeling to be conducted either by state officials or the sources to demonstrate compliance with all applicable air quality criteria. The intent of this section is to describe the modeler's choices in atmospheric dispersion modeling methods.

3.2. Mathematical Theory

Approaches to modeling air pollution can be broken into two large classes: physical and mathematical. Physical modeling involves the use of wind tunnels or water tanks to simulate atmospheric dispersion for complex flow situations. Physical modeling has been used in the development and validation of mathematical models. However physical modeling methods will not be discussed futher in this paper since mathematical models make up the bulk of the atmospheric dispersion models in use for regulatory purposes.

Mathematical modeling can be further broken down to deterministic or statistical models. Deterministic models start their calculations at the source to establish a cause-and-effect relationship, while statistical models start their calculations with measured air quality data at receptor sites to establish a relationship to the pollutant source. Deterministic and statistical models are two different complementary methods for providing an assessment of the responsibility of each pollution source to each receptor area. When measured concentration trends are better than those obtained from deterministic models then statistical models may be more appropriate than deterministic models. However deterministic models are used more extensively used for regulatory purposes than statistical models due to the lack of actual measurements and the inability of statistical models to provide a prediction of the impact of a proposed pollutant source.

This paper will focus on deterministic models due to their extensive use for regulatory purposes. Deterministic models can be broken down into three classes of models: Eulerian, Lagrangian, and Gaussian. These modeling methods will be discussed further in this section to

provide a basic understand of their theories, while a brief discussion of statistical models will be provided.

3.2.1. Statistical Models

3.2.1.1. Receptor Models. Receptor models attempt to apportion measured concentrations of aerosols to each source or group of sources by relating observations at the receptor site to known source characteristics. Receptor models use finger prints of a source or group of sources which are based on the known unique chemical composition of the source or group of sources. The finger print is used to attribute measured concentrations at the receptors to the source or group of sources. The mathematical formula for finding source contribution is

$$C_{ik} = \sum f_{ij} a_{ij} D_{jk} E_{jk} \qquad 3\text{-}1$$

where the coefficients are:

C_{ik}	Concentration of species i at the k-th receptor sample.
f_{ij}	Fraction that represents modifications to a_{ij} due to process like settling between the source and the receptor. (when neglecting assumed to be = to 1)
a_{ij}	Fraction of species i in emissions from source j.
D_{jk}	Atmospheric dispersion term between the j-th source and the k-th sample.
E_{jk}	Emissions rate from the j-th source that can be attributed to the receptor sample.
S_{jk}	Total mass concentration of material from source j to the receptor k. ($S_{jk} = D_{jk}E_{jk}$)

The C_{ik}, f_{ij}, and a_{ij} coefficients are assumed to be known from measurements and are used to solve for S_{jk}. Three more advanced receptor model versions are described in Zannetti (1990) and a more detailed description of these models can be found in Henry et al., (1984). Zannetti (1990) indicates

that receptor modeling techniques are becoming a major analysis tool and are extremely powerful even though they are empirically developed and highly theoretical.

3.2.2. Deterministic Models

Deterministic models are used for describing atmospheric dispersion processes. The most common application of deterministic models is for the dispersion of continuous point sources. Figure 3.1 illustrates the plume rise and dispersion behavior of an elevated plume after injection into the atmosphere. The physical stack height is represented by h, while the plume rise is represented by Δh. The effective stack height is represented by H and is the sum of h and Δh. As shown in the figure, the plume is bent over by the horizontal wind resulting in the centerline height being achieved some distance downwind of the stack. The plume then randomly spreads out in the atmosphere as it travels downwind along the x-axis due to the entrainment of the surrounding air by turbulence and diffusion.

When choosing a deterministic model, an analysis of the problem must be conducted along with the appropriate selection and use of the model. The analysis of the problem includes defining the type of pollutant to be modeled, choosing the appropriate averaging time, defining the type of terrain in which the model is to be used, and knowing the computional limitations of the modeler's equipment. Once these requirements have been defined, a list of the suitable models should be developed and one should be chosen based on a cost-effective analysis. The model chosen then should be calibrated and evaluated with local air quality monitoring data to ensure its applicability and minimize errors (Zannetti, 1990).

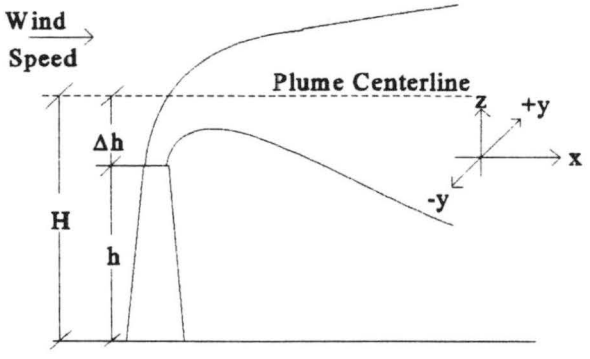


Figure 3.1: Plume Behavior.

This section of the paper will examine

deterministic modeling theories. It will begin by looking at the mathematical theories that describe how the plume enters the atmosphere and is dispersed. Next, Eulerian and Lagrangian numerical methods for modeling atmospheric dispersion process and the Gaussian dispersion models which are the most frequently used models for regulatory purposes will be reviewed.

3.2.2.1. Plume Rise Models. Plume rise resulting from hot and/or lighter-than-air gases being emitted vertically into a cooler-temperature atmosphere, is determined by both the momentum and buoyancy of the stack gases. The momentum term is related to the stack gases vertical velocity and its mass, while the buoyancy term is due to stack gases having a density less than the surrounding atmosphere. Turner (1994) suggests that the buoyancy term may have a greater effect than the momentum term. He suggests that as a rule-of-thumb that if the exit termperature is 10 to 15 °C higher than the ambient temperature, that the buoyance rise will be the dominant plume rise force. Further, the momentum rise effects dissipate within 30 to 40 seconds, while the buoyancy rise effects will presist for approximately three to four minutes when a sufficient amount of ambient air has been entrained into the plume which acts to lower the plume temperature to the surrounding air temperature. This section of the paper will present the commonly-used formulas for estimating plume rise.

One of the earliest plume rise equations, which is only good for neutral conditions, is the Holland formula which is

$$\Delta h = (v_s d_s/u)[1.5 + 2.68(10)^{-3} P_a((T_s - T_a)/T_s) d_s] \qquad 3\text{-}2$$

where

v_s Stack gas velocity, m/s.

d_s Stack inner diameter, m.

u Wind speed, m/s.

P_a Atmospheric Pressure, mb.

T_s Stack gas temperature, K.

T_a Atmospheric temperature, K.

(Source: Cooper and Alley, 1994.)

For conditions other than neutral conditions, a correction factor of 1.2, 1.1, 0.9, and 0.8 can be multiplied to the equation for classes A, B, E, and F respectively. These classes will be discussed further in a later section of this paper.

The most commonly used plume rise model is the Briggs model which is dependent upon the atmospheric stability. This method is currently the EPA's recommended method since it appears to perform better at estimating thermally induced plumes and it recognizes that plumes still continue to rise after they are bent over. This method of estimating the plume rise depends on the comparison of the estimated buoyant and momentum plume rises. The estimate producing the highest value is assumed to be the dominant mechanism and this value is used in the dispersion calculations that follow.

Neutral and Unstable Conditions. Turner (1994) suggests that for neutral and unstable conditions the final plume rise is estimated by the following method. The buoyancy flux parameter (F_b, m^4/sec^{-3}) is defined as

$$F_b = gvd^2(T_s - T_a)/(4T_s) \qquad 3\text{-}3$$

where

g is the gravitational constant, 9.8 m/sec^2.

v stack gas exit velocity, m/sec.

d top inside stack diameter, m.

T_s Stack gas temperature, K.

T_a ambient air temperature, K.

Then the empirically derived plume rise (Δh, m) depend on whether the conditions are neutral or unstable. If the conditions are neutral then F_b will be greater than 55 and the final plume rise is calculated from equation 3-4.

$$\Delta h = 38.71 F_b^{3/5}/u_h \qquad 3\text{-}4$$

where u_h is the wind speed at the stack top. If the conditions are unstable then F_b will be less than 55 and the final plume rise will be calculated by equation 3-5.

$$\Delta h = 21.425 F_b^{3/4}/u_h \qquad 3\text{-}5$$

The momentum rise for neutral and unstable conditions is calculated by the following equation.

$$\Delta h = 3dv/u_h \qquad 3\text{-}6$$

Stable Conditions. For stable conditions the buoyant final plume rise is calculated by using equation 3-3 and an intermediate variable called the stability parameter, S. The stability parameter is calculated using equation 3-7.

$$S = (g/T_a)(D\Theta/Dz) \quad \text{units of } sec^2 \qquad 3\text{-}7$$

where $D\Theta/Dz$ is the potential temperature gradient in units of K/m. The potential temperature gradient is used to relate the stability to the atmospheric temperature profile. It is calculated by equation 3-8.

$$D\Theta/Dz = dT/dz + \Gamma \qquad 3\text{-}8$$

where Γ is the adiabatic lapse rate which is equal to 0.0098 K/m. Cooper and Alley (1994) suggest that if the potential temperature gradient is unavailable, it is recommended to use 0.02 K/m for class E and 0.035 K/m for class F. The final plume rise is then calculate by using equations 3-9 for stable conditions and 3-10 for calm conditions. The buoyant plume rise equation that gives the lowest value is the value that is saved to compare with the momentum rise.

$$\Delta h = 2.6[F_b/(u_h S)]^{1/3} \qquad 3\text{-}9$$

$$\Delta h = 4F_b^{1/4} S^{-3/8} \qquad 3\text{-}10$$

The stable momentum final plume rise is estimated by comparing the value obtained from equation 3-6 to value obtained from equation 3-11. The lowest value is chosen and compared to the outcome of the buoyant plume rise to detemine which method is the dominant mechanism.

$$\Delta h = 1.5[(v^2 d^2 T)/(4T_s u_h)]^{1/3} S^{-1/6} \qquad 3\text{-}11$$

Gradual Plume Rise. For buoyant plumes the period for the temperature dissipation of the plume may still occur after the plume has bent over. To account for this plume behavior Turner (1994) reports Briggs's 1972 finds that are shown in equation 3-12.

$$\Delta h = (1.60F_b^{1/3} x_f^{2/3})/u_h \qquad 3\text{-}12$$

where F_b is calculated from equation 3-3 and the downwind distance to final plume rise, x_f, is calculated by equation 3-13

$$x_f = 3.5x^* \qquad 3\text{-}13$$

Where the critical downwind distance (x^*) is calculated in the following manner

$$x^* = 34(F_b)^{2/5} \qquad \text{for } F_b \geq 55 \text{ m}^4/\text{sec}^3 \qquad 3\text{-}14$$

$$x^* = 14(F_b)^{5/8} \qquad \text{for } F_b < 55 \text{ m}^4/\text{sec}^3 \qquad 3\text{-}15$$

If this method calculates a final plume rise greater than that for the normal (unstable, neutral, or stable) plume rise then this method is applied for the downwind distance.

It should be pointed out that there are several methods of determining the plume rise. What has been shown in this section represents methods that have been used in regulatory models. Currently the Briggs model has been incorporated into most U.S. EPA models because of its relative accuracy and simplicity. Other methods of representing plume rise will not be discussed further due to the large amount of available and proposed models. For further information on advanced and special use plume rise models, refer to Turner's 1994 book, the 1975 Briggs article and Zannetti's 1990 book.

3.2.2.2. Diffusion Theories. As mentioned earlier, after a plume has been injected into the atmosphere it is randomly dispersed throughout the atmosphere. This is a result of thermally and/or mechanically induced atmospheric turbulence. This random dispersion behavior results in time averaged plume concentrations that are normally distributed perpendicular (±y,±z directions) to the direction of the wind (x-direction). Two ways to represent plume diffusion in the atmosphere are the K-theory and the statistical theory. K-theory is based on the atmospheric diffusion equation shown as equation 3-16.

$$\frac{\partial \langle c \rangle}{\partial t} + u\frac{\partial \langle c \rangle}{\partial x} = K_{xx}\frac{\partial^2 \langle c \rangle}{\partial x^2} + K_{yy}\frac{\partial^2 \langle c \rangle}{\partial y^2} + K_{zz}\frac{\partial^2 \langle c \rangle}{\partial z^2} + S(x,y,z,t) \qquad 3\text{-}16$$

Where

$\langle c \rangle$ Ensemble mean concentration.

u Time-averaged fluid velocity.

K_{xx} Eddy diffusivity in the direction of the wind.

K_{yy} Cross-wind eddy diffusivity which is dependent upon the pollutant travel time.

K_{zz} Vertical eddy diffusivity which is a function of altitude z.

S Source and sink term of pollutants.

In general, K-theory is used with Eulerian grid type models to represent the vertical and horizontal transport and diffusion of pollutants. In some applications of Lagrangian models, particularly photochemical and particle models, K-theory is used to simulate diffusion processes. When used in grid models, it is applicable when the change in the turbulent transport is smaller than the change in the mean concentration field. In most cases, the eddy diffusivity values are a function of how accurate the dispersion models are at estimating the unresolved velocity component which will be discussed further in the next section.

The statistical theory of diffusion is concerned with the actions of individual particles in stationary, homogeneous turbulence. They provide a statistical estimate of the particle behavior. Statistical theory for diffusion processes are typically used in Lagrangian models to simulate pollutant diffusion. Their basic limitations are in the determination of the Lagrangian time scale of turbulence. Gaussian plume models which really are a subset of Lagrangian models also use statistical theory to model diffusion processes based on a Gaussian concentration distribution and the atmospheric stability condition. Both types of models will be discussed further in the following sections.

3.2.2.3. Eulerian Models. Eulerian models are based on a material balance approach, using a fixed reference system with respect to the earth. Eulerian models use velocity measurements at fixed points to formulate pollutant concentration statistics. The basic Eulerian dispersion model equation for N species is

$$\frac{\partial C_i}{\partial t} + V_j \frac{\partial C_i}{\partial x_j} = D_i \frac{\partial^2 C_i}{\partial x_j^2} + R_i(C_1,\ldots C_N,T) + S_i(x,t) \qquad 3\text{-}17$$

where

C_i Concentration of species i.

V_j Fluid velocity in the jth component.

D_i Molecular diffusivity of species i (approx. 1.5×10^{-5} m^2/sec for air).

R_i Rate of chemical generation of species i

S_i Sources and sinks other than chemical sources.

t Time.

T Temperature is needed since the rate of chemical reaction is a function of temperature.

As mentioned earlier, K-theory is used to represent the unresolved components of the diffusion of pollutants in the atmosphere. These unresolved components of diffusion are a result of the fluctuating random fluid turbulence. In the case of fluid velocity, V_j, the unresolved component, is represented by u_j' in the following equation,

$$V_j = u_j + u_j' \qquad 3\text{-}18$$

where u_j is the average resolvable fluid velocity. In the case of the pollutant concentration, C_i, the unresolved component is represented by c_i' in the following equation,

$$C_i = \langle c_i \rangle + c_i' \qquad 3\text{-}19$$

where $\langle c_i \rangle$ is the theoretical ensemble mean concentration that is resolvable. When introducing equations 3-18 and 3-19 into equation 3-17 and neglecting molecular diffusion (small when compared to turbulent diffusion) and assuming an incompressible atmosphere with no chemical reactions, the following equation results:

$$\frac{\partial \langle c_i \rangle}{\partial t} + u_j \frac{\partial \langle c_i \rangle}{\partial x_j} + \frac{\partial \langle u_j' c_i' \rangle}{\partial x_j} = S_i(x,t) \qquad 3\text{-}20$$

where $\langle u_j' c_i' \rangle$ represents the unresolved portion that can be modeled using K-theory, appling the

following relationship

$$\langle u_j' c_i' \rangle = -K_{jk} \frac{\partial \langle c_i \rangle}{\partial x_j} \qquad 3\text{-}21$$

where K_{jk} is a tensor that is a function of location and time where only the main three diagonal elements K_{11}, K_{22}, and K_{33}, are nonzero. It is important to note that the unresolved components, $\langle u_j' c_i' \rangle$, cannot be eliminated but can be minimized by reducing the grid size. When considering one species and plugging equation 3-21 into the equation 3-20, the result is the Eulerian atmospheric diffusion equation,

$$\frac{\partial \langle c \rangle}{\partial t} + u_j \frac{\langle c \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} K_{jj} \frac{\partial \langle c \rangle}{\partial x_j} + S(x,t) \qquad 3\text{-}22$$

where the second term on the left hand side represents advection. The first term on the right hand side represents the diffusion term using K-theory, and the last term on the right hand side represents the sources and sinks of the pollutant. This equation is usually solved using a finite difference approach, due to the difficulty in integration. Eulerian models are difficult and expensive to run since they are dependent upon the initial conditions (for finite difference) and the numerous data required to run them.

3.2.2.4. Lagrangian Models. In a Lagrangian model, the reference system moves by following the average atmospheric motion. The basic Lagrangian equation for atmospheric dispersion of a single pollutant is

$$C(r,t) = \int_{-\infty}^{t} \int p(r,t|r',t')S(r',t')dr'dt' \qquad 3\text{-}23$$

where

r'	Source location or previous receptor location.
r	Receptor site of interest.
t'	Initial time of pollutant release or time previous to time of interest.
t	Time of interest.
C(r,t)	Average concentration at r at time t.
p(r,t|r',t')	Probability density function that the air moves from r' at t' to r at t.
S(r',t')	Source term (units as mass/volume/time).

(Source: Zannetti, 1990.)

The first integral in Equation 3-23 is in space and is to be performed over the atmospheric domain of interest. The most important term in equation 3-23 is the probability density function p, which is only a function of meteorology and the type of pollutant. It is used to describe the atmospheric transport and diffusion processes in probabilistic terms.

Lagrangian models are useful in representing photochemical processes, particle models, segmented Gaussian plume models, and Gaussian puff models. Equation 3-23 can be modified to represent a Gaussian plume and puff algorithm by portraying the probability density function, p, as a Gaussian distribution, and making several other simplifying assumptions of the probability density function, as shown in Zannetti, 1990.

Lagrangian box models are used to simulate photochemical reactions using a moving air mass with a defined volume ("box"). This box is then advected horizontally according to the local time-varying average wind speed and direction. Two major problems with this type of model is that it ignores dilution effects from wind shear and it is difficult to compare its output with fixed air quality monitoring data.

Lagrangian particle models can properly simulate physical particle dynamics on a range from an atomic scale to an astronomical scale. Particle models that simulate atmospheric motion use a set of formulas to generate realistic trajectories of imaginary particles. These particles represent masses

of pollutants that are either held constant or are time-varying due to chemical reactions or deposition. Each particle is moved at every time step by pseudo-velocities which account for fluid velocity transport, turbulent fluctuations in both horizontal and vertical directions, and molecular diffusion. The use of pseudo-velocities reduces the amount of assumptions made about the atmospheric motion by using fixed measurements of air quality monitoring data on the variance of wind velocity fluctuation and inferring a numerical perturbation to account for turbulence. For further information on Lagrangian particle modeling see Zannetti (1990).

3.2.2.5. Gaussian Plume Models. Gaussian plume models are the most widely used atmospheric dispersion models due to their ease of understanding and simple mathematics that are easily convertible to computer programs. They were orginally developed for point sources but most Gaussian plume models have been modified to represent multiple sources, and area sources while some Guassian plume models have been modified to model line sources. Gaussian plume models represent the bulk of the U.S. EPA recommended models for regulatory use.

The steady state Gaussian equation is

$$C = [Q/(2\pi u\sigma_y\sigma_z)]\exp[-(y^2/2\sigma_y^2)]\{\exp[-(H-z)^2/2\sigma_z^2)] \qquad 3\text{-}24$$

where

C	Downwind concentration at any point (x,y,z) in $\mu g/m^3$.
Q	Source emission rate in $\mu g/sec$.
u	Average wind speed at the stack height in m/sec.
y	Horizontal distance from the plume centerline in m.
z	Vertical distance from the plume centerline in m.
x	Downwind distance in m.

σ_y, σ_z Horizontal and vertical standard deviations of the plume concentration distribution in m.

Equation 3-24 represent a true double Guassian equation where the modeled plume would not be reflected back into the atmosphere after intercepting a boundary condition such as the surface of inversion layer. Figure 3.2 helps to illustrate physically each of these variables. It is fundamentally derived using a Lagrangian approach. However, it can also be derived using an Eulerian approach. The fundemental assumptions of Gaussian plume models are:

i. The source emission are taking place continueously and do not vary over time.

ii. The mass of the pollutants emitted from the source stays in the atmosphere and is not removed via chemical reaction or deposition processes which statifies the continuity equation.

iii. The meterogical conditions remaining unchanged over the time period of transport to satify the steady state assumption.

iv. The vertical and horizontal distributions of pollutants represents a Gaussian of normal distribution over the averageing time of interest.

v. The mean wind direction defines the x-axis and the wind speed at the release hieght defines the diluting wind.

(Source: Turner, 1994.)

The first exponential term in equation 3-24 represents the distribution in the ±y directions (horizontal directions) while the last exponential terms represents the distribution in the ±z directions (vertical directions).

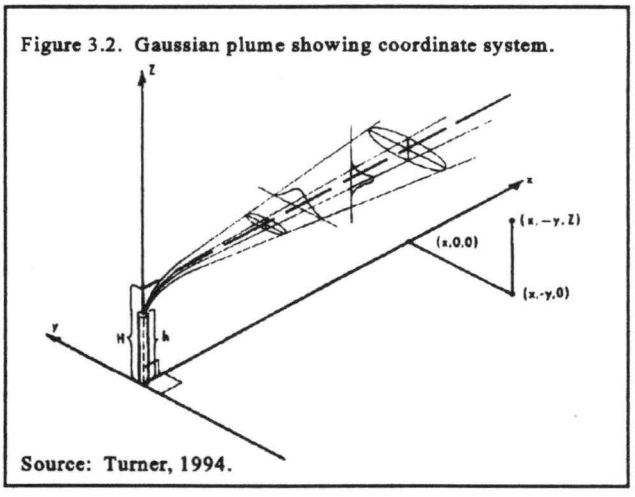


Figure 3.2. Gaussian plume showing coordinate system.
Source: Turner, 1994.

Dispersion Parameters. The σ_y and σ_z values can be found by either making use of the

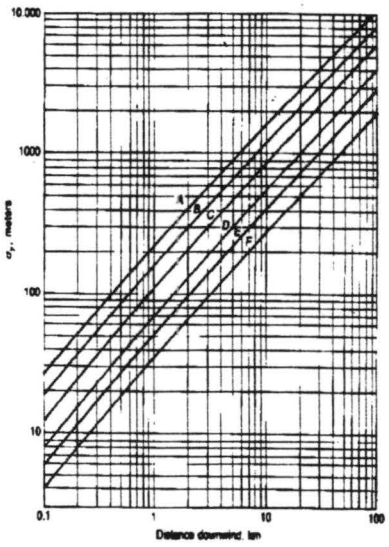
turbulence intensity measurements or stability classifications. The turbulent intensity measurements are used to to determine standard deviations of the wind vector azimuth (σ_θ) and elevation angles (σ_ϕ) which are used to determine the σ_y and σ_z by the following equations.

$$\sigma_y = s_q x S_y(t/T_i) \qquad 3\text{-}25$$

$$\sigma_z = s_f x S_z(t/T_i) \qquad 3\text{-}26$$

where x is the downwind distance, t is the travel time, and T_i is a normalization factor which is proportional to the lagrangian time scale (T_L) and is equal to $1.64T_L$. S_y and S_z are nondimensional functions of the diffusion or travel time. Currently research involves determining more accurate methods for determining S_y and S_z by using more descriptive boundary layer characteristics. This type of horizontal and vertical standard deviation determination will not be covered further in this paper since most regulatory models make use of the semiempirical standard deviation calculations that are described in the rest of this section.

Figure 3-3: Horizontal dispersion parameter.



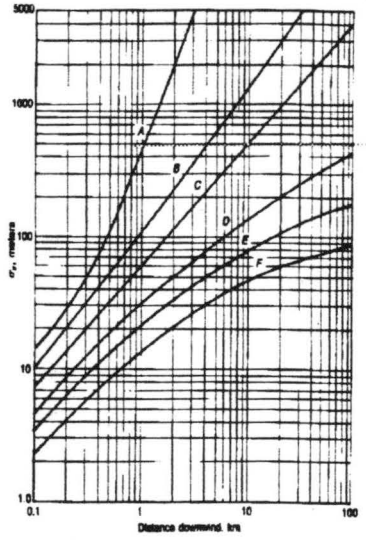
Source: Cooper and Alley, 1994.

The stability classification method is the most common method used for defining the dispersion spread capabilities of the atmosphere. There are six stability classes that are used when using this method, as illustrated below.

A	Very unstable
B	Moderately unstable
C	Slightly unstable
D	Neutral
E	Slightly stable
F	Stable

These six stability classes are used in several ways to find the dispersion parameters. In all cases Table 3.1 is used to determine the stability classification which is dependent upon the sun angle, the amount of cloud cover, and the surface wind speed.

Figure 3-4: Vertical dispersion parameters.



Source: Cooper and Alley, 1994.

Table 3.1. Stability Classifications.

10 m Height	Day Incoming Solar Radiation			Night Cloudiness[d]	
Surface wind speed (m/sec)	Strong[a]	Moderate[b]	Slight[c]	Cloudy (≥4/8)	Clear (≤3/8)
<2	A	A-B	B	E	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Notes:

a. Corresponds to clear summer day with sun higher than 60° above the horizon.

b. Corresponds to a summer day with few broken clouds, or a clear day with sun 35° to 60° above the horizon.

c. Corresponds to a fall afternoon, or a cloudy summer day, or clear summer day with the sun 15° to 35° above the horizon.

d. Cloudiness as defined by the fraction of clouds covering the sky.

For day or night overcast conditions Class D should be assumed regardless of wind

speed.
(Source: Cooper and Alley, 1994.)

Figures 3-3 and 3-4 represent the Pasquill-Gifford method for estimating the horizontal and vertical dispersion parameters for rural conditions as a function of downwind distance. The Pasquill-Gifford method is the most widely used method for estimating the dispersion parameters for rural conditions. When using these figures the stability class is found first, which establishes the dispersion parameter at any downwind distance of interest. The concentration found using equation 3-24 represents the 10 minute average concentration. To find average concentrations other than the 10 minute average concentration, the following equation should be used

$$C_t = C_{10}(10/t)^{1/2} \qquad 3\text{-}27$$

where

t	Average time of interest in minutes. (good for times between 10 min to 5 hours)
C_{10}	10 minute average concentration.
C_t	Average concentration for the average time of interest.

Other methods attempt to analytically represent Figures 3.3 and 3.4 by fitting the curves to equations, with different coefficients for each stability class. An example of one of these methods is shown in the following equations and Table 3.2.

$$\sigma_y = ax^b \qquad 3\text{-}28$$

where b = 0.894 for all stability classes and values of x.

$$\sigma_z = cx^d + f \qquad 3\text{-}29$$

Table 3.2. Curve fit coefficients.

		x < 1 km			x > 1 km		
Stability	**a**	**c**	**d**	**f**	**c**	**d**	**f**
A	213	440.8	1.941	9.27	459.7	2.094	-9.6
B	156	106.6	1.149	3.3	108.2	1.098	2
C	104	61	0.911	0	61	0.911	0
D	68	33.2	0.725	-1.7	44.5	0.516	-13
E	50.5	22.8	0.678	-1.3	55.4	0.305	-34
F	34	14.35	0.74	-0.35	62.6	0.18	-48.6

(Source: Cooper and Alley, 1994.)

Another more recent method used for determining the dispersion parameters depends on whether the area being modeled is either urban or rural. The dispersion parameters derived from this method are called Briggs sigmas and are illustrated in Tables 3.3 and 3.4 and in Figure 3-5. The urban Briggs sigmas are currently the U.S. EPA recommended sigmas and are also called McElroy-Pooler sigmas.

Table 3.3. Urban Dispersion Parameters.

Stability Class	σ_y (m)	σ_z (m)
A-B	$0.32x(1 + 0.0004x)^{-1/2}$	$0.24x(1 + 0.001x)^{1/2}$
C	$0.22x(1 + 0.0004x)^{-1/2}$	$0.20x$
D	$0.16x(1 + 0.0004x)^{-1/2}$	$0.14x(1 + 0.0003x)^{-1/2}$
E-F	$0.11x(1 + 0.0004x)^{-1/2}$	$0.08x(1 + 0.00015x)^{-1/2}$

(Source: Zannetti, 1990.)

Table 3.4. Rural Dispersion Parameters.

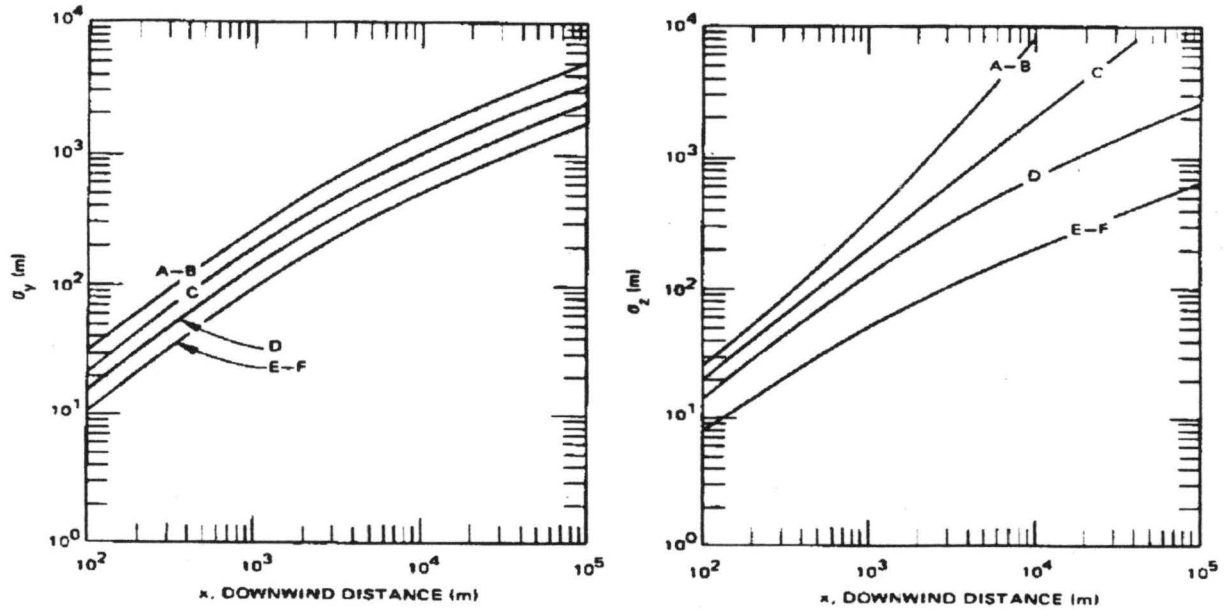
Stability Class	σ_y (m)	σ_z (m)
A	$0.22x(1 + 0.0001x)^{-1/2}$	$0.20x$
B	$0.16x(1 + 0.0001x)^{-1/2}$	$0.12x$

C	$0.11x(1 + 0.0001x)^{-1/2}$	$0.08x(1 + 0.0002x)^{-1/2}$
D	$0.08x(1 + 0.0001x)^{-1/2}$	$0.06x(1 + 0.0015x)^{-1/2}$
E	$0.06x(1 + 0.0001x)^{-1/2}$	$0.03x(1 + 0.0003x)^{-1}$
F	$0.04x(1 + 0.0001x)^{-1/2}$	$0.016x(1 + 0.0003x)^{-1}$

(Source: Zannetti, 1990.)

These methods represent only a few of the methods that are employed in today's dispersion models. The majority of the current U.S. EPA approved regulatory models rely on the stability classification method due to its simplicity.

Figure 3-5: Briggs urban dispersion parameter.



Source: Turner, 1994.

Wind Speed. In most cases the wind speed is only known at the standard 10 meter anemometer height. In cases when the wind speed is required at heights other than the anemometer height, for example stack height, the power law equation 3-30 can be used to estimate the wind speed at different heights

$$(u_2/u_1) = (z_2/z_1)^p \qquad 3\text{-}30$$

where

z_1, z_2 Elevations 1 and 2.

u_1, u_2 Wind speed at z_1 and z_2.

p Exponent.

(Source: Cooper and Alley, 1994.)

The exponent p in the equation is dependent upon the atmospheric stability class and the surface roughness. Surface roughness is usually classified as having either rough or smooth. Urban and suburban areas are considered rough surfaces, while flat, open country, lakes and seas where the geostrophic wind and surface winds are similar are considered smooth surfaces. Table 3.5 illustrates how p varies with atmospheric stability for a rough surface. The exponent values in Table 3.5 can be multiplied by 0.6 for use in smooth terrain conditions.

Table 3-5. Wind Profile Exponent for Rough Surfaces.

Stability Class	Exponent (p)
A-B	0.15
C	0.20
D	0.25
E	0.40
F	0.60

(Source: Cooper and Alley, 1994.)

Ground Reflection. Equation 3-24 can be altered to include total or partial concentration reflection at the surface by adding the expression below into the {} of the last term

$$+ r_g \exp[-(H+z)^2/2\sigma_z^2)]\}$$

where r_g is the ground reflection coefficient, which varies from 1 to 0 for total reflection and no reflection, respectively. The term with (z+H) represents a mirror image of the source beneath the ground level which accounts for increased above ground level concentrations after the lower plume edge hits the ground. In cases where the ground level concentration is desired, with total ground reflection, the term in the {} of equation 3-24 reduces to become

$$\{2\exp[-(H^2/2\sigma_z^2)]\}$$

Inversion Reflection. In cases where there is an inversion layer above the stack height, the plume becomes trapped and is reflected downward. Equation 3-24 can be altered by including the following term into the {}of the last term

$$+ r_i\exp[-(z + H + 2L)/\sigma_z]\}$$

where r_i is the inversion reflection coefficient and L is the height of the inversion layer. However, since there are multiple reflections occurring from the ground and the inversion barriers, the last term will be changed to the following expression, which better represents the behavior of the plume:

$$\{\sum\{\exp[(-(z + H - 2jL)/(2\sigma_z))2] + \exp[(-(z + H + 2jL)/(2\sigma_z))2]\}\}$$

where j is the summation index (usually -2 to +2 for convergence). In cases of uniform vertical mixing equation 3-24 ca be further modified to the following experssion:

$$C = [Q/((2\pi)^{1/2}u\sigma_y H)]\exp[(-1/2)(y/\sigma_y)^2] \qquad 3\text{-}31$$

Equation 3-31 can be used by substituting H with L when the downwind distance x is two times the downwind distance where the first top plume edge intercepts with the inversion layer x_L. The x_L distance can be found by using Figure 3.4 and the following equation

$$\sigma_z = 0.47(L-H) \qquad 3\text{-}32$$

Therefore equation 3-24 can be used for $x < x_L$, equation 3-27 can be used for $x > 2x_L$, and distance between x_L and $2x_L$ must be interpolated.

Other Conditions. The Gaussian model can be manipulated in several ways to better represent atmospheric motion and dispersion phenomena. The original equation can be multiplied by an exponential term to represent dry and wet deposition and chemical transformations. It can be modified to represent line, area, and volume sources, concentrations in the wake of buildings, plumes trapped in valleys, tilted plumes, coastal diffusion and shoreline fumigation, and complex terrain.

The Gaussian model can be modified to simulate the time-varying concentration fields for climatological models. This method uses the steady-state Gaussian equation repeatedly with a series of hourly emissions and meteorological input to produce long-term or short term concentration averages.

The Gaussian equation can also be modified to represent time-varying transport conditions in which the wind direction changes. This type of model is called a segmented plume model because the plume is segmented into independent elements which generate individual concentration fields. Another method of representing time varying transport conditions is the use of puff models, which use a centroidal approach to calculate the receptor concentration of a particular mass of pollutants injected into the atmosphere. In addition, both of these methods can be combined to produce a mixed segment-puff model which simulates plume dispersion.

4.0 APPROACHES TO AIR POLLUTION MODEL VALIDATION AND EVALUATION

This section of the paper will focus on deterministic models and ignore statistical models since they are beyond the scope of the paper. The sources of modeling uncertainties and the different methods of evaluating and verifying models are outlined and discussed, along with three examples of the use of a few of these methods.

At this point it is important to define some of the key terms involved in this section. Model verification is proof of the accuracy, reality, or truth of the model. Model evaluation is the process of examining and estimating the performance of the model by comparing modelled output to measured air quality data. Model validation is the establishment of a conclusion, by detailed analysis of evidence, that leads to formal recognition (Fox, 1980).

4.1. Sources of Modeling Uncertainties

Modeling uncertainties arise from the fact that any measurement has a characteristic error associated with it, and from the stochastic (turbulent) nature of the atmosphere, which can not easily be physically modeled. The stochastic nature of the atmosphere introduces unknown variable that must be represented statistically and through ensemble concentrations. Hanna (1993) suggests that as a rule of thumb, the uncertainty in typical air quality model applications is about a factor of two, and that the uncertainty in high-grade research programs is about ±20%.

The two types of uncertainty are reducible error and inherent uncertainty. Reducible errors arise from inappropriate or insufficient meteorological and air quality data inputs and from inadequacies of the model formulations. Inherent uncertainty is irreversible and is a result of the stochastic nature of the turbulent atmosphere, which can not be fully described mathematically. Inherent uncertainty will always remain in air pollution models, even for models with good representations of the atmospheric physics and chemistry.

Hanna (1988) presents the equation below for the total model uncertainty, which is made up of three main components

$$\overline{(C_p - C_o)^2} = \overline{(C_p - C_{oa})^2} + \sigma^2_{Co} + \sigma^2_{Cp} + \overline{\Delta C_o^2} + \overline{\Delta C_p^2} \qquad 4\text{-}1$$

Total Model Uncertainty	Model Physics I	Stochastic Uncertainty II	Data Errors III

where

C_p The predicted concentration.

C_o The observed concentration.

C_{oa} The actual ensemble average (without instrument errors).

σ Magnitude of the turbulent or stochastic fluctuations in concentrations.

ΔC_o Data error in C_o (instrument, human, and other).

ΔC_p Data input error.

and where the bar indicates an average over a certain number of pairs of C_p and C_o observed at various points and/or times. This section will discuss the sources of these errors.

4.1.1. Data Input Errors

As stated above, every measurement has a characteristic error associated with its estimate of the true value. Air pollution modeling inputs include emission and meteorological input data measurements which have error associated with them. In addition, as Zannetti (1990) states, they possess space and time limitations that prevent their use beyond their "representativeness" regions (usually very small) around the monitoring point.

Hanna (1988) suggests that most input parameters are known only to an accuracy of 10 percent, at best. One of the largest sources of error in air pollution models is in the wind direction measurement which can vary as much as 20° (Hanna, 1988). This results in poor correlation between predicted short term average concentrations and observed concentrations at the same time and location.

Input error can have the result of limiting how complex an air pollution model can become. Input error increases as the model includes more information to improve model physics and time and space resolution, and reduce the overall modeling uncertainties. However, as will be discussed later, irreversible uncertainties limit ability to decrease the overall modeling uncertainty.

In addition, most model evaluation studies use observed pollutant concentration measurements from monitoring sites to compare to predicted (modeled) concentrations. These observed monitoring site measurements include a characteristic error around the true value. Hanna (1988) suggested that monitored concentrations have an accuracy of ±5 to 10 percent. Therefore, there is an error that is introduced and carried through in the evaluation and development of performance measurements such as the model confidence limits.

Meteorological data error many times is a result of the use of nonrepresentative meteorological data in air pollution models. In most cases this is due to our inability to measure the atmosphere with sufficient spacial resolution to provide adequate input data for air pollution models (Fox, 1982). Another source of error is caused by discretizing of the atmospheric conditions which in reality are constantly varying, such as the use of stability categories. The inability of measurement devices to accurately measure variables such as wind speed and wind direction is another source of error.

Emissions data errors are the result of variations in fuel supply and variations in production level. In some cases the emissions are spatially dispersed and their location is not well known, like

in the case of fugitive dust. Another source of emission errors is caused by the use of conservative maximum emission estimates being used as input to models instead of time varying emission inputs.

4.1.2. Model Formulation Errors

Model formulation errors arise from inadequate or incorrect representation of the atmospheric dispersion physics. Every model has limitations on the physical representation of the atmosphere and the space and time resolution. Model formulation errors can be categorized on the basis of the model components, such as modeling the pollutant source introduction to the atmosphere and the treatment of the pollutant transport.

Model formulation errors are considered reducible errors as long as it is possible to better model or represent the atmospheric physics through the use of more complex model formulations and meteorological data. However, the inherent uncertainty associated with the stochastic nature of the atmosphere limits our ability to better represent pollutant dispersion in modeling and thus model formulation errors are also considered irreducible errors.

Errors associated with the model formulation of how the pollutant is initially injected into the atmosphere mainly come from how the model represents the source aerodynamic interactions and the source's plume rise. Source aerodynamic interactions, such as building wakes, downdrafts, and complex emission fluctuations, are not well simulated by models, and can be responsible for maximum ground level concentration at up to five building height downwind distances (Fox, 1982). Source plume rise can have a significant effect on downwind concentrations since they are highly dependent on the actual plume rise. Plume rise is very difficult to model because it depends on the initial stack conditions, the ambient wind speed, and the stability of the atmosphere between the stack height and the final plume rise height. The latter is a source of significant error since the atmospheric conditions between 10-1000m of plume rise are quite variable (Fox, 1982).

Errors associated with how the model handles pollutant transport come from how the model represents vertical wind shear, horizontal variations in wind, mixing depth and stability, and dispersion coefficients. Vertical wind shear is a result of wind speed and direction changes with height. Wind shear can have a large effect on how the plume spreads out. In most cases wind speed at different heights is estimated by a power law relationship whose coefficients vary with the stability class, while wind direction at different heights is usually an unknown variable.

Variations in horizontal wind speed and direction contribute largely to errors in ground level concentration estimates. This is due to the use of the straight-line transport assumption used in many dispersion models. In reality, the mean wind field varies with the level above the surface, the heating and cooling of the surface, the interaction with physical obstructions, and the interaction with synoptic winds aloft.

The mixing depth and stability class of the atmosphere can be large sources of error, since they depend largely on the highly variable incoming solar radiation intensity on the ground surface. The grouping of stability into discrete classes is thus a large contribution to the modeling error. The mixing depth is a source of error because many models do not allow pollutants that have risen above the mixing layer to return to the surface and the top of the mixing layer is used as a reflection boundary for pollutants below the mixing layer. However, improvements have been made in this area by using convective scaling concepts which allow layer-by-layer calculations so that changes in the vertical structure of the atmosphere, such as wind and temperature are represented.

Dispersion coefficients have been another source of model formulation error since the Pasquill-Gifford dispersion coefficient formulations are universally accepted and used under conditions for which they were not validated. This error has been reduced by the use of different dispersion coefficients for different conditions such as rural, urban, and complex terrain conditions.

4.1.3. Stochastic Nature of the Atmosphere

The stochastic nature of the atmosphere is caused by the practical impossibility of including certain processes in our description of the atmosphere (Venkatram, 1988). Therefore, inherent uncertainty will always be present in atmospheric modeling because of the randomness of the atmosphere which allows for an infinite number of statistically possible outcomes. It is estimated that inherent uncertainty may represent a large fraction of the total uncertainty.

In deterministic models, an attempt is made to develop a cause-and-effect relationship between the source and receptor. This is done by using a chain of mathematical expressions that simulate the atmospheric dispersion processes. In every step of the chain some noise is being injected into the system that models are unable to model accurately due to the purely random outcomes that exist. This noise is a result of both monitoring and processing unknowns that cloud our ability to predict the true outcome. Therefore the more sophisticated a model becomes, the more steps are included in the model and thus more error is injected into the model unless empirical scaling parameters are added and/or the model is a better representation of the actual processes.

Venkatram (1988) addressed the different causes of inherent uncertainty in different types of modeling domains. His findings were that inherent uncertainty in models that are used on the scale of the order of kilometers is essentially caused by inability to describe the turbulent motion in detail. This forces use of statistics like the Gaussian distribution to describe these processes. The inherent uncertainty associated with models that are used on the scale of hundreds of kilometers is primarily caused by mesoscale motions such as sea/land breezes that cannot be resolved by the grid. These types of uncertainty can be modeled deterministically but because of computational constraints they are dealt with statistically.

4.2. Choices of Parameters to Evaluate

The choices of performance parameters to evaluate are either operational or scientific. Operational performance measurements are comparisons with predicted data and measured data to determine how good a model is at predicting some concentration. Scientific performance measurements attempt to measure how well a model estimates the cause-and-effect relationship of the model and involves testing the model components such as model input effects, model physics, and model inherent uncertainties (Fox, 1980).

4.2.1. Operational Performance Evaluations

Operational performance evaluations are used to evaluate the ability of the model to estimate concentration statistics for regulatory purposes, such as the network-wide highest concentrations. Operational evaluations are mainly used to determine the best performing model by comparing observed concentrations, C_o, to predicted concentrations, C_p.

4.2.1.1. Early Methods. The method recommended by the 1980 American Meteorological Society (AMS) Steering Committee made use of the difference, d, between the non-ensemble-mean observed c_o, and the nonensemble-mean predicted, c_p, concentration.

$$d = C_o(x,T) - C_p(x,T) \qquad 4\text{-}2$$

This residual is used to measure the average or bias,

$$\bar{d} = (1/N)\sum_{i=1}^{N} d_i \qquad 4\text{-}3$$

and the variability can be measured by the variance, σ_d^2, the mean-square error, MSE, and the average absolute gross error $|d|$ as illustrated below

$$\sigma_d^2 = (1/N\text{-}1)\sum_{i=1}^{N}(d_i - \bar{d})^2 \qquad 4\text{-}4$$

$$MSE = (1/N)\sum_{i=1}^{N} d_i^2 \qquad 4\text{-}5$$

$$|\bar{d}| = (1/N)\sum_{i=1}^{N} |d_i| \qquad 4\text{-}6$$

where N is the number of observations and the overbar represents the average. Note the square root of the σ_d^2 is the standard deviation and the square root of the MSE is the root mean square, RMS. For normally distributed variables the bias has a normal distribution, the variance has a chi-squared distribution, and the mean square error has a compound distribution.

These methods were recommended for determining the correlation between the maximum observations and predictions that were paired in time, space, and the combination of time and space. However, the determination of the correlation and the above differences was recommended for only the 25 maximum concentrations (unpaired in time and space) since (1) the differences yielded little or no information due to uncertainties in the plume transport, and (2) the regulatory concern was placed on maximum concentrations, over designated averaging times. The regulatory concerns were and are only concerned with how well the model predicts maximum concentrations without concern for when and where they occur. The lack of success in distinguishing model performance when using these methods has led to many improvements in model performance evaluations which will be discussed in the following sections.

4.2.1.2. Recent Methods. More recent methods use improved statistical analysis techniques to estimate model operational performance. This involves the use of more straight forward measures of model operational performance. These measures are estimated by calculating the fractional bias, FB, and the fractional scatter, FS, which emphasize the model effectiveness at the upper end of the concentration distributions. The FB and the FS are calculated by

$$FB = 2(\bar{C}_o - \bar{C}_p)/(\bar{C}_o + \bar{C}_p) \quad 4\text{-}7$$

$$FS = 2(\sigma_{co} - \sigma_{cp})/(\sigma_{co} + \sigma_{cp}) \quad 4\text{-}8$$

where the overbar represents the average over the 25 highest concentrations that are not paired in time and space and the σ_c is the standard deviation of the concentrations about the average. The FB indicates how well the model reproduces the average of the highest observed concentrations while the FS signifies how well the model reproduces the spread of the highest observed concentrations. Typical values of FB and FS are between +2 (extreme underprediction) and -2 (extreme overprediction), with a desired value of zero (free from bias) where ±0.67 corresponds to a prediction within a factor of 2 of the observations. The uncertainties of these variables can be calculated using resampling techniques to improve estimates of the means, variances, and other aspects of the distribution of FB and FS.

4.2.2. Scientific Performance Evaluations

The scientific component is used to evaluate the model's ability to perform accurately throughout a wide range of expected meteorological conditions and the immediate geographical area that surrounds the source(s). This type of evaluation may analyze the model input, model physics, and the model inherent uncertainties in attempting to estimate the representativeness of the model for the actual physical conditions. Scientific evaluations of models are important in determining areas of model improvement and in determining the range of conditions for model application.

Useful statistical parameters used to evaluate pairs of predicted and observed concentrations are listed below and their use is demonstrated in Section 4.3. Note all these statistical parameters evaluate the scientific component as long as the predicted and observed concentrations are paired in either space, time, or space and time. When they are not paired in time and space then they can be used to evaluate the operational component of a model analysis.

The normalized mean square error, NMSE

$$NMSE = \overline{(C_p - C_o)^2}/\bar{C}_o\bar{C}_p \qquad 4\text{-}9$$

The geometric mean bias, MG

$$MG = \exp(\overline{\ln C_o} - \overline{\ln C_p}) \qquad 4\text{-}10$$

The geometric mean variance, VG

$$VG = \exp[\overline{(\ln C_o - \ln C_p)^2}] \qquad 4\text{-}11$$

The correlation coefficient, R

$$R = \overline{(C_o - \bar{C}_o)(C_p - \bar{C}_p)}/\sigma c_p \sigma c_o \qquad 4\text{-}12$$

The fraction within a factor of two, FAC2

$$FAC2 = \text{fraction of data for which } 0.5 \leq Cp/Co \leq 2 \qquad 4\text{-}13$$

An additional method that can be used to evaluate the scientific credibility is the use of residual plots, where the residual is defined as the ratio of the predicted to the observed concentration (C_p/C_o). This residual is then plotted against any variable used in the model, such as wind speed. For a good model the residual plot should not show any trend with the variable, and it should not show large deviations from unity.

4.2.2.1. Model Input Analysis. As noted in equation 4-1 the input error is $\Delta C_o^2 + \Delta C_p^2$, where ΔC^2 can be quantified by using a Taylor series that retains terms up to the second order, as shown below (Hanna, 1988).

$$\overline{\Delta C^2} = \sum_{i=1}^{n}(\partial C/\partial x_i)^2\overline{(\Delta x_i)^2} + (1/2)\sum_{i=1}^{n}(\partial^2 C/\partial x_i^2)^2\overline{(\Delta x_i)^4} + \sum_{i=1}^{n}\sum_{j=1}^{n}(\partial^2 C/\partial x_i\,\partial x_j)^2\overline{\Delta x_i}^2\overline{(\Delta x_j)^2}$$

4-14

where x_i could be any parameter, such as wind speed, wind direction, and stability, to name a few. The first, second and third terms represent the first, second, and third order effects, which are nonzero only when the second partial derivative with respect to x_i and x_j is nonzero. Note that as n increases this method becomes cumbersome and it might become necessary to estimate the data errors by using model sensitivity tests like the computerized Monte Carlo procedures (Hanna, 1988).

4.2.2.2. Model Physics Analysis. In order to estimate the model physics errors, the model error (residual difference between the observed, C_o, and the predicted, C_p, ensemble mean concentrations) must be separated from the natural variability of the atmosphere and the data input errors (Weil et al., 1992). This section will summarize two approaches outlined by Weil et al., (1992) for estimating the model physics errors. The first approach is a simple, more practical method to use than the second approach, which involves the use of models which estimate the natural or stochastic variability in concentrations, σ_c.

The practical approach involves the use of calculating the residual, d, by $d = \ln C_p - \ln C_o$ since it was found that C_p/C_o approximates a lognormal distribution. Then, $\ln[C_p/C_o]$ is plotted on the y-axis against individual model inputs such as the buoyancy flux, F* or the downwind distance. These scatter plots are then broken up into intervals for which the geometric mean (GM) and the geometric standard deviation (GSD) are calculated to estimate the uncertainty. The uncertainty is estimated by the 95% confidence interval, which is developed from the GSD and the number of points in each interval, and then plotted in the same manner as above to determine significant trends of C_p/C_o. This method will clearly show if the model has a tendency to make overpredictions ($C_p/C_o>1$) or underpredictions ($C_p/C_o<1$) by knowing where the GM and the confidence interval of C_p/C_o lies when plotted against the input variable on the x-axis. In addition, it is also useful to plot $\ln C_p$ verses $\ln C_o$ to determine the correlation between predicted and observed concentrations to measure the

performance of two or more models with the same data set. This method is useful in determining the best model by determining the model with the least bias and the greatest confidence that the error is small. Weil et al., (1992) suggests that this method can be used in an iterative process to determine deficiencies for improvement within models.

The second method is a more complex rigorous evaluation involving more calculations and an additional model to determine errors in the model physics. The fundamental problem in this method is the definition of the ensemble of realizations for determining the observed concentration statistics. This paper defines the ensemble in terms of model inputs since the model inputs define the physics of the dispersion problem. This ensemble can be used to isloate the model error from the other contributions to the variability in performace measures such as the mean square error (MSE). This method breaks model predictions into the model inputs, ξ_n, and model input uncertainties, ξ_n', as follows:

$$c_p(\xi_n,\xi_n') = C_p(\xi_n) + c_p'(\xi_n,\xi_n') \qquad 4\text{-}15$$

where c_p' is the prediction uncertainty due to ξ_n', C_p is the predicted ensemble-mean concentration, and c_p is the decomposed model prediction. The observed concentration can be broken down into measurement error fluctuations, c_o', natural variability fluctuations, c_r', and variables not included in the model formulation, μ_m. The μ_m is also known as the realization index which varies from realization to realization. The observed concentration algorithm is represented in the following equation

$$c_o(\xi_n,\mu_m) = C_o(\xi_n) + c_o' + c_r'(\xi_n,\mu_m). \qquad 4\text{-}16$$

When plugging in these decomposed equations into the equation for the residual, d, the expression becomes

$$d = C_o + c_o' + c_r' - C_p - c_p' \qquad 4\text{-}17$$

which then changes the expression for the mean square error to

$$\langle MSE \rangle = \langle d \rangle^2 + \langle c_p'^2 \rangle + \langle c_o'^2 \rangle + \langle c_r'^2 \rangle \qquad 4\text{-}18$$

where $\langle d \rangle = C_o - C_p$, which is the square of the model error. The second and third terms are the fluctuations in measurement errors, while the last term is the natural variability which is irreducible and is approximated by σ_c^2. Weil et al., (1992) represents σ_c^2 as

$$\sigma_c^2 = \langle [c(x,t) - C(x,t)]^2 \rangle^{1/2} \qquad 4\text{-}19$$

where x is the downwind location, t is the time, c(x,t) is the concentration in any realization of the experiment, and C(x,t) is the time-averaged quantity. Weil et al., (1992) indicates that σ_c is difficult to obtain due to limitations in replicating field experiments and in general must be obtained from laboratory experiments and models. However, σ_c is important in estimating errors in model physics because it can be used to isolate errors in model physics and it has been shown by Weil et al. (1992) that c_r'/σ_c has a self-similar probability distribution in the upper part of the cumulative distribution function, cdf, for different model inputs. In addition, c_r'/σ_c can be assumed to be equal to d/σ_c when σ_c^2 is the dominant contributor to the residual and it is measured over several averages. This allows residual plots of d/σ_c verses model inputs to be constructed to evaluate model error without the effects of the natural varibility. These residual plots can be analyzed in the same manner as the practical method where an ideal situation will be symmetrically distributed around $d/\sigma_c = 1$.

4.2.2.3. Model Inherent Uncertainties Analysis. As noted in equation 4-1 the model inherent uncertainty (stochastic uncertainty) is the $\sigma_{co}^2 + \sigma_{cp}^2$ term. The σ_c^2 term expresses the turbulent fluctuations in any geophysical parameter. It characterizes the natural variability and is strongly dependent upon the sampling time and averaging time. Weil (1992) suggests that estimating this parameter for advanced model physics errors is the main problem in actual situations due to the lack of repetitive similiar conditions to determine representative ensemble properties of σ_c. He suggests that laboratory experiments provide the best way to obtain σ_c estimates and models.

Hanna (1988) suggests that σ_c^2 can be estimated through Taylors' equation, shown below, if the integral time scale, T_I, the averaging time, T, and the concentration fluctuations are known.

$$\sigma_c^2(T)/\sigma_c^2(0) = (2T_I/T)\{1 - (T_I/T)[1 - \exp(-T/T_I)]\} \quad 4\text{-}20$$

For cases when the plume intermittently affects monitoring sites, it is useful to calculate the cumulative distribution function, cdf, from an exponential probability distribution function, pdf, as shown below:

$$P(C) = 1 - I\exp(-IC/\bar{C}) \quad 4\text{-}21$$

where P is the cdf and I is the fraction of time that the observed monitor readings are nonzero. This is helpful because the probability of occurrences of any concentration can be predicted once P is known. The variance, σ_c^2, for instantaneous averaging times can be calculated, as illustrated below, when the exponential distribution is valid.

$$\sigma_c^2 = \bar{C}^2[(2/I) - 1] \quad 4\text{-}22$$

where I is calculated as follows

$$I = (\sigma_{zi}/\sigma_{zT})(\sigma_{yi}/\sigma_{yT}) \quad 4\text{-}23$$

and where subscript i indicates instantaneous and subscript T indicates time-averaged. The σ_z and σ_y values describe the turbulent fluctuations in wind speed in the vertical and lateral directions, respectively. For conditions when the T_I for the vertical and lateral turbulences are equal, then I can be calculated by

$$I = \exp(-1.2t/T_I)\exp(-y^2/2\sigma_{yT}^2) \quad 4\text{-}24$$

4.2.3. Current Regulatory Practice

The current regulatory practice of model evaluation in determining the best performing model involves the use of a two stage processes. The first stage is a screening test which eliminates models that fail to perform at a minimum operational level. This minimum operational level of the model prediction is suggested to be within a factor-of-two of the observed concentrations. The second step is then applied to those models that pass the first stage. This step is called the statistical test step which involves more comprehensive statistical comparisons and bootstrapping procedures described in the next section, and which is used to produce a probability distribution of the feasible data outcomes. This probability distribution is then used to calculated confidence intervals to aid in the comparison of two or more models.

In the screening stage the fractional bias, FB, is calculated to determine if the model is operating within a factor of two. The FB is used for both the average of the highest 25 observed and predicted values and the standard deviation of the 25 highest observed and predicted values. The FB is useful in determining if the model is biased towards overpredicting or underpredicting. However, for regulatory purposes the most important factor is whether or not the model is operating within a factor of two so the calculations can be simplified by determining the absolute fractional bias (AFB), which is the absolute value of the fractional bias. The absolute fractional bias should not exceed a value of 0.67 to satisfy the factor of two requirement. If the model exceeds the AFB of 0.67, then it should be excluded from further evaluation.

The statistical test step involves statistical comparisons of both operational and scientific components of model evaluations. It uses a test statistic called the robust highest concentration (RHC), which uses the upper end of the concentration distribution within a given data category to determine the performance of a model. The RHC is useful because it mitigates the unacceptable effects of unusual events in the actual peak values and it represents a smoothed estimate of the highest concentrations (typically the annual second highest concentration at each monitor for the whole

network) which is not artificially bound by maximum concentrations of the bootstrap distribution of the RHC. The expression for the RHC is

$$RHC = X(N) + [\bar{X} - X(N)]\ln[(3N - 1)/2] \qquad 4\text{-}25$$

where $\bar{X}$ is the average of the N - 1 largest values, X(N) is the N^{th} largest value, and N is the number of values exceeding the threshold value ($N \leq 26$). The threshold value is defined as the near background concentration which has no impact on the determination of the RHC. Whenever N is less than 3, then the threshold value is used as the RHC statistic.

The RHC is considered to be a direct measure of the central location of the highest values and their spread about the central location. This is supported by the fact that the magnitude of the highest 25 concentrations tends to increase as the central location and the spread increase, due to increasing values of the average and standard deviations.

Once the RHC test statistic is calculated for each monitoring station within the actual network and the model network, the absolute fractional bias (AFB) performance measures can be calculated. The network wide RHC test statistic for the 3-hour and 24-hour averaging periods are used to calculate the AFB for the operational component measurement. The scientific component is measured by determining the 1-hour averaging period RHC for each meteorological condition and monitoring station. The AFB is then calculated from the spatially paired observed and predicted RHCs. The six meteorological conditions used are:

i. below 4.0 m/s

ii. above 4.0 m/s

iii. unstable (Classes A, B, and C)

iv. neutral (Class D)

v. Stable (Classes E and F)

Once the performance measures are computed, they can be combined by determining the composite performance measure (CPM)

$$CPM = (1/3)\overline{(AFB)_{ij}} + (2/3)\{[(AFB)_3 + (AFB)_{24}]/2\} \qquad 4\text{-}26$$

where

$(AFB)_{ij}$ The average AFB for meteorological category i and station j.

$(AFB)_3$ The AFB for the 3-hour averages.

$(AFB)_{24}$ The AFB for the 24-hour averages.

The 1/3 and the 2/3 are included in the equation because the operational component is two times as important than the scientific component for regulatory use. The CPM measures the overall tendency of the model to over or underpredict the measured values. The CPM's purpose is to compare the performance of two or more models by using the model comparison measure (MCM) which compares pairs of models by calculating the difference in the CPM of two models, as shown in equaiton 4-27.

$$(MCM)_{A,B} = (CPM)_A - (CPM)_B \qquad 4\text{-}27$$

where the subscripts A and B refer to model A and Model B respectively.

Once the models have been compared using the MCM procedure then the determination of significant difference between models (standard error) is determined by using the blocked bootstrap method. The standard error is determined by the standard deviation of the bootstrap-generated outcomes for the MCM.

The blocked bootstrap method is a resampling technique (outlined further in section 4.2.4) which recalculates the performance measure for a number of trial years. The original data is broken up into seasonal and 3-day blocks (approximately 30 blocks per season). The 3-day blocks are

randomly sampled, recorded, and replaced back into the seasonal data pool from each season until a whole season is created. This process is repeated until four seasons are reconstructed and a complete bootstrap year has been produced. The purpose of three day blocks is to ensure that day to day meteorological conditions are preserved, while the seasonal sampling is done to ensure that seasonal bootstrap data will represent that season. The bootstrap data is used repeatedly to calculate the CPM for each model until a meaningful standard error can be calculated for each model performance statistic.

The selection of the best model is done by comparing the CPM of two or more models. The model with the smallest CPM is the better model, which means that when calculating the MCM of two models, the sign of the MCM indicates the better model.

When determining the significant difference between two models, the ratio of the MCM to the standard error is calculated. For approximately a 90 percent confidence level, a ratio less than 1.7 indicates no significant difference, while ratios larger than ±1.7 indicate a significant difference between the models. For more than two models the significant difference between models is found by calculating simultaneous confidence intervals for each pair of model comparisons. If the confidence interval overlaps zero then the two models are not significantly different. Confidence levels of 90 to 95 percent are suggest by the EPA in the "Protocol for Determining the Best Performing Model" manual. In section 4.3 an example of this procedure from the article by Cox and Tikvart (1990) will be presented.

4.2.4. Resampling Techniques.

Resampling procedures are used to develop confidence limits on performance measures to estimate significant differences between the model predictions and observations or between the predictions of two models. Air quality data and model performance measures are estimated using resampling procedures because standard analytical procedures found in statistics textbooks, such as the Chi-Square formulas, are inadequate. This inadequacy arises from the fact that

air quality data and model performance measures are rarely normally distributed and are not easily transformed to a Guassian shape (Hanna, 1989).

This section will describe a few resampling procedures that were evaluated by Hanna (1989)in a study to determine the best method in the development of confidence intervals for performance measures. This study used a concocted data set which had a Gaussian parent distribution with known confidence limits to determine the best resampling procedure. The study found that the jacknife method was the most efficient procedure, requiring only a few seconds to perform 1000 resamples for the data set consisting of 30 hours of seven model predictions, while the bootstrap method required 15 minutes. The moment bootstrap method produced the best confidence limit results, while the leave-out-one jackknife method tended to slightly overestimate the known confidence limits.

4.2.4.1. Bootstrap Resampling Methods. The bootstrap resampling method involves randomly drawing a new set of N values from the original set of particular performance measures. Once one measurement is drawn from the set, it is recorded and then replaced back into the original data set pool. Therefore it is possible to redraw this measurement again. This method gives the multinomial distribution for the probability of certain combinations of N original values in the development of the cdf. The typical number of resamples that are drawn range from 100 to 1000. However, this method can give inaccurate results at the tails of the distribution function, due to an extreme value being resampled repeatedly to produce an unrealistic distribution function. This bootstrap method is also known as the *seductive bootstrap method*. Problems with this method have led to the development of the other resampling procedures discussed in this section.

Blocking Bootstrap Resampling. This method attempts to get around the seductive bootstrap weaknesses by blocking or dividing the data set into two or more blocks. Each block contains data which have similar characteristics such as the time of day or season. This ensures that for each block, such as a season, the reproduced performance measure distribution represents the data in that block. This method is used in the current EPA evaluation method which is described further in section 4.2.3.

The Moment Bootstrap. This method uses the original bootstrap method to estimate the mean and the variance of the distribution of any parameter, y, because these two measures are less susceptible to the influence of outliers. To alleviate the effects of small sample sizes the variance should be multiplied by N/(N-1) when calculating the 95% confidence limit around parameter y. The 95% Student-t value is used to calulate the 95% confidence limit as follows.

$$y - t_{95}\sigma_y(N/(N-1))^{1/2} < x < y + t_{95}\sigma_y(N/(N-1))^{1/2} \qquad 4\text{-}28$$

4.2.4.2. Jackknife Resampling Methods. The jackknife resampling method has been used for a long time and is less time consuming. It calculates the confidence intervals by determining the variance of a particular performance measure over N "leave-out-one" passes through the data set of size N. A pseudo-value, y_{*j}, is calculated from a statistic, y_{all}, which is derived from the whole data set. The y_{all} can be the variance, correlation, etc. Equation 4-29 uses the y_{all} and a statistic calculated when the jth entry is omitted from the data set, y_j, to calculate the mean, y_*, and the variance of the mean, s_*^2.

$$y_{*j} = Ny_{all} - (N-1)y_j \qquad 4\text{-}29$$

$$y_* = \sum y_{*j}/N \qquad 4\text{-}30$$

$$s^2 = \{\sum y_{*j}^2 - Ny_*^2\}/\{N-1\} \qquad 4\text{-}31$$

$$s_*^2 = s^2/N \qquad 4\text{-}32$$

The 95% confidence interval is then calculated by using the Student-t statistic shown below

$$[y^* - t95s^*, y^* + t95s^*] \qquad 4\text{-}33$$

This method is known as the *leave-out-one jackknife method,* and should be used for statistics that are narrowly estimated, such as the mean and variance, since the jackknife estimate is easily affected by outliers.

The Blocked Jackknife. The blocked jackknife method is used when data can be broken up into two or more well defined blocks to remove differences not caused by sampling. Once the blocks are developed equations 4-32 through 4-36 are used to calculate average values of the mean and the variance. Confidence intervals are then calculated for the entire data set and the individual blocks. These values are compared to determine which confidence interval is smaller. The smaller confidence interval values will most likely be the correct values if the blocks are appropriately chosen for the analysis.

Jackknifing by Halves-the Multihalver. The multihalver method is used when a block of data includes only two data points. The data set is divided into (N/2) blocks with two points per block. Resampling involves assigning "+" or "-" to each block. A "+" sign means that the first value in the block goes into the left hand half of a resampled set and the second value goes into the right hand half and the reverse if a "-" sign is assigned. Then g sequences of +s and -s are used to calculate statistics y_{Lg} and y_{Rg} which are calculated from the left half of the halvings g and the right half respectively. The mean and the variance is then estimated by

$$y_* = 2y_{all} - (1/G)\sum(1/2)(y_{Lg} + y_{Rg}) \qquad 4\text{-}34$$

$$s_*^2 = (1/G)\sum(1/4)(y_{Lg} - y_{Rg})^2 \qquad 4\text{-}35$$

where G is the number of rehalvings which is equal to N/2. The confidence interval can then be calculated by using Student-t values.

4.3. Some Proposed Validation and Evaluation Methods

This section of the paper will outline and review three air quality evaluation methods that have been conducted in the research of air quality model evaluation procedures. The first case will review Hanna's 1988 simplified method for evaluating models. The second case will review the current EPA method for evaluating models which is illustrated by Cox and Tikvart in their 1990 publication. The third case will review Hanna's 1993 method for quantifying the minimum achievable model uncertainty based on several independent exercises in which model predictions were compared to observed concentrations.

4.3.1. Case 1.

4.3.1.1. Methodology. This case will review Hanna's (1988) proposed method for evaluating models. It emphasizes the estimation of confidence limits around each performance measure used in the evaluation process. In this article Hanna (1988) suggested calculating the bias, normalized mean square error (NMSE), the correlation, and the development of confidence limits around these performance measures.

The bias is calculated from the highest top ten predicted and observed concentrations that are not paired in time and space by the following equation.

$$\text{bias} = \bar{C}_p - \bar{C}_o \text{ (top ten)} \qquad 4\text{-}36$$

The normalized mean square error (NMSE) is calculated to emphasize the scatter in the entire data set by equation 4-9, which is repeated here as equation 4-37.

$$\text{NMSE} = \overline{(Cp - Co)2}/\bar{C}o\bar{C}p \qquad 4\text{-}37$$

The NMSE is used because it is not biased towards models that typically overpredict or underpredict. This is useful in determining whether one model is significantly different from another in model

comparisons. The NMSE can be used for data paired in time and space, paired in space, or paired in time.

Once the bias, NMSE, and the correlation is calculated, it is helpful to calculate the confidence limits of these model performance measures. The confidence limits are constructed by using the seductive bootstrap resampling procedure outlined in section 4.2.4. In this example the bootstrap resampling method is applied to the bias, NMSE, and the correlation to determine the confidence limits around comparisons of model predictions to observed concentrations and for model to model comparisons to determine significant differences. Significant differences between two models and model predictions to observations are determined by whether or not the confidence interval includes zero. If the confidence interval includes zero, it is said that the model is not significantly different from the observed concentrations or from another model's predictions.

4.3.1.2. Case Example. Hanna uses the above outlined procedure on two air quality modeling studies which have been reported in *Atmospheric Environment* by Davis *et al.* (1986) and Stunder and Sethuraman (1986). The Davis *et al.* (1986) data included 23 comparisons of observed concentrations to four different model predictions, while the Stunder and Sethuraman (1986) data included 58 comparisons of observed concentrations to four different model predictions. Performance measures such as the bias, NMSE, and the correlation were calculated by Hanna (1988) for both studies which are shown in Tables 4-1 and 4-2.

Table 4-1: Davis *et al.* data.

Model	Cp - Co	NMSE	Correlation, r
1	-7.7	1.81	0.63
2	-46.6	44.82	0.60
3	-14.6	2.24	0.73
4	11.6	1.49	0.54

(Source: Hanna, 1988.)

Table 4-2: Stunder and Sethuraman data.

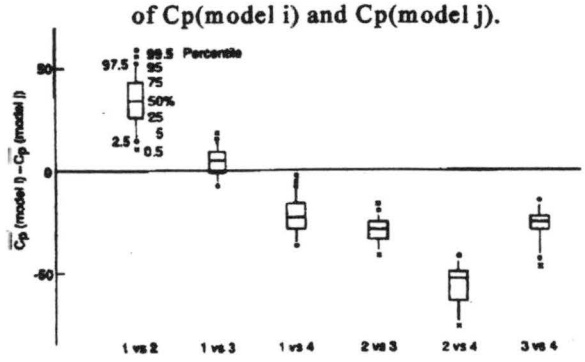
Table 4-2: Stunder and Sethuraman data.

Model	Cp -Co	NMSE	Correlation, r
1	22.6	0.60	0.59
2	-36.5	1.28	0.17
3	-115.4	3.83	0.16
4	-53.7	1.85	0.15

(Source: Hanna, 1988.)

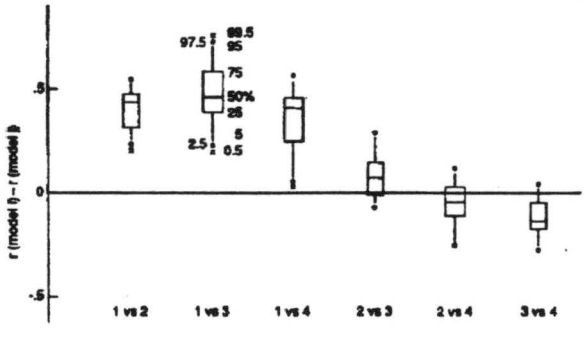
From Tables 1 and 2 we can determine which models have the lowest bias, NMSE, and the best correlation. However, they do not tell us anything about the significant differences between models, which must be estimated using confidence limits as discussed in the previous section. Figures 4-1 and 4-2 give some of the results found from the Davis *et al.* data and the Stunder and Sethuraman data respectively. Figure 4-1 gives results of the bias analysis which indicates that models 1 and 3 are not significantly different from each other. A similar plot of NMSE indicates that model 4 is not significantly different from model 1 and model 3 at the 95% confidence interval. A plot of the correlations shows that none of the models are significantly different from each other. This means that the best model can not be chosen.

Figure 4-1: Expected distribution of the comparison of $\overline{Cp}$(model i) and $\overline{Cp}$(model j).



Source: Hanna, 1988.

Figure 4-2: Expected distribution of the Correlation comparison of models i and j.



Source: Hanna, 1988.

Figure 4-2 shows that the correlations of models 2, 3, and 4 are not significantly different from each other and that model 1 has a slightly higher correlation coefficient than the other models since all of its comparisons between the other models are above zero. In addition, the bias analysis indicates that model 1 has the lowest bias and is not significantly different from zero. A similar plot of the analysis of the NMSE indicates that models 1 and 2 are not significantly different from zero at the 95% confidence interval. This allows us to determine that model 1 is the best model for this application.

In summary, Hanna suggests that we are able to make the conclusion that model 1 is the best model from the Stunder and Sethuraman data because of the size of the data set (n=58), while conclusions from the Davis *et al.* data set are inconclusive because of the small data set (n=23). Hanna goes on to suggest that the results from this study indicate that model uncertainty is very large since the NMSE is on the order of unity. He suggests for this reason that model uncertainty should be analyzed and predicted. He then proceeds to suggest a few methods for analyzing model uncertainties in data input and stochastic uncertainties which have been discussed in previous sections of this paper.

4.3.2. Case 2

4.3.2.1. Methodology. This example will illustrate the current EPA method for evaluating models to determine the best performing model for a particular regulatory application. The methodology used in this example has been outlined in Section 4.2.3 of this paper. The example shown here is a summary of Cox and Tikvart's example which was demonstrated in their 1990 publication in *Atmospheric Environment*. This method focuses on the model's ability to accurately predict peak concentrations and is primarily an operational performance evaluation of models.

4.3.2.2. Case Example. In this example, Cox and Tikvart compare the EPA's MPTER Version 6 model and an alternative model which contained a number of features not presently included in the MPTER model. The model evaluation uses 1-hour, 3-hour, and 24-hour

average measured and predicted concentration data obtained from four different power plant sites which are described further in Table 4-3.

Table 4-3: Power Plant Characteristics.

Plant Location	Source Characteristics	Terrain	Monitoring Network
Cliffy Creek, Indiana	1300 MW	Rolling hills	Six SO2 stations
	Three 208 m stacks	Low ridges	3-15 km from plant
		Below stack height	Data: 1975 and 1976
Muskingum River,	1460 MW	Rolling hills	Four SO2 stations
Ohio	Two 252 m stacks	Low Ridges	4-20 km from plant
		Below stack height	Data: 1975 and 1976
Paradise, Kentucky	2560 MW	Rolling hills	Twelve SO2 stations
	Two 183 m stacks	Below stack height	3-17 km from plant
	One 244 m stack		Data: 1980/1981
Kincaid, Illinois	1260 MW	Relatively isolated	Thirty SO2 stations
	One 187 m stack	In flat terrain	3-20 km from plant
			Data: 1976

(Source: Cox and Tikvart, 1990.)

Cox and Tikvart begin by performing the evaluation procedures on the Clifty Creek 1975 data for the two models. Threshold values of 25 $\mu g/m^3$ for the 1-hour data and 5 $\mu g/m^3$ for both the 3-hour and 24-hour data were determined by monitors outside the 90° area downwind of the source and were used in determining the robust highest concentrations (RHC) for the three averaging times. The RHC were used to construct Figures 4-3 and 4-4.

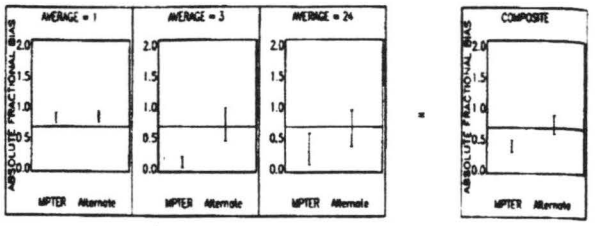
Figure 4-3 illustrates the absolute fractional bias for each model and the three averaging times, while Figure 4-4 illustrates the difference in the absolute fractional bias between the two model predictions, which is known as the model comparison measure, MCM, when all averaging times are put together into the composite performance measure (CPM). The 1-hour averaging time subfigures

represent the composite average which was constructed from the individual stations and the six meteorological conditions discussed in Section 4.2.3, while the 3-hour and 24-hour averaging time subfigures were developed from the maximum concentrations across the six monitoring stations.

Figure 4-3 shows that from the 1-hour averaging time the absolute fractional bias (ABS) is approximately the same for the two models. The other averaging times shows that the MPTER model is the better model since its confidence limits do not overlap and are within the area beneath the absolute fractional bias of 0.67. This results in the composite performance measure (CPM) plot indicating that the MPTER model is the better performing model, which is shown as the last subfigure in Figure 4-3.

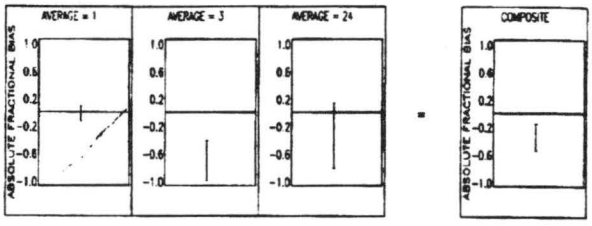
Figure 4-4 indicates that, for the 1-hour averaging time, there is no significant difference between the MPTER and the alternative model, since the confidence limits overlap zero. The 3-hour and 24-hour averaging times subfigures indicate that the MPTER model is the better performing model since the difference is

Figure 4-3: Performance comparison between model predictions and observations.



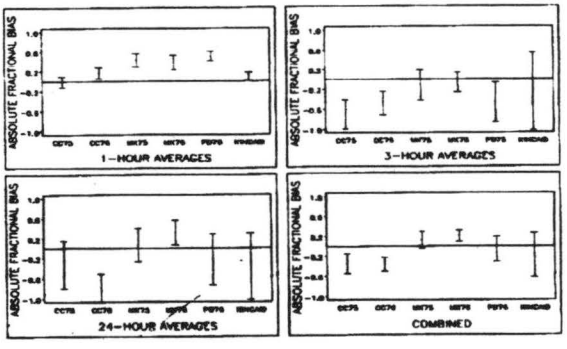
Source: Cox and Tikvart, 1990.

Figure 4-4: Difference in performance between models.



Source: Cox and Tikvart, 1990.

Figure 4-5: Performance comparisons between MPTER and the alternative model for six rural data bases.



Source: Cox and Tikvart, 1990.

negative. This carries over to the MCM plot, which also shows that the MPTER model is the better performing model.

Cox and Tikvart then go on to compare the results of the two models for the other six areas used to determine the best performing model. The result of the difference in the absolute fractional bias is shown in Figure 4-5. Figure 4-5 indicates that the alternative model appears to be the better performing model for the 1-hour averaging time, while MPTER appears to be the better performing model for the 3-hour averaging time. The results of the 24-hour averaging time are mixed since the MPTER model performs better for the 1976 Clifty Creek data, while the alternative model appears to perform better for the 1976 Muskingum River data. The composite of all the averaging times, the MCM, indicates that the MPTER model is the best performing model for the Clifty Creek site, while the alternative model appears to perform better at the Muckingum River site. At the other three sites it is impossible to determine the best performing models since the confidence limits overlap zero, indicating that there is no significant difference between them.

Cox and Tikvart suggest combining the above results from the six data bases to determine the overall better performing model. They recommend simply averaging the composite results of each model comparison since each data base is obtained independently. This is done by using the following equation

$$CMCM = [\sum(W_i * MCM_i)]/[\sum W_i] \qquad 4\text{-}37$$

where

CMCM	Composite Model Comparison Measure
MCM_i	Model Comparison Measure for the ith model data base
W_i	$= 1.0/S_i**2$
S_i	Bootstap estimated standard error for the ith model data base.

The standard error for this composite measurement is then calculated by

$$S = SQRT[1.0/(\sum W_i)] \qquad 4\text{-}38$$

When performing this exercise, Cox and Tikvart found that the composite model comparison measurement equalled -0.04 ± 0.03, which indicates that there is no significant difference between the models and no one model can be chosen as the best performer. Cox and Tikvart suggest that, to obtain meaningful results for the composite model comparison measure, that factors that influence differences between models be accounted for in the data base.

This method of evaluating models primarily focuses on how accurately a model predicts peak concentrations. The results of this analysis demonstrate that there are differences between the performance of the models for different averaging times, but the difference in the overall performance of the models indicates no significant difference. The authors suggest that this method could be adapted to include a more scientific evaluation by pairing observations and predictions in time and space for all the data, not just the 1-hour averaging time data.

4.3.3. Case 3

4.3.3.1. Methodology. This case reviews Hanna's (1993) method for evaluating models. The objective of this study is to quantify the "minimum achievable model uncertainty" based on 21 independent field site exercises in which predictions from 21 air quality models are compared to observations. The purpose of this study is to demonstrate that models need to be evaluated at different sites and under different situations to determine how well they perform over a large range of circumstances. Four separate model evaluation programs are demonstrated and the results are summarized in Hanna (1993). This section will review one of the four studies which illustrates Hanna's (1993) point. The parameters used in this paper to evaluate the models are:

i. A plot of the observed C/Q verses the predicted C/Q, where C/Q is defined as the maximum normalized concentration along a given monitoring arc or at any location on the monitoring network.

ii. Residual plots which are defined as the ratio of predicted to observed concentrations which are plotted verses any variable used in the model. For a good model the residual plot should show no trend with the variable and it should not exhibit large deviations from unity.

iii. The fractional bias, FB, as defined by equation 4-7.

iv. The geometric mean bias, MG, as defined by equation 4-10.

v. The normalized mean square error, NMSE, as defined by equation 4-9.

vi. The relative mean square error, RMSE, which is the square root of the NMSE and is an indication of the scatter.

vii. The geometric variance, VG, as defined by equation 4-11.

viii. The correlation coefficient,R, as defined by equation 4-12.

ix. The fraction within a factor of two, FAC2, as defined by equation 4-13.

4.3.3.2. Case Example. As mentioned above, the intent of this study is to quantify the minimum achievable model uncertainty by using a large number of independent exercises which are expected to result in the appearance of consistent patterns. Four model evaluation programs are outlined in this paper are:

i. The use of the Offshore and Coastal Dispersion (OCD) model evaluation.

ii. The Hybrid Plume Dispersion Model (HPDM) for power plant stacks.

iii. The Similarity model applied to continuous ground-level tracer gas releases.

iv. 14 Hazardous gas models applied to 8 databases.

Only the Offshore and Coastal Dispersion (OCD) model evaluation will be presented to illustrate Hanna's 1993 point that models should be evaluated at more than one site and for more than

one condition or situation. For more information on the other three studies refer to Hanna's 1993 article in *Boundary-Layer Meteorology*.

The OCD model evaluation took place at four independent sites where several tracer studies had been conducted to develop databases to improve coastal dispersion models. Two versions of the OCD model were evaluated at these sites during two different seasons for the Ventura, Pismo Beach, and Cameron sites and three different conditions at the Carpinteria site. The performance measures used to evaluate the two models at these location and conditions are the maximum C/Q, the FB, the NMSE, and the RMSE. Results for the OCD-4 version are summarized in Table 4-4.

Table 4-4: Summary of OCD-4 model performance for nine independent experiments.

Dataset	Hours, this analysis	Maximum C/Q, ($\mu s/m^3$)		FB	NMSE
		Observed	Predicted		
Ventura, Fall	9	2.8	1.9	-0.35	0.36
Ventura, Winter	8	3	3.7	0.22	0.17
Pismo Beach, Summer	16	7.8	15	-0.32	0.81
Pismo Beach, Winter	15	9.2	13.7	0.02	0.89
Cameron, Summer	9	3	2.4	-0.46	0.52
Cameron, Winter	17	37	31.4	-0.21	0.36
Carpinteria SF_6 Complex Terrain	18	109	231	-0.22	1.38
Carpinteria Freon Terrain	9	25	26.7	-0.32	0.43
Carpinteria Fumigation	9	15.2	9.8	0.16	0.97

Source: Hanna, 1993.

From Table 4-4 it is apparent that the OCD-4 model tends to overpredict the mean since the FB is negative for six of the nine conditions evaluated. Another important trend which shows up from doing model evaluations at different sites for differenct conditions are indicated in the mean FB and the median NMSE. The mean value of the FB for the OCD-4 model is 0.22 and is calculated as the median absolute magnitiude of the FB. This measure indicates that at any site the typical uncertainty of the mean prediction will vary by ±22%. Table 4-4 also shows that the median value of the NMSE is 0.52 and it ranges from 0.17 to 1.38. This measure is an indication of the scatter of the predicted values. This results in the median relative root mean square error (the square root of the NMSE) of about 70% which is expected to range from 40% to 100% from site to site.

This example shows how the relative bias in the mean predictions varies by ±22% from site to site but may vary as much as 46% or as little as 2% at any given site. This illustrates the tendency of one model evaluation to either give poor or excellent performance measures. This is also the case for the NMSE or the relative RMSE which may indicate a high or low amount of scatter at a particular site but a limited amount of scatter for several sites. This limited amount of scatter is approximately 70 % for the relative RMSE or 0.5 for the NMSE since it becomes impossible to demonstrate statistically significant improvements in the models using these performance measures due to the data errors and stochastic fluctuations (Hanna, 1993). The other three examples illustrate similar trends in model evaluations and support this conclusion.

5.0 FUTURE IMPROVEMENTS TO AIR POLLUTION MODELS

5.1. Defining Current Modeling Problems and Limitations

The current generation of regulatory and research models are relatively mature in their frameworks, with respect to their first development in the early 1970's and 1980's. These models include mathematical descriptions of emissions, atmospheric chemical dynamics, and/or pollution transport mechanisms. They are useful in setting emission limits on proposed sources, the scientific defense of future air pollution control strategies, and expanding our knowledge of how pollutants function in the atmosphere. Heavy reliance by the regulatory community on Gaussian type dispersion models has led to many improvements in these types of models even though they can be up to 50 percent inaccurate. Some of the current limitations associated with the use of Gaussian plume models are:

i. temporal and spatial changes in wind speed and direction,

ii. extrapolation of dispersion parameters beyond their empirical basis, for example, applying parameters derived from other sites, and

iii. the statistical nature of a turbulent atmosphere.

(Source: Robertson and Barry, 1989.)

The failure of Gaussian plume models to accurately model atmospheric conditions, chemical reactions, and physical removal processes will ultimately lead to the use of more advanced methods of modeling plume dispersion, such as Eulerian grid models which are capable of being more physically thorough and giving a more complete view of the air pollution problem causes and cures. This is not to say that Gaussian models will be phased out. In many situations it is much easier and cheaper to arrive at the correct answer from a simpler incorrect model. However, getting the wrong or incomplete answer is becoming unacceptable with the rising costs of implementing control strategies and decisions.

Currently, Eulerian grid models for regulatory uses are either urban-scale or regional-scale models and are primarily used to model photochemical processes. Urban grid models have horizontal grid sizes of about 5 km and cover 4×10^4 to 4×10^5 km^2 areas with 4 to 10 vertical levels. Regional grid models have larger horizontal grid sizes of about 18.5 km to 80 km and cover 1000 to 5000 km on each side of the area modeled with 3 to 15 vertical levels (Russell and Odman, 1993). Urban grid models are capable of handling sharp pollutant gradients where regional models cannot. This incompatibility prevents the interchangeable use of both types of fixed grid models. This presents a major problem for simulating long-range transport of precursor secondary pollutants, such as NO_x and hydrocarbons which may participate in the formation of O_3 outside the original modeling domain.

Another limitation of the current grid models is the use of homogeneous gas phase chemistry that may differ between urban and regional areas, where the chemistry of one species, such as NO_x, may be unknown in low concentrations (rural or isolated areas) and well known in high concentrations. In addition, Russell and Odman (1993) estimate that computational time involved in solving chemical reactions may take up as much as 85% of the total time. This high proportion of computational time has led to simplifications in the chemical mechanisms used in these models to reduce the time.

Other limitations of current models include input uncertainties, such as anthropogenic and biogenic source contributions, or meteorological variables that are not characterized spatially and may be highly biased. Another limitation is the manner in which models are evaluated. Traditionally this has involved the comparison of computed and observed concentrations of one chemical, with less attention placed on other trace species. In addition, the typical methods for determining modeling uncertainties, such as sensitivity analyzes, are performed using a brute force method. Other limitations are the lack of multiphase pollutant modeling and simplified deposition processes modeling. The use of multiple models to confront different facets of air quality problems in a single area can lead to compounding errors. The inability to accurately measure hazardous air pollutant (HAP) emissions is a severe limitation to the downwind HAP concentrations and risk assessment values. An additional related problem is the lack of individuals that are capable of operating these models, conducting

model evaluations, and enhancing models due to the expertise required and the lack of user friendly computer interfaces and easily interpretable model results.

5.2. Future Solutions.

In the future, attempts will be made to solve many of the problems associated with air quality modeling. This section will describe where the current and future research is going in attempting to overcome limitations of current models. It will discuss, where possible, the currently used research modeling efforts that may be incorporated into future regulatory models to better simulate atmospheric dispersion processes.

5.2.1. Improvements in Model Framework

5.2.1.1. Improved Grid Resolution. Some current research models are attempting to resolve the difficulties of modeling both urban and regional areas where long range transport is important by embedding urban models within the domain of a coarser regional model. This embedded urban model is called a nested grid model. The use of nested grids within regional grid models improves the resolution of the model. These multiscale grid models can either be a one-way or two-way nested grid. A one-way grid model allows information to travel from the regional model to the urban model. The regional grid model follows the pollutant transport into the urban area and calculates the appropriate boundary conditions for the urban model. A two-way grid model uses variably spaced grids that are adapted by the model to match the concentration gradients. This allows improved resolution of the chemistry in urban areas. It will improve chemical reaction mechanisms by permitting the flow of long-range pollutants that may affect the chemistry in these urban areas. Future regulatory models should include this type of modeling technique and framework to model not only oxidants but also other atmospheric compounds, and should be applicable to both small and large scales.

5.2.1.2. Improvements in Scientific Detail. Improvements in computational power are expected to allow more scientific detail within the air quality models, by including more detailed chemical mechanisms, multiphase pollutant modeling capabilities, and improved parameterization of deposition processes (Russell and Odman, 1993). The number of chemical species that can be modeled will be increased to include organic gases and radical species. This will allow chemical mechanisms within the models to reflect the current explicit mechanisms, instead of simplified chemical mechanisms that are included in the current regulatory models.

Multiphase pollutant modeling, including aerosol dynamics, particulate matter concentrations, visibility, and acid rain production, is becoming increasingly important in evaluating the air quality. These processes are computationally very intensive, and the lack of understanding of the thermodynamics and kinetics of multiphase atmospheric chemistry may inhibit their implementation. However, as our knowledge of multiphase atmospheric chemistry grows and computational power increases, they will inevitably be included in the next generation of models.

Other increasingly important processes to be modeled are deposition processes and particle chemical interactions. These processes are also limited by computational power and knowledge. The fluid dynamics of particles is well understood but complicated to model, while chemical surface interactions are not well understood. Some current "state-of-the-science" research models model deposition processes by a series of deposition resistances

$$r_{deposition} = r_a + r_b + r_c = 1/v_{dep}$$

where

$r_{depostion}$	deposition resistance
r_a	aerodynamic resistance
r_b	boundary layer resistance

r_c chemical resistance

v_{dep} deposition velocity

Source: Russell and Odman, 1993.

This method of modeling deposition processes will increasingly be used in regulatory models instead of using exponential models to estimate the amount of pollutants deposited from the atmosphere.

Another improvement in the physical representativeness of air pollution models is the linking of air pollution models to comprehensive atmospheric meteorological models to allow physiographic forcing of flow fields. Pielke, et al. (1992) present an example of this with Colorado State University, Department of Atmospheric Science's Regional Atmospheric Modeling System (RAMS). RAMS was developed to merge several numerical weather simulation codes into one computer package with hopes to facilitate more effective scientific research (Pielke, et al., 1992). In addition to the meteorological codes, a mesoscale Lagrangian particle dispersion model (MLPDM) was include to operate in conjunction with RAMS to model point, line, area, and volume sources in a variety of situations. This was done to minimize errors caused by homogeneous assumptions about the air flow in simple models (Gaussian type) and temporal and spatial resolution difficulties in more complex models used to simulate long-range transport of air pollutants. It is expected that the linking of MLPDM to RAMS will decrease these errors by allowing RAMS to predict the time-dependent, three-dimensional meteorological fields for use in the MLPDM to calculate the dispersion and transport of air pollutants in the atmosphere.

5.2.2. Incorporation of Uncertainty Analysis.

Russell and Odman (1993) suggest that the next generation of models should attempt to provide some kind of sensitivity analysis technique to determine uncertainties in model formulation. This would be beneficial in interpreting results and identifying key uncertainties. Currently the EPA's Atmospheric Research and Exposure Assessment Laboratory is developing a third-generation

modeling system, called Model-3, which includes an automatic differentiation for sensitivity estimations of the model.

As discussed in Section 4 of this paper, many researchers (such as Weil, Venkatram, and Hanna) are stressing the use of confidence limits around model predictions due to the many uncertainties in air pollution model predictions. Currently these researchers are developing methods for determining modeling uncertainties and estimating confidence limits around model predictions. In addition many researchers are stressing the evaluation of the scientific component of model evaluations instead of the operational component. Venkatram, (1988) suggests that an increase in computational power will allow brute force computer simulations to determine model inherent uncertainties. Weil *et al.*, (1992) suggests that future model evaluation activities will include the development of σ_c models in determining cumulative distribution functions, cdf, of the random fluctuations in model predictions. Hanna (1993) suggests that future research should be conducted in an attempt to develop and test predictive equations for the quantification of the scatter caused by data errors and natural stochastic fluctuations. The development and implementation of improved methods for determining air pollution modeling uncertainties will result in improved model predictions and better estimates of confidence limits around model predictions.

Improvements in emission inventories from both anthropogenic and biogenic sources are also expected to improve modeling efforts for predicting the effectiveness of future control strategies. Studies such as the 1987 Southern California Air Quality Study are expected to help in the development of new and more detailed data bases which will aid modeler's in improving air quality models by allowing them to better analyzing modeling weaknesses and uncertainties (Russell and Odman, 1993). The Title V permit program will be instrumental in assisting in the development of improved anthropogenic emission inventories by creating centralized databases of industrial activities and by forcing industry to incorporate improved monitoring systems, such as continuous emission monitors, for their stack emissions.

5.2.3. Improvements in Computational Power

As mentioned, most of the improvements in how air quality models represent atmospheric chemistry and dynamics depends on the utilization of advanced modeling architecture that takes advantage of recent and future advances in computer power. This is due to the computational time constraints of representing the complex atmospheric chemistry and the physics of air pollution transport.

Parallelization of model code and the use of multiple processors is a possible remedy to the time constraints of computationally intensive air quality modeling problems. This is expected to speed up the computational time to operate air quality models and increase the available memory which will allow for more grid points to be represented and thus reduce truncation error (Pai and Tsang, 1993). Research performed by Shin and Carmichael (1992) to determine if parallel processing actually provided significant improvements in the computational power of air pollution modeling found that the computational time was significantly reduced. Shin and Carmichael found for a 3-D regional scale grid model which was capable of calculating concentrations of 55 chemical species that by performing concurrent calculations the speed-up ratio (serial verses parallel code) ranged from 1.8 to 2.5 for gas-only and gas-liquid calculations, respectively when operating on an eight processor computer.

Shin and Carmichael (1992) indicate that multi-tasking applications to air pollution models will be exploited further in the future as our knowledge of atmospheric processes grows. However, for these multi-tasking efforts to be successful, new computer designs, software tools, and algorithms must be developed to take advantage of parallel processing. In addition, the new codes should be easily upgradeable to allow models to be modified when physical and chemical improvements are made.

Other future advances in air quality modeling include improved, easily understood results, such as graphical output. Increased computational power will allow models to be able to analyze

input and output graphically and numerically to help illustrate air quality problems to the modeler. In addition, improvements in input and output devices will allow further growth in the use of air quality models and thus increase the number of competent modelers which will eventually lead to a greater understanding of pollutant dynamics. In response to these needs, the Galson corporation of Syracuse, N.Y. is combining their nongraphical Air-1 ISCST based model with Environmental Systems Research Institute's (ESRI) Acr/Info geographical information system (GIS) to present output information in a manner which can be easily understood and analyzed (Puttre', 1994). This will allow pollution concentration data to be presented in map form and be analyzed in a new ways to yield improved accuracy at pinpointing areas with air pollution problems.

6.0 SUMMARY AND CONCLUSION

The primary focus of this paper has been to determine the future directions of atmospheric dispersion modeling for regulatory use in the United States. This was done by reviewing the past and current United States air pollution regulations, the available air pollution modeling methods, some of the current model evaluation and validation methods, and some of the future improvements to air pollution models. These topics will be put together in this section to illustrate where air pollution modeling fits into future air pollution control strategies.

Section two of this paper illustrates how air pollution regulations have been a driving force in air pollution modeling. Historically, air pollution models began their use as a regulatory tool in the late 1960's to early 1970's. Air pollution models were the only way regulatory authorities could develop emission limits on sources, since the NAAQS were set for the atmosphere. This is still the case today, however the current regulations have expanded the use of air pollution models.

Today air pollution models are used to determine where a proposed source may be built, its emission limits, and its control technology requirements. States must use air pollution models when submitting their SIPs to demonstrate compliance with all federal standards within the state. States with nonattainment areas must use regional and urban models to demonstrate that their air pollution control strategy will satisfy the reasonable further progress goals of eventually bringing the nonattainment area into compliance with all federal regulations. Air pollution models are also used by regulatory authorities and researchers to determine future air pollution control strategies when studying specific air pollution problems, such as acid rain, visibility degradation, ozone depletion, and global warming.

The 1990 CAAAs are designed to improve these efforts by providing a more comprehensive database on anthropogenic air pollutants that are emitted into the atmosphere. This has been done through the Title V operating permit program and the use of better monitoring and reporting methods. In addition, the NAAQS for particulate matter is currently being reviewed and may be

altered to include a lower particulate matter diameter standard which would be more representative of the health and visibility effects of particulate matter. This will require extensive regearing of air pollution measurement devises and air pollution control strategies. However, this will provide a better database on smaller particulate matter emissions and will allow air pollution models to provide improved output on the visibility and health effects of particulate matter.

Air pollution models have gone through many improvements and have become more complex as the regulations have grown and become more stringent. The future of air pollution modeling will continue to mature as the regulations continue to become more complex and the costs of implementing control strategies increase.

The high costs associated with implementing new control strategies has required and will require models to become more detailed in their physical description of the atmosphere. Gaussian plume models have been extensively modified over the years to include complex flow situations, such as building wake effects or complex terrain effects. However, Gaussian models have many limitations due to their underlining assumptions. These limitations will eventually lead to the use of more complex models, such as Eulerian grid models and Lagrangian models which are capable of incorporating more detailed physical descriptions of the atmosphere. Currently, the complexities and difficulties in operating these models have limited their introduction into regulatory use. As computers become more advanced and the capabilities of modelers increase, these problems will be overcome.

Improvement in model evaluation and validation methods are expected to identify the weaknesses and strengths of air pollution models. This will allow air pollution models to be improved so that they yield a better representation of the atmospheric dispersion processes which will provide more accurate predictions of pollutant concentrations. This will also allow improvements in the identification of the best performing model for a particular situation so that models are only used for those conditions in which they operate best.

The large number of available air pollution models currently requires the use of model evaluation methods to demonstrate which model is the best performing model for the particular situation. However, the current EPA methods are primarily interested in which model best estimates the maximum pollutant concentration anywhere in the modeling domain. This operational evaluation does not provide information on how well the model is estimating the maximum concentration at the correct receptor area. Improved and more comprehensive model evaluation methods will be used in the future as the number of models increases and as it becomes more important to estimate pollutant concentrations at the correct locations.

The next generation of models will provide easy to use input and output interfaces, they will be easy to update and they will include methods for evaluating the input and output information. The algorithm efficiency of the models will be improved by the use of advanced computers and the development of modeling frameworks that take advantage of the current and future computer architecture.

In summary, air pollution modeling will be increased in the future, due to the rising costs of implementing control strategies, the inability to perform thorough air pollution control pilot studies on the atmosphere, and improvements in the input and output interfaces of air pollution models which will allow more modelers to use these complex models.

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