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COMPUTER MODELING OF TRANSPORTATION- GENERATED AIR POLLUTION

A STATE-OF-THE-ART SURVEY

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16. Abstract

This report surveys the state-of-the-art in air pollution modeling with particular emphasis on the modeling of dispersion from transportation sources. Models which have actually been implemented are stressed and the computational aspects of these models are treated in detail. Applications are discussed and validations are critically assessed. It was found that Gaussian and conservation of mass models are currently the most widely used tools for analyzing the dispersion of pollutants in the atmosphere. Models presently in operation are run on medium to large-scale computers of the IBM 360/50 class or greater and nearly all of these models are programmed in FORTRAN IV. Although existing models have been applied to a wide variety of air pollution problems, their performance has not been adequately evaluated. This deficiency is primarily due to the fact that, until recently, instrumented transportation test sites have not existed and hence very little validation data have heretofore been generated. However, such test sites do now exist and data from them is beginning to become available, hence the validation of dispersion models will soon be feasible.

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PREFACE

In response to recent legislation requiring that each department of the Government take steps to carefully and systematically consider the environmental effects of its actions, the Office of the Secretary of Transportation (TST-8) initiated a program at TSC in FY72 to develop unified technological capabilities in air pollution control as part of a family of techniques and capabilities necessary to support the development in the Office of the Secretary, and in the operating administrations, of planning procedures related to the environmental impact of transportation systems and facilities.

The initial effort on this program was devoted to surveying the state-of-the-art of dispersion models suitable for analyzing transportation-generated air pollution. That survey is the subject of this report.

In FY72 TSC also developed a long-range plan to acquire and test transportation-related air pollution models. In addition, the Center initiated liaison and coordination activities with the DOT operating administrations and with the Environmental Protection Agency in order to ensure that pertinent information and data are disseminated among groups with responsibilities in the air pollution field.

In preparing this survey the author benefited from the work of Mr. Mark Caruso, a student at the University of Wisconsin, who, in 1971 as a summer employee of the Office of the Assistant Secretary for Systems and Technology, DOT, compiled a bibliography on air pollution modeling and wrote a preliminary version of Section 3. The author is also indebted to a number of individuals in the Department of Transportation who took time to read the draft version of this report and who were kind enough to forward their many helpful suggestions.

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1.0 INTRODUCTION

1.1 BACKGROUND

Under a series of recent laws relating to the preservation of environmental quality, the Secretary of Transportation must take certain actions aimed at curbing the impact of transportation-generated air pollution on the environment. Compliance with these laws requires that techniques be developed to analyze air pollution from transportation sources. This report is a state-of-the-art survey of air pollution models for predicting the dispersion of transportation emissions.

Since a knowledge of the new environmental laws is essential to understanding the role of the Secretary in air pollution abatement, a brief summary of the pertinent acts is included here, followed by a section on relevant court decisions under the National Environmental Policy Act of 1969. The Introduction concludes with a section on the content and structure of this report.

1.2 PUBLIC LAWS GOVERNING THE ENVIRONMENTAL IMPACT OF TRANSPORTATION

The six major public laws which deal with the environmental impact of transportation are summarized below.

1.2.1 Title 49, U.S.C. (1970), The Department of Transportation Act

"It is hereby declared to be the national policy that special effort should be made to preserve the natural beauty of the countryside and public park and recreation lands, wildlife, and waterfowl refuges, and historic sites." To this end the Secretary of Transportation must cooperate with designated Federal officials and with the States in developing plans which enhance natural beauty. Furthermore, the Secretary will not approve any program or project requiring use of publicly owned land from parks, recreation areas, wildlife refuges, and the like, unless there is no alternative to the use of such land, or unless all possible planning has been done to minimize harm to the land from such use.

1.2.2 Title 49, U.S.C. (1970), The Urban Mass Transportation Act of 1964, as amended

As in the Department of Transportation Act, the same national policy to preserve natural beauty is stated, but here with reference to the, "planning, designing, and construction of urban mass transportation projects for which Federal assistance is provided." The role of the Secretary of Transportation is to see that, "adequate opportunity was afforded for the presentation of views by all parties with a significant economic, social, or environmental" interest in the project. He must also review the project application to determine either that no adverse environmental effect will result or, if there is no feasible alternative to such an adverse effect, that the effect is minimized.

1.2.3 PL 91-190, The National Environmental Policy Act of 1969

This Act declares, "a national policy which will encourage productive and enjoyable harmony between man and his environment" and also, "promote efforts which will prevent or eliminate damage to the environment and biosphere and stimulate the health and welfare of man." All agencies of the Federal Government are required to "include in every recommendation or report on proposals for legislation and other major Federal actions significantly affecting the quality of the human environment, a detailed statement by the responsible official on the environmental impact of the proposed action." The Act also creates in the Executive Office of the President a Council on Environmental Quality, "to formulate and recommend national policies to promote the improvement of the quality of the environment."

1.2.4 PL 91-258, The Airport and Airway Development Act of 1970

Herein the Congress states its findings that, "the Nation's airport and airway system is inadequate to meet the current and projected growth in aviation" and that, "substantial expansion and improvement of the airport and airway system is required." The Secretary of Transportation is made responsible for formulating a national transportation policy which considers:

"(1) the coordinated development and improvement of all modes of transportation, together with the priority which shall be assigned to the development and improvement of each" and

"(2) the coordination of recommendations made under this title relating to airport and airway development with all other recommendations to the Congress for the development and improvement of our national transportation system."

The Secretary must consult with designated Federal officials "with regard to the preservation of environmental quality" and "shall, to the extent that (he) determines to be feasible," incorporate their recommendations in the "national airport system plan." Furthermore, "the Secretary shall not approve any project application for a project involving airport location, a major runway extension, or runway location unless the Governor of the State in which such project may be located certified in writing to the Secretary that there is reasonable assurance that the project will be located, designed, constructed and operated so as to comply with applicable air and water quality standards."

1.2.5 PL 91-604, The Clean Air Amendments of 1970

In this Act, the Congress finds, "that the growth in the amount and complexity of air pollution brought about by urbanization, industrial development, and the increasing use of motor vehicles, has resulted in mounting dangers to the public health and welfare, including injury to agricultural crops and livestock, damage to and deterioration in property, and hazards to air and ground transportation." In order to safeguard the environment, the Administrator of EPA is granted broad powers in the field of air pollution prevention and control.

This act also specified the future standards for emissions of carbon monoxide, hydrocarbons and oxides of nitrogen from light duty vehicles and engines. The EPA Administrator is required to report annually to Congress "with respect to the development of systems necessary to implement the emission standards." Also, the Administrator is charged with investigating, "emissions of air pollutants from aircraft" and subsequently with issuing, "proposed emission standards applicable to emissions of any air pollutant from any class or classes of aircraft or aircraft engines which in his judgment cause or contribute to or are likely to cause or contribute to air pollution which endangers the public health or welfare." The role of the Secretary of Transportation is defined as follows: "The Secretary of Transportation, after consultation with the Administrator, shall prescribe regulations to insure compliance with all standards prescribed......by the Administrator."

1.2.6 PL 91-605, Federal-Aid Highway Act of 1970

Under this Act the Secretary of Transportation is assigned certain responsibilities relating to the environmental impact of highway projects. Specifically, the Act states that, "the Secretary, after consultation with appropriate Federal and State officials, shall submit to Congress, and not later than 90 days after such submission, promulgate guidelines designed to assure that possible adverse economic, social and environmental effects relating to any proposed project on any Federal-aid system have been fully considered in developing such project, and that the final decisions on the project are made in the best overall public interest." Among the environmental effects which must be considered are air, noise, and water pollution. Furthermore, "the Secretary, after consultation with the Administrator of the Environmental Protection Agency, shall develop and promulgate guidelines to assure that highways constructed pursuant to this title are consistent with any approved plan for the implementation of any ambient air quality standard for any air quality control region designated pursuant to the Clean Air Act, as amended."

1.2.7 Timetable for Action

The timetable for air pollution actions which the above laws require is shown in Table 1. Note that the States were required to submit implementation plans to the EPA Administrator by January 1972, showing how the national primary and secondary air quality standards will be met in 1975. The Administrator was then responsible for approving or disapproving these plans. Also, in 1972 the Secretary of Transportation must promulgate guidelines relating to adverse environmental effects of Federal-aid highway projects and in the same year he must publish a national airport system plan which takes environmental quality into account. In addition, the Secretary (after consultation with the Administrator) must prescribe regulations to insure compliance with all aircraft emissions standards proposed by the Administrator. Note also that the principal automotive emissions must be drastically reduced by the 1975-76 period.

1.3 COURT DECISIONS UNDER THE NATIONAL ENVIRONMENTAL POLICY ACT (NEPA) OF 1969

Recent court decisions under NEPA have clarified the role of the Government in the environmental impact field. The main thrust of these decisions is to place responsibility on individual Federal Agencies for the development of their own environmental research programs. This burden falls heavily on the Department of Transportation because of the fact that transportation is currently a major emitter of air pollution in the United States (see Section 2).

The three decisions which are pertinent here deal with the following points:

1. The requirement for agency research into environmental impact. (Case: EDF v. Hardin 2 ERC 1425, 1426 (D.D.C 1971).
2. The NEPA mandate of a rather finely tuned, systematic balancing of environmental factors in decision making. (Case: Calvert Cliffs v. AEC, 2 ERC 1779, 1781-82, 1788 (CA D.C. 1971).

TABLE 1. TIMETABLE FOR AIR POLLUTION ACTIONS AS REQUIRED BY LAW

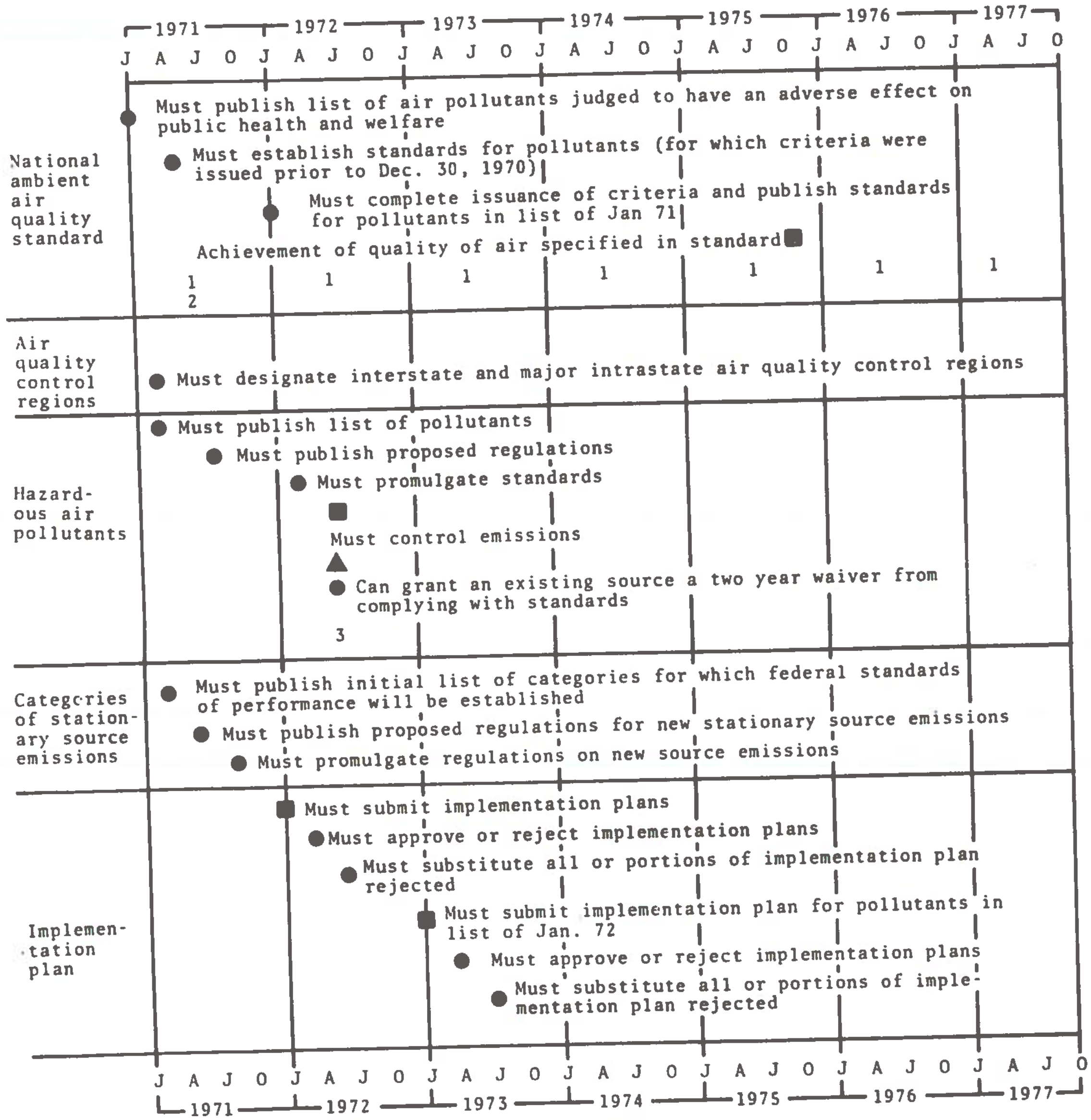
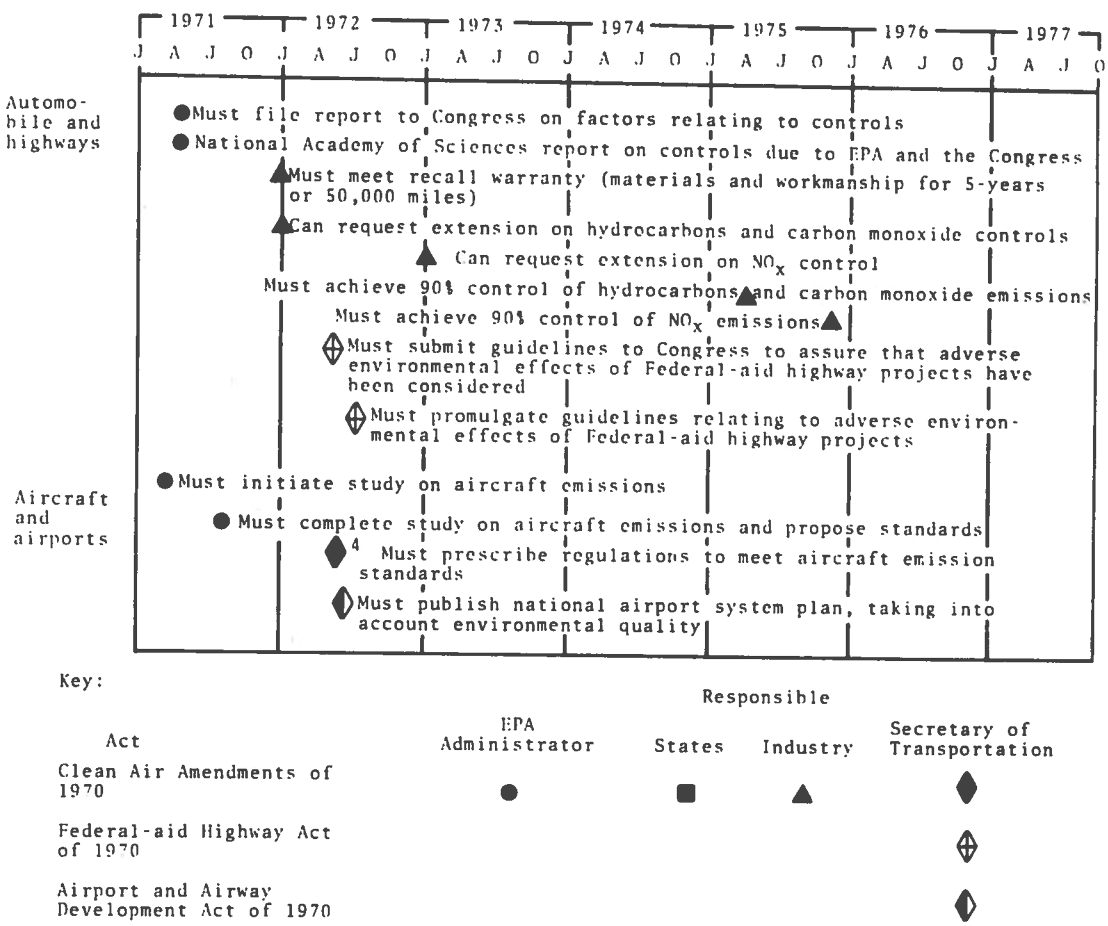


TABLE 1. TIMETABLE FOR AIR POLLUTION ACTIONS AS REQUIRED BY LAW (CONTINUED)



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1. The President's annual report on environmental quality required by the National Environmental Policy Act of 1969.
2. All agencies must propose to the President those measures required to bring their authority and policies into conformity with the National Environmental Policy Act of 1969.
3. Under the Clean Air Amendments of 1970, the President can exempt any stationary source from compliance with the standards for a period of two years or less. The exemption can be extended for one or more additional two year periods.
4. Date not specified in the Act.

3. Agency responsibility not to sit back like an umpire to resolve environmental issues others may raise, but rather to take the initiative itself in probing environmental considerations. (Case: same as 2).

1.4 THIS REPORT

The material for this report was obtained from an extensive survey of the literature, as well as from responses to the following Commerce Business Daily announcement placed by TSC. This announcement appeared in the CBD issue of December 21, 1971.

> "R--SOURCE SOUGHT, ANALYTIC CAPABILITY NECESSARY TO SUPPORT DEVELOPMENT, IN THE OPERATING DOT ADMINISTRATIONS, OF PROCEDURES FOR PLANNING DECISIONS RELATED TO TRANSPORTATION SYSTEM AIR POLLUTION. TSC is seeking firms with existing computer programs for modeling air pollution produced by transportation sources. Programs which compute the following quantities are of interest: wind field, stability indices, source emissions, pollutant dispersion and other related variables. TSC invites firms with operating computer programs either developed for, or readily adaptable to, the modeling of transportation source air pollution to submit their program specifications. TSC will only consider information about a firm's existing computer programs if it is submitted on a TSC questionnaire.
>
> Requests for this questionnaire should be addressed to:
> Department of Transportation
> Transportation Systems Center
> Information Sciences Division, Code TCD
> 55 Broadway, Cambridge, MA 02142
>
> For identification purposes requests for the questionnaire should cite Code MAP-01. Supplemental material may be submitted with the questionnaire, but is not required. The closing date for submission is 14 Jan 72.
>
> In this questionnaire firms will be required to state that the information submitted is not proprietary and must further agree that the Government is free to make any use of said

information it deems appropriate, including publication with proper acknowledgements in Government technical reports.

This is not a request for proposal. Firms which are deemed qualified to support TSC's program in this field will be considered if and when requests for proposals are solicited. No formal results of the evaluation of responses to this request will be furnished." (R351)

The questionnaire cited was used in order to assure that the same information would be obtained from each respondent. In order to clarify the level of detail and the format desired, a sample completed questionnaire for a hypothetical model was furnished to each firm responding to the announcement. The questionnaire called for specific information on the following topics:

I. General Description of the Model
II. Flow Diagram of the Model
III. Implementation of the Model
IV. Program Operation
V. Validation

Both the questionnaire and the sample appear in Appendix A.

It was felt that a public announcement of this type was the surest way to give all potentially interested sources an equal opportunity to make their capabilities known to the Government. This decision was more than vindicated by the magnitude of the response. Seventy-one (71) firms requested copies of the questionnaire, and 44 completed questionnaires were returned to TSC. Thirty four (34) of the completed questionnaires pertained to dispersion models.

The body of this report consists of five sections. Section 2 summarizes air pollution facts and standards. The dispersion models which have been used to analyze air pollution are discussed in Section 3. The computational aspects of these models, including input, hardware and software requirements, and output are treated in Section 4. A variety of applications of the models to both transportation and non-transportation pollution problems are described in Section 5. Finally, Section 6 examines the validation of the models with real-world data.

2.0 AIR POLLUTION FACTS AND STANDARDS

Table 2 summarizes the EPA data[1] on air pollution emissions in the United States for the year 1969. Of the 281.2 million tons emitted into the atmosphere during that year, transportation accounted for 144.4 million tons or 51.4%. The principal source of transportation-generated air pollution is the motor vehicle, as Table 3 shows. Note that the motor vehicle contributed 44.2% of the total U.S. emissions and 86.1% of all transportation emissions in the year 1969. However, these 1969 motor vehicle emissions are slightly lower than those of the previous year, thus indicating that the peak emission year from this source may have already been reached (probably due to the fact that newer model cars with emission control devices are replacing older models without such controls).

It should be noted that statistics on pollutants in terms of tons emitted give no information about their geographic distribution or concentration. However, it is the concentration of pollutants at a particular place which determines the level of hazard to public health and public welfare, and it is in terms of concentrations that the national air quality standards are stated. The dispersion models considered in this report calculate the concentrations resulting from the transport and diffusion of pollutants in the atmosphere.

This Section deals with emission sources, emission products and national air quality standards.

2.1 EMISSION SOURCES

Emissions from stationary and mobile combustion sources in the United States have been extensively documented by EPA in a recent publication[2] and the material in this section is taken from that reference. Table 4 lists the principal pollutants emitted (without controls) by a number of the major sources in the U.S.

TABLE 2. ESTIMATED EMISSIONS OF AIR POLLUTANTS IN THE UNITED STATES, 1969

10^6 TONS

Source	CO	HC	NO_x	Particulates	SO_x	Source Total
Transportation	111.5	19.8	11.2	0.8	1.1	144.4
Fuel combustion in stationary sources	1.8	.9	10.0	7.2	24.4	44.3
Industrial processes	12.0	5.5	.2	14.4	7.5	39.6
Solid waste disposal	7.9	2.0	.4	1.4	.2	11.9
Miscellaneous	18.2	9.2	2.0	11.4	.2	41.0
U.S. Total	151.4	37.4	23.8	35.2	33.4	281.2

Source: Environmental Protection Agency.

TABLE 3. TRANSPORTATION CONTRIBUTION TO THE TOTAL AIR POLLUTION EMISSIONS IN THE UNITED STATES, 1969

	CO		HC		NO_x		Particulates		SO_x		Source Total		
	10^6 Tons	% of U. S. Total	10^6 Tons	% of U. S. Total	10^6 Tons	% of U. S. Total	10^6 Tons	% of U. S. Total	10^6 Tons	% of U. S. Total	10^6 Tons	% of U. S. Total	% of Transportation Total
Motor Vehicles	97.8	64.6	17.1	45.7	8.7	36.5	0.4	1.2	0.3	0.9	124.3	44.2	86.1
Aircraft	2.9	1.9	0.4	1.1	0.4	1.7	0.1	0.3	0.1	0.3	3.9	1.4	2.7
All Other Transportation	10.8	7.1	2.3	6.1	2.1	8.8	0.3	0.8	0.7	2.1	16.2	5.8	11.2
Transportation Total	111.5	73.6	19.8	52.9	11.2	47.0	0.8	2.3	1.1	3.3	144.4	51.4	100.0
U. S. Total	151.4	---	37.4	---	23.8	---	35.2	---	33.4	---	281.2	---	----

Source: Environmental Protection Agency

TABLE 4. EMISSIONS FROM TYPICAL STATIONARY AND MOBILE SOURCES[2]

Combustion Source	Principal Pollutants Emitted (without controls)				
STATIONARY	CO	HC	NO_x	Part.	SO_x
Coal Burning			X	X	X
Fuel Oil Burning			X	X(1)	X
Natural Gas Burning	X(2)	X(3)	X	X	
Incineration, Municipal, Multiple Chamber	X			X	
Incineration, Domestic, Single Chamber	X	X		X	
Incineration, Municipal, Conical Burners	X	X		X	
MOBILE					
Gasoline-powered Motor Vehicles	X	X	X		
Diesel-powered Trucks and Buses	X	X	X	X	X
Diesel-Powered Locomotives	X	X	X	X	X
Aircraft(4), Turbofan, Jumbo Jet	X			X	
Aircraft(4), Turbojet	X	X		X	
Aircraft(4), Piston, Transport	X	X		X	
Steamships, Underway			X		X
Steamships, In-Berth			X	X	X

(1) Not a major constituent in power plant emissions

(2) A major constituent for domestic and commercial heating only

(3) Not a major product of domestic and commercial heating

(4) Calculated for landing/take-off cycle which includes ground operations

2.1.1 Stationary Combustion Sources

Included in the category of stationary combustion sources are: steam-electric generating plants, industry, commercial and institutional buildings, domestic furnaces, and incineration. Coal, fuel oil, and natural gas are the major fossil fuels used for power and heating, accounting for 95% of the total heat energy in the United States. The burning of these fuels is a major source of NO_x, particulates and SO_x. Controls for particulate emissions are now being used. Emissions of sulfur oxides can be reduced by the use of low-sulfur fuels. Nitrogen oxide emissions are produced under conditions of high temperature combustion which tends to occur when the process is most efficient. These emissions are not controlled at present.

Approximately 50% of all waste generated in the United States is disposed of by burning in open or enclosed incinerators. Both gaseous and particulate emissions result from incineration, but the output is variable because of the heterogeneous character of the refuse being burned.

2.1.2 Mobile Combustion Sources

As mentioned previously, transportation is currently the largest source of CO, HC, and NO_x emissions in the United States (Table 2). The primary mobile source of these three pollutants is the gasoline-powered motor vehicle, a category which includes passenger cars, light-duty trucks and heavy-duty vehicles. Other lesser sources are aircraft, diesel-powered trucks and buses, locomotives,and ships.

Diesel engines are used by heavy duty trucks, buses and locomotives. These engines emit not only the three pollutants produced by gasoline-powered vehicles, but also significant amounts of particulates and SO_x. Particulates are emitted in the form of both black and white smoke, while SO_x arises because the sulfur content of diesel fuel is 10 times that of gasoline.

Aircraft engines are of two types: reciprocating (i.e. piston) and gas turbine, including turbofan, turboprop, turbojet and turboshaft. CO is the principal pollutant emitted by all aircraft engines except the turboprop. HC and particulates are also produced, with the amount depending upon the engine type.

Fuel oil is the principal fuel for both steamships and motor ships. (Steamships have steam turbines driven by an external combustion engine, while motor ships have diesel internal combustion engines). Ships generate one to two orders of magnitude more pollutants when in-berth than when underway, mainly because boilers are operated under reduced draft and at lower fuel rates - hence at lower efficiency - when ships are in port. NO_x, particulates and SO_x are the principal pollutants emitted by ships.

2.2 EMISSION PRODUCTS

In this section the five major pollutants: CO, HC, NO_x, particulates and SO_x are each discussed, briefly. The production of these constituents by transportation is emphasized and applicable emission standards are stated.

2.2.1 Carbon Monoxide, CO

CO is the most common and most widely distributed of all pollutants. It is the product of incomplete combustion. In amount, CO emissions exceed the combined emissions of all other pollutants (see Table 2). In the internal combustion engine the two factors that determine the total CO emissions are the concentration of CO in the exhaust and the exhaust volume[3], the former depending on the air-to-fuel ratio and the latter on the power output. These two factors combine in such a way that total CO emissions decrease as average route speed increases. Under the Clean Air Amendments of 1970, the CO emissions from light duty vehicles and engines manufactured during or after model year 1975 must be reduced by at least 90% in comparison to the standards applicable to 1970 model light-duty vehicles and engines.

Aircraft contribute less than 2% to the total U. S. emissions of CO (see Table 3). For jet aircraft, CO emission is highest during ground operations (taxiing, idling, queuing for take off or for a gate) where the engine is operating at minimum efficiency[4]. It is customary to only consider aircraft operations below 3500 feet in computing aircraft emissions. The EPA is currently developing proposed emission standards for aircraft engines as required by the Clean Air Amendments of 1970. Standards will be proposed for any air pollutant emitted by aircraft engines which is adjudged to pose a hazard to public health or welfare.

2.2.2 Hydrocarbons, HC

Air pollution problems associated with these constituents are not due to hydrocarbons, themselves, but rather are caused by the products of their photochemical reactions in the atmosphere under the influence of sunlight. The ultimate products of photooxidation of hydrocarbons in urban air, after sufficiently long irradiation by sunlight, would be carbon dioxide and water vapor[5]. However, the products which produce photochemical air pollution all occur at intermediate stages in the photooxidation process. These products vary widely in reaction rate. The photochemical constituents which have the longest lives and highest concentrations in the atmosphere are ozone, nitrogen dioxide, aldehydes, and the peroxyacyl nitrates of which the most abundant is peroxyacetyl nitrate (PAN).

Hydrocarbon pollutants result primarily from the inefficient combustion of fuels, especially gasoline. For automobiles without emission controls, 60% of the unburned hydrocarbons comes from the exhaust, 20% from crankcase blow by and 20% from fuel tank and carburetor evaporation[6]. In the case of aircraft jet turbine engines, the main source of unburned hydrocarbons is the exhaust. These emissions are most serious at low power settings where the combustion efficiency of the turbine engine is low. However, it should be noted that aircraft hydrocarbon emissions account for only about 1% of the U. S. total (Table 3) and hence are negligible, except in the immediate vicinity of airports.

Under the Clean Air Amendments of 1970, the HC emissions from light duty motor vehicles and engines manufactured during or after model year 1975 must be reduced by at least 90% in comparison with the standards applicable to 1970 model light-duty vehicles and engines.

2.2.3 Oxides of Nitrogen, NO_x

The oxides of nitrogen which cause air pollution occur as NO and NO_2 [7]. Nitric Oxide, NO, is the primary product of high temperature combustion in automobile engines and furnaces. Nitrogen Dioxide, NO_2, is produced by the chemical reaction of nitric oxide and oxygen, as well as by other reactions involving NO, O_2 and NO_3. During daylight hours the atmospheric NO_2 photolytic cycle governs the interactions between NO and NO_2 under the influence of ultraviolet energy. When generated by combustion, NO_x consists mainly of NO which is then oxidized to NO_2.

It is interesting to note that NO_x emissions from internal combustion engines can be effectively minimized by reducing the air-fuel ratio (which will lower the combustion temperature, since more heat is required to warm the incoming excess fuel and hence less heat is available for combustion of gases in the chamber[6]). However, such a fuel-rich mixture would produce greatly increased emissions of both CO and HC. An alternative procedure would be to use a very high air-fuel ratio which, theoretically at least, would minimize the emissions of NO_x, CO and HC, simultaneously. However, such a fuel-lean mixture would cause operating difficulties (including stalling and misfiring) with presently available engines which, in turn, would actually result in high emissions of CO and HC, as well as poor performance.

The Clean Air Amendments of 1970 require that NO_x emissions from light-duty motor vehicles and engines manufactured during or after model year 1976 must be reduced by at least 90% in comparison to the average emissions of oxides of nitrogen actually measured from light-duty vehicles manufactured during model year 1971.

2.2.4 Particulates

Transportation contributes only about 2% of the total particulate emissions in the United States (Table 3). The bulk of particulate emissions results from fuel combustion in stationary sources, industrial processes, and incineration. Most atmospheric particles range between 0.1 and 10μ in diameter and are generally classified as aerosols. Particles occurring in motor vehicle exhaust include lead compounds, carbon particles, motor oil, and nonvolatile products formed from motor oil in the combustion zone[8]. Particulates discharged through the blowby are mainly unchanged lubricating oil. Tests at cruising speeds have shown that: concentrations of particulates in dilute exhaust range from 40 to 52 μg/liter; at unit density 62 to 80% of these particles have diameters below 2μ; and the lead content averages 40% of the total particulate emissions.

At present, because of the relatively small production of particulates by transportation, there are no transportation-related standards for this source.

2.2.5 Sulfur Oxides, SO_x

Transportation emits negligible amounts of the sulfur oxides. The principal emitters of these pollutants are industry, electric utilities, refineries, ore smelters and other similar sources. In the case of aircraft, SO_2 emissions have been minimized by the use of low-sulfur fuel. In fact, a recent survey of emissions within the Boston Metropolitan Air Pollution Control District shows that aircraft contribute only 0.1% of the total SO_2 emissions[4]. Nationwide SO_x emissions by motor vehicles are similarly low, accounting for less than 1% of the total emissions of SO_x in the U. S. (Table 3).

Because transportation produces so little SO_x, there are presently no transportation-related standards for this source.

2.3 AIR QUALITY STANDARDS

Under the Clean Air Amendments of 1970 the EPA Administer was made responsible for publishing, "proposed regulations prescribing a national primary ambient air quality standard and a national secondary ambient air quality standard for each pollutant for which air quality criteria have been issued." National primary ambient air quality standards are those judged necessary to protect public health, while the secondary standards are those judged necessary to protect the public welfare from known, or anticipated, adverse effects of air pollution.

Such primary and secondary standards have now been established for CO, HC, NO_2, photochemical oxidants, particulate matter and SO_2 [9]. Each standard specifies an averaging time, frequency, and concentration. The averaging times are 1, 3, 8, and 24 hours, and 1 year. These standards are stated in Table 5. The frequency parameter column specifies either the annual maximum concentration for averaging times of 24 hours or less, or the arithmetic or geometric mean for a 1-year period. The standards require that the maximum concentrations are not to be exceeded more than once per year.

A methodology for relating measured air pollution concentrations to the air quality standards has been developed by R. I. Larsen [10].

Under the Clean Air Amendments of 1970 the EPA Administrator has responsibility for designating interstate, and major intrastate, air quality control regions. Examples of such regions[11] are shown in Table 6. Note that these major regions are quite large, encompassing many townships, cities or counties. Each State was required to submit an implementation plan to the EPA Administrator by January 1972 that showed how the national primary and secondary air quality standards will be met in all its air quality control regions by the year 1975. This plan may have been supported by a measurement program to determine current emission levels; a statement of proposed control procedures and an estimate of their impact on future emissions; and an assessment of what additional control measures, if any, are required to meet the air quality standards.

TABLE 5. NATIONAL PRIMARY AND SECONDARY AMBIENT AIR QUALITY STANDARDS

Pollutant	Type of Standard	Averaging time	Frequency Parameter	Concentration µg/m³	ppm
Carbon monoxide	Primary and secondary	1 hr 8 hr	Annual maximum[a] Annual maximum	40,000 10,000	35 9
Hydrocarbons (nomethane)	Primary and secondary	3 hr (6 to 9 a.m.)	Annual maximum	160[b]	0.24[b]
Nitrogen dioxide	Primary and secondary	1 yr	Arithmetic mean	100	0.05
Photochemical oxidants	Primary and secondary	1 yr	Annual maximum	160	0.08
Particulate matter	Primary	24 hr 24 hr	Annual maximum Annual geometric mean	260 75	-- --
	Secondary	24 hr 24 hr	Annual maximum Annual geometric mean	150 60[c]	-- --
Sulfur dioxide	Primary	24 hr 1 hr	Annual maximum Arithmetic mean	365 80	0.14 0.03
	Secondary	3 hr 24 hr 1 yr	Annual maximum Annual maximum Arithmetic mean	1,300 260[d] 60	0.5 0.1[d] 0.02

[a]Not to be exceeded more than once per year.

[b]As a guide in devising implementation plans for achieving oxidant standards

[c]As a guide to be used in assessing implementation plans for achieving the annual maximum 24-hour standard.

[d]As a guide to be used in assessing implementation plans for achieving the annual arithmetic mean standard.

Source: Environmental Protection Agency[9]

TABLE 6. AN EXAMPLE OF AN AIR QUALITY CONTROL REGION DESIGNATED BY EPA[11]

a. Metropolitan Boston Intrastate Air Quality Control Region. The Metropolitan Boston Intrastate Air Quality Control Region (Massachusetts) consists of the territorial area encompassed by the boundaries of the following jurisdictions or described area (including the territorial area of all municipalities (as defined in section 302(f) of the Clean Air Act, 42 U. S. C. 1857h(f) geographically located within the outermost boundaries of the area so delimited):

In the State of Massachusetts:

CITIES

Beverly.	Medford.
Boston.	Melrose.
Brockton.	Newton.
Cambridge.	Peabody.
Chelsea.	Quincy.
Everett.	Revere.
Gloucester.	Salem.
Lynn.	Somerville.
Malden.	Waltham.
Marlborough.	Woburn

TOWNSHIPS

Abington.	Easton.	Middleton.	Stoneham.
Acton.	Essex.	Millis.	Stoughton.
Arlington.	Framingham.	Milton.	Stow.
Ashland.	Hamilton.	Nahant.	Sudbury.
Avon.	Hanover.	Natick.	Swamscott.
Bedford.	Hanson.	Needham.	Topsfield.
Belmont.	Hingham.	Norfolk.	Wakefield.
Bolton.	Holbrook.	North Reading.	Walpole.
Boxborough.	Holliston.	Norwell.	Watertown.
Braintree.	Hopkinton.	Norwood.	Wayland.
Bridgewater.	Hudson.	Pembroke.	Wellesley.
Brookline.	Hull.	Randolph.	Wenham.
Burlington.	Ipswich.	Reading.	West Bridgewater.
Canton.	Lexington.	Rockland.	Weston.
Cohasset.	Lincoln.	Rockport.	Westwood.
Concord.	Lynnfield.	Saugus.	Weymouth.
Danvers.	Manchester.	Scituate.	Whitman.
Dedham.	Marblehead.	Sharon.	Wilmington.
Dover.	Marshfield.	Sherborn.	Winchester.
Duxbury.	Maynard.	Southborough.	Winthrop.
East Bridgewater.	Medfield.		

3.0 MODELING THE DISPERSION OF POLLUTANTS

A dispersion model may be defined as a mathematical structure which accepts data on source emissions, meteorological conditions, geographic boundaries, etc. as inputs; computes the dispersion of pollutants by the atmosphere (as well as chemical reactions and removal by sinks where appropriate); and produces output data on the concentration of pollutants over the area of interest for specified time periods. The model is thus a mechanism for translating emission data into air quality data and, as such, is an invaluable tool for environmental impact analysis.

The problem is to calculate the environmental impact (in terms of pollutant concentrations) of a particular transportation system operating in a prescribed manner. Input data for such problems are of two types: variable and fixed. The variable inputs are those which affect emissions (e.g. traffic density, traffic speed and vehicle mix). The fixed data define the physical environment into which pollutants are emitted. These include the geography, topography, meteorology*, and background pollution** of the area under study.

The environmental impact of transportation is both local and regional in scale. Local effects, consisting of pollutant concentrations greater than the background level, are felt within a few thousand feet of the transportation system (i.e. within 2000 feet of a roadway[12,13] or within one mile of an airport[14,15]). Regional air pollution from transportation occurs as a result of the action of sunlight on hydrocarbons over a period of several hours which produces such photochemical products as ozone, nitrogen dioxide and peroxyacetyl nitrate (PAN), the constituents of photochemical smog. Roadways are the principal transportation source

*Of course it is the statistics of meteorological variables that are fixed (i.e. stationary), not the variables themselves.

**The existing level of pollution from sources other than the transportation system(s) being analyzed.

for this type of pollution since motor vehicles emit 86% of all the hydrocarbons produced by transportation (Table 3). In modeling local pollution it may be necessary to take into account the turbulence generated by the vehicles, themselves. This effect is certainly important at the edge of a roadway or runway. Farther away from the source, atmospheric dispersion predominates. In modeling the pollution distribution over a region the combined effects of dispersion and photochemical reactions must be considered.

A dispersion model can be used to compute the pollutant concentrations produced by any existing, or projected, transportation system as a consequence of the implementation of any desired operating strategy. Here we distinguish between the physical identity of the system --- e.g. a highway plus its vehicles --- and the manner in which the system operates --- e.g. highway speed limits, vehicle restrictions, and traffic control procedures. It is clear that the environmental impact of a transportation system can be minimized by adopting the proper operating strategy, or mix of strategies. Three categories of operating strategies can be identified:

1. Vehicle strategies which modify the vehicle (usually its engine) in order to reduce its emissions. The use of control devices for light-duty motor vehicle emissions (as required to meet the 1975 standards for CO and HC, and the 1976 standards for NO_x as prescribed in the Clean Air Amendments of 1970) is a vehicle strategy.
2. System strategies which operate on groups of vehicles in the system. These are of three types:
    a. Measures which regulate the entry of vehicles into the system,
    b. Controls which govern the flow of vehicles within the system, and
    c. Policies which influence the point at which vehicles exit from the system.

3. Intermodal strategies which deal with interrelations among two or more transportation systems. An example is a personal rapid transit (PRT) system such as UMTA's Demonstration A at Morgantown, West Virginia[16,17] which provides an alternative to automobile travel.

We will now proceed to a detailed discussion of dispersion models which have been used to analyze air pollution.

3.1 TYPES OF MODELS

Dispersion models are of two broad types:

1. Physical models which simulate atmospheric motions in wind tunnels[18], or which make use of irradiation reaction chambers for simulating photochemical processes in smog[19], and
2. Mathematical models based on equations which represent atmospheric and photochemical processes.

This paper only deals with mathematical models since these are by far the most widely used tools for air pollution analysis. Most mathematical models fall into one or more of the following categories:

1. Gaussian models which assume that the dispersion of pollutants can be represented by a Gaussian process,
2. Conservation of mass models which require the solution of the partial differential equations governing turbulent diffusion,
3. Box models[20] which assume that pollutant concentrations are homogeneous throughout a prescribed region,
4. Statistical methods which use regression theory to develop an empirical relationship between concentrations and emissions[21],
5. Solutions of differential equations representing photochemical processes[22], or
6. Solutions of the complete Navier-Stokes equations for turbulent fluid motions. These solutions contain the

field of turbulence, turbulent fluxes, and pollutant dispersion rates, computed from input data on the vertical profiles of temperature and mean wind speed in the atmospheric boundary layer.[23]

Reviews of the literature by myself and others[24] as well as the completed questionnaires returned to TSC, reveal that nearly all the dispersion models being used in the air pollution field today are either Gaussian or conservation of mass models. Table 7, which summarizes the 34 dispersion models reported in the TSC questionnaire, shows that 21 of these models are Gaussian, 10 are conservation of mass, 1 uses a combination of the two, and 2 are of other types. Consequently, the remainder of this report will mainly consider these two predominent types of air pollution models.

3.2 THE CLASSICAL GAUSSIAN MODELS

Gaussian techniques for modeling the dispersion of pollutants in the atmosphere, based upon the pioneering work of Taylor[25] and Sutton[26] as later developed by Cramer[27], Pasquill[28] and Guifford[29], are still the most widely-used tools in the field (see Table 7). In this section the various Gaussian equations are stated; methods of solution are discussed; and the limitations of these equations are examined.

3.2.1 The Gaussian Puff Model

The Gaussian Puff equation is considered first since all other Gaussian equations can be derived from it. This equation deals with the instantaneous emission of a finite puff of material from a point source at height H. The concentration, $\chi_1(x,y,z,t)$, of material is expressed by the equation:

$$\chi_1(x,y,z,t) = \frac{Q}{(2\pi)^{3/2}\,\sigma_x\sigma_y\sigma_z}\,\exp -\left[\frac{(x-\bar{u}t)^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2}\right] \cdot \left\{\exp -\left[\frac{(z-H)^2}{2\sigma_z^2}\right] + \exp -\left[\frac{(z+H)^2}{2\sigma_z^2}\right]\right\} \quad (1)$$

TABLE 7. DISPERSION MODELS CURRENTLY OPERATING

Company	Type of Model: Gaussian	Type of Model: Conservation of Mass	Type of Model: Other	Emission Source
Aeronautical Research Associates of Princeton Inc.			Complete Navier Stokes	Airport
Argonne National Lab (1)	x	x		Airport
Argonne National Lab (2)	x			Region
Argonne National Lab (3)	x			Single Source
Argonne National Lab (4)	x			Area, Point
AVCO Systems Division	x			Point Source Jet
Battelle, Columbus Labs	x			Point
Boeing Computer Services Inc.	x			Airport
Center for the Environment and Man Inc. (1)		x		Arbitrary Array
Center for the Environment and Man Inc. (2)	x			Point
Computer Sciences Corporation	x			Airport, Highway
Environmental Research and Technology Inc. (1)	x			Airport, Highway
Environmental Research and Technology Inc. (2)		x		Airport, Highway
ESL Inc.	x			Airport, Highwav
Euclid Research Group			Global Balance	Nuclear Explosion

TABLE 7. DISPERSION MODELS CURRENTLY OPERATING (CONTINUED)

Company	Type of Model: Gaussian	Type of Model: Conservation of Mass	Type of Model: Other	Emission Source
General Research Corporation (1)		x		Highway
General Research Corporation (2)		x		Airport, Highway
GEOMET INC	x			Urban Area, Point
Grumman Aerospace Corporation	x			Airport, Highway
IBM-FSD	x			Roads
INTERCOMP		x		Highway
Kaman Sciences Corporation	x			Highway
Lockheed, Huntsville	x			Point, Line, Area
Mt. Auburn Research Assoc.	x			Nuclear Explosion
Northern Research and Engineering	x			Airport
Pacific Environmental Services Inc.		x	Chemical Kinetics	Any Vehicle
Systems Applications Inc.		x		Airport, Highway
Systems Control Inc.		x		Point, Line
Systems, Science and Software (1)		x		Airport, Highway
Systems, Science and Software (2)		x		Highway
Texas Instruments Inc.	x			Point, Area
TRC	x			Point,Line,Area
Walden Research Corporation	x			Area, Point
Westinghouse Research Labs	x			Point

Q, amount of material emitted (g).

x, y, z, Cartesian coordinates with positive x being the downwind direction

t, time since emission of the puff

$\bar{u}$, mean wind transporting the material

$\sigma_x, \sigma_y, \sigma_z$, standard deviations of the material concentration distribution in the three coordinate directions relative to the puff center with origin ($\bar{u}t$, o, H)

Figure 1 shows a conceptual sketch of the Gaussian puff model. Note the Gaussian character of the component distributions of pollutant material.

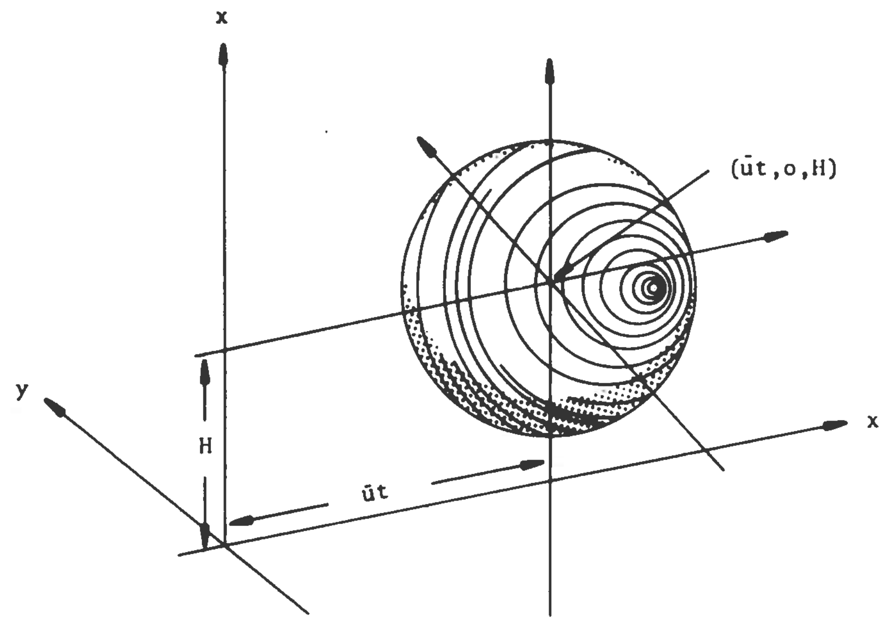
3.2.2 The Gaussian Plume Model

Continuous emission from a point source may be regarded as an infinite series of puffs which spread out into a continuous plume (see Figure 2). Thus, the Gaussian Plume equation is the steady state version of the Gaussian Puff equation and is derivable by integrating Equation 1 with respect to time and keeping σ_x constant as the puff passes any point:

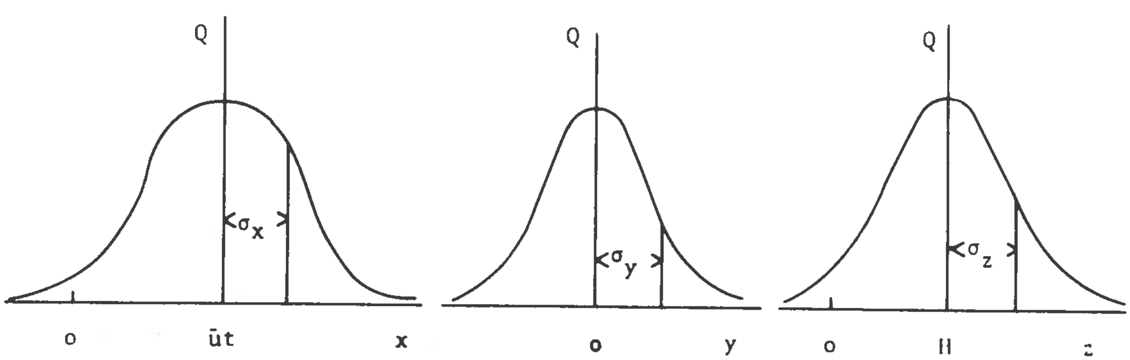
$$\chi_2(x,y,z) = \int_{-\infty}^{\infty} \chi_1(x,y,z,t)dt$$

$$= \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp - \left[\frac{y^2}{2\sigma_y^2}\right]$$

$$\cdot \left\{ \exp - \left[\frac{(z-H)^2}{2\sigma_z^2}\right] + \exp - \left[\frac{(z+H)^2}{2\sigma_z^2}\right] \right\} \qquad (2)$$

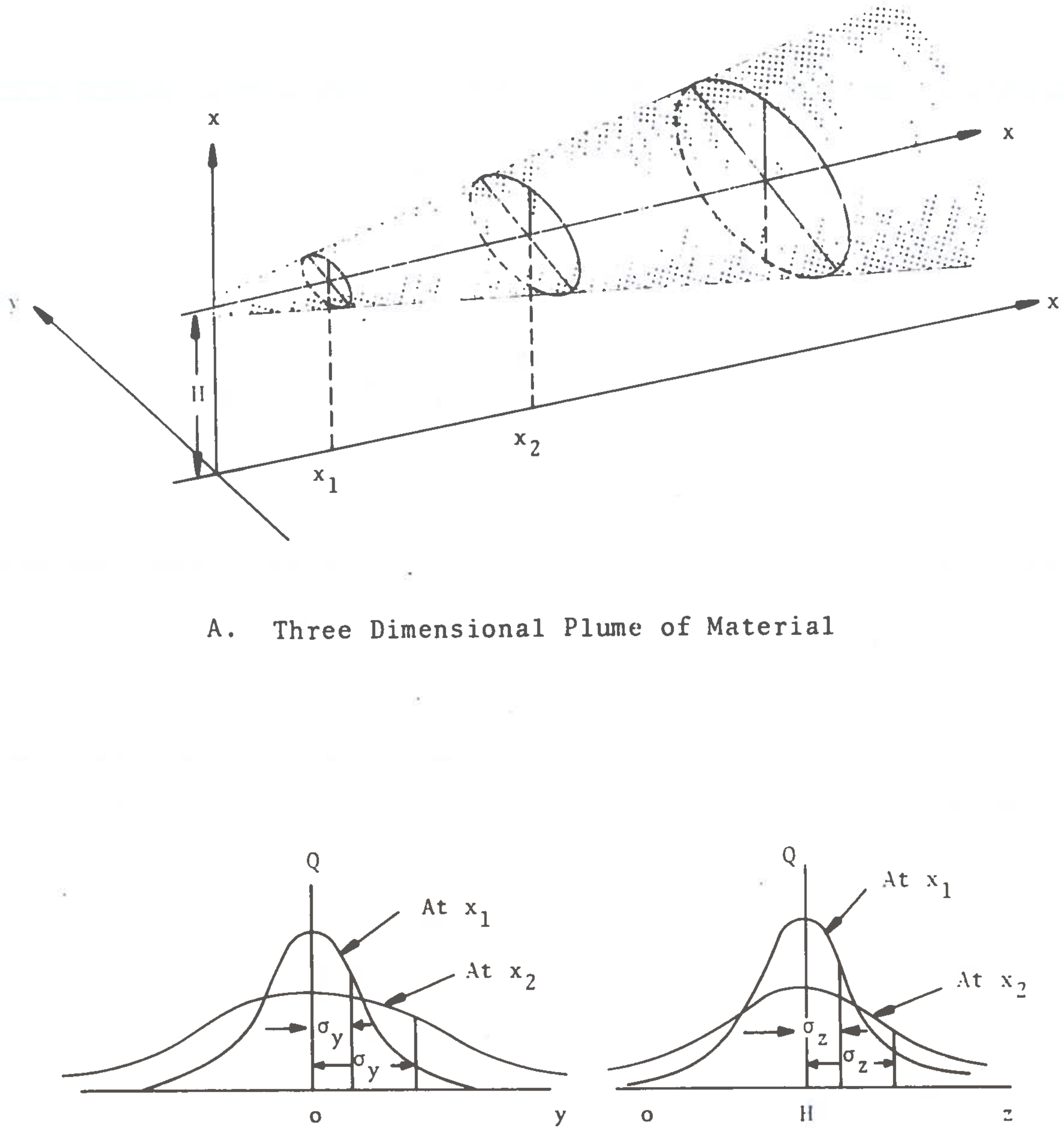


A. Three Dimensional Puff of Material



B. Component Distributions of Material about Axes through ($\bar{u}t$,o,H)

Figure 1. Schematic Representation of the Gaussian Puff Model



A. Three Dimensional Plume of Material

B. Component Distribution of Material About (x_1,o,H) and (x_2,o,H)

Figure 2. Schematic Representation of the Gaussian Plume Model

where Q is now the source emission rate of material (g/sec)

x is in the downwind direction along the plume axis

σ_y, σ_z are standard deviations of the material concentration distribution in the y and z directions relative to the plume axis

The Gaussian Plume equation can readily be modified to handle both linear and area sources as shown below.

3.2.3 The Gaussian Line Source Models

Consider a finite line at height H extending from y_1 to y_2, $y_1 < y_2$, perpendicular to the mean wind which blows in the x direction. The line emits at a constant rate, q, per unit length (g sec^{-1} m^{-1}). Then

$$\chi_3(x,y,0) = \frac{2q}{\sqrt{2\pi}\,\sigma_z \bar{u}} \exp - \left[1/2 \left(\frac{H}{\sigma_z}\right)^2 \right]$$

$$\int_{p_1}^{p_2} \frac{1}{\sqrt{2\pi}} \exp - \left(\frac{p^2}{2}\right) dp \qquad (3)$$

where $p_i = \frac{y_i}{\sigma_y}$, i = 1,2

If the finite line source is on the ground, as would be the case for a road or airport runway,

$$\chi_3(x,y,0) = \frac{2q}{\sqrt{2\pi}\,\sigma_z\, \bar{u}} \int_{p_1}^{p_2} \frac{1}{\sqrt{2\pi}} \exp -\left(\frac{p^2}{2}\right) dp \qquad (4)$$

If the line is of infinite length,

$$\chi_4(x,y,0) = \frac{2q}{\sqrt{2\pi}\,\sigma_z\,\bar{u}} \exp - \left[1/2\left(\frac{H}{\sigma_z}\right)^2\right] \quad (5)$$

If the infinite line is on the ground, there results the simple form:

$$\chi_4(x,y,0) = \frac{2q}{\sqrt{2\pi}\,\sigma_z\,\bar{u}} \quad (6)$$

Finally, if the wind is blowing at an angle ϕ (<45°) with respect to the infinite line, Equations 5 and 6 become

$$\chi_4(x,y,0) = \frac{2q}{\sin\phi\,\sqrt{2\pi}\,\sigma_z\bar{u}} \exp - \left[1/2\left(\frac{H}{\sigma_z}\right)^2\right] \quad (5a)$$

$$\chi_4(x,y,0) = \frac{2q}{\sin\phi\sqrt{2\pi}\,\sigma_z\bar{u}} \quad (6a)$$

3.2.4 The Gaussian Area Source Model

An area may be treated as a cross-wind line source with a normal distribution of material, σ_y. The area source is assumed to have an initial standard deviation, σ_{yo}. The area can be treated using Equation 2 by defining a virtual upwind distance for a point source which would produce the desired σ_{yo} at the initial position of the area source. The initial vertical variation of emissions due to the distribution of source heights is represented by an initial σ_{zo} which can also be handled by defining an upwind virtual point source at the proper distance.

3.2.5 Solution of the Gaussian Equations

The Gaussian equations are receptor oriented, which is to say that they are best suited to computing the concentrations of pollutants at specific locations due to emissions from a given source.

The principle of superposition is used to compute the concentration at a receptor of pollutants from multiple sources. If the number of source/receptor combinations is small, the problem can readily be solved using the graphs and nomograms in the reports by Taylor[30] and Beals.[31] On the other hand, large dispersion problems, involving multiple sources and many receptors, must be solved on a digital computer. If concentrations at a large number of receptors are required, the computation time can be reduced by calculating backward trajectories from each receptor and then determining the appropriate weighted contribution of all sources along that trajectory during the time period in question.

The Gaussian equations are not well suited to computing concentrations over a rectangular grid. On the other hand, the conservation of mass models to be described later are well suited for that purpose.

3.2.6 Limitations of the Gaussian Models

The simplicity of the classical Gaussian models has been achieved at the expense of assumptions which restrict their application to real-world dispersion problems. Various assumptions and resulting limitations are discussed below.

It should be noted that the downwind dimension x does not appear in Equation 2 although χ_2 is a function of x,y, and z. This is because the equation is derived in such a way that both σ_y and σ_z are functions of x, hence the dimension x is implicit. In turn, σ_y and σ_z are functions of atmospheric turbulence, topographic characteristics, wind speed, sampling interval, and other variables. In order to solve the equation, these complex dependencies must somehow be taken into account. The standard approach has been to define a set of five atmospheric stability classes in terms of quantities which are readily observable, namely surface wind speed and incoming solar radiation for daytime situations; or surface wind and degree of cloudiness for the night. For each stability class, $\sigma_y(x)$ and $\sigma_z(x)$ have been determined empirically. These relationships obtain for a sampling interval of ten minutes, for the lower several hundred meters of the atmosphere, and over flat terrain. Their use under other conditions, though frequently undertaken, is questionable.

The Equations 2 - 6 apply only to the continuous emission from a source, be it a point, line, or area. Also, dispersion in the downwind direction x is neglected. Therefore, the equations in their original form are not strictly applicable to many real-world problems, especially those involving transportation sources which tend to vary in both space and time. Furthermore, the equations deal only with the diffusion of stable gases or aerosols (i.e., particles of <20μ diameter) which are assumed to remain suspended in the atmosphere in the atmosphere indefinitely. Hence photochemical reactions are not considered. In addition, since mass continuity is maintained, the Gaussian equations require that no material be removed from the plume as it moves downwind (i.e. total reflection of the plume takes place at the earth's surface).

The requirement that a single mean wind $\bar{u}$ over the entire three dimensional area of concern be introduced to transport the emitted material is contrary to the known behavior of winds. In fact, it is known that the wind generally increases with height in the lower several hundred meters of the atmosphere, hence the use of a single mean wind will tend to result in an underestimate of concentrations at lower levels and an overestimate at higher levels. Also, since $\bar{u}$ appears in the denominator of Equations 2 - 6 it is apparent that all of these equations become unstable in the case of very light or calm winds.

Problems are posed by the existence of a temperature inversion, or stable layer, in the atmosphere which prevents the upward spread of pollutants. The region below such an inversion is called the mixing layer (since, in general, the atmosphere is completely mixed by turbulence in such a layer) and the inversion is called the mixing level. When such conditions exist, the equations are modified in such a way that the plume material distribution in the vertical becomes uniform at a certain distance downwind from the point where the plume encounters the mixing level. The distribution in the horizontal remains Gaussian.

Also, the use of the superposition principle is questionable in the case of turbulent atmospheric flow.

3.2.7 Modern Improvements in the Gaussian Equations

Some of the limitations cited above have been minimized by improvements in the basic Gaussian equations. A number of these improvements were reported in the TSC questionnaires returned by current investigators. One problem not solved by anyone, however, is how to improve the representation of σ_y and σ_z as functions of x and stability. The approach reported by Turner is still universally used. Also, emission rates are still considered constant although great sophistication in representing emissions is evidenced by many investigators. These will be reported in the section on input data.

The Gaussian Plume equation has been modified to include an exponential half-life decay function for inert gases and/or a settling time for particles. (With these changes the equation of mass continuity for the plume is only satisfied when these sinks are taken into account). Two investigators have succeeded in incorporating photochemical reactions into the Gaussian formulation, one by a hybrid scheme using a finite difference algorithm to treat the chemical kinetics (C. Michael Hogan, ESL Inc.) and the other by introducing arbitrary functions of time to represent simple chemical reactions (P. J. Cefola, Computer Sciences Corporation).

Several versions of the Gaussian Plume equation have replaced the single constant transport wind $\bar{u}$ with a vertical wind profile obtained either from actual measurements, or from an assumed power law function of height. Also, in some models a new wind is entered periodically (typically every one or two hours) so that changes in the plume axis with time can be taken into account.

3.3 THE CONSERVATION OF MASS EQUATION

A number of investigators have adopted a more fundamental approach to the dispersion problem by attempting to solve the equations governing the conservation of pollutant mass. Table 7 contains the names of companies which reported their efforts in this direction by submitting completed TSC questionnaires. In the literature, work on the conservation of mass equations is described by Sklarew[32], Eschenroeder and Martinez[33], Roth et al[34] and Egan and Mahoney[35].

The general conservation equation for a particular pollutant may be written in vector form, as follows:

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot (\vec{V} c_i) + \nabla \cdot (D \nabla c_i) + R_i + S_i \qquad (7)$$

with c_i concentration of species i

$i = 1,2,3...p$ species

$\vec{V}$, the wind velocity with components u,v, and w in the x,y, and z directions

$$\nabla = \frac{\partial}{\partial x} \vec{i} + \frac{\partial}{\partial y} \vec{j} + \frac{\partial}{\partial z} \vec{k}$$

x, y, z, component directions

$\vec{i}$, $\vec{j}$, $\vec{k}$, unit vectors in directions x, y, z, respectively

D, molecular diffusivity tensor

R_i, rate of generation of species i by photochemical reactions

S_i, emission source strength for species i

Equation 7 governs changes in concentration of a particular species i at a point in the atmosphere. It states that the concentration change, $\frac{\partial c_i}{\partial t}$, is equal to the net effect of four processes: The advection (or transport) of pollutant, $\nabla \cdot (\vec{u} c_i)$; the molecular diffusion, $\nabla \cdot (D \nabla c_i)$, of pollutant; the change due to photochemical reactions, R_i; and the emission source strength, S_i, of the pollutant.

The concentration and the wind can be expressed in terms of turbulent deviations from their time-averaged values:

$$c_i = \overline{c}_i + c_i'$$

$$\vec{V}_i = \overline{\vec{V}}_i + \vec{V}_i'$$

thus

$$u_i = \overline{u_i} + u_i'$$

$$v_i = \overline{v_i} + v_i'$$

$$w_i = \overline{w_i} + w_i'$$

where bars above quantities denote time-averaged values and primes indicate turbulent eddy fluctuations.

By introducing the above expressions into Equation 7, taking time averages of each term, expanding, and rearranging terms the following equation is obtained for the conservation of mass of species i in a turbulent atmosphere:

$$\frac{\partial \bar{c}_i}{\partial t} + \frac{\partial (\overline{u c_i})}{\partial x} + \frac{\partial (\overline{v c_i})}{\partial y} + \frac{\partial (\overline{w c_i})}{\partial z} + \frac{\partial (\overline{u' c_i'})}{\partial x} + \frac{\partial (\overline{v' c_i'})}{\partial y} + \frac{\partial (\overline{w' c_i'})}{\partial z}$$

$$= D_i \left(\frac{\partial^2 \bar{c}_i}{\partial x^2} + \frac{\partial^2 \bar{c}_i}{\partial y^2} + \frac{\partial^2 \bar{c}_i}{\partial z^2} \right) + R_i + S_i \qquad (8)$$

In order to reduce Equation 8 to a form tractable for solution, the following assumptions are made:

1. Molecular diffusion is negligible in comparison to turbulent diffusion, hence $D_i = 0$.
2. Atmospheric flow is incompressible, hence

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0$$

3. The turbulent eddy diffusion coefficients K_x, K_y, K_z may be defined as follows:

$$\overline{u' c_i'} = -K_x \frac{\partial \bar{c}_i}{\partial x}$$

$$\overline{v' c_i'} = -K_y \frac{\partial \bar{c}_i}{\partial x}$$

$$\overline{w' c_i'} = -K_z \frac{\partial c_i}{\partial z}$$

Introducing these assumptions into Equation 8:

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}\frac{\partial \bar{c}_i}{\partial x} + \bar{v}\frac{\partial \bar{c}_i}{\partial y} + \bar{w}\frac{\partial \bar{c}_i}{\partial z}$$

$$= \frac{\partial}{\partial x}\left(K_x \frac{\partial \bar{c}_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \bar{c}_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \bar{c}_i}{\partial z}\right) + R_i + S_i \qquad (9)$$

Even further simplification can be achieved by introducing the following additional assumptions:

1. The horizontal wind field is a uniform flow in the x-direction,
2. The vertical velocity component $\bar{w}$ can be neglected, and
3. Horizontal eddy diffusion can be neglected.

With these assumptions Equation 9 reduces to:

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}\frac{\partial \bar{c}_i}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \bar{c}_i}{\partial z}\right) + R_i + S_i \qquad (10)$$

A salient feature of these equations is that they represent conditions over a three-dimensional grid and hence do not require the source-receptor formulation of the Gaussian equations. Instead, all sources enter cells of the grid and all concentrations are computed for those same cells. Thus, the model is spatially-oriented which greatly simplifies computations for a large number of sources since each additional source affects only a single cell (or at most a few cells).*

3.3.1 Solution of the Conservation of Mass Equations

There are two basic approaches to solving these equations: the fixed coordinate or Eulerian method, and the moving cell or Lagrangian method. In the Eulerian method, the air space is subdivided into a fixed three-dimensional grid with cells a few miles on a side in the horizontal and a few hundred feet in the vertical. The solution is obtained for each cell in this fixed grid at short intervals of time. In the Lagrangian method, columns of air are advected through the air space and solutions are obtained within the moving columns. There are many mathematical subtleties in both the Eulerian and Lagrangian solutions to these equations. Detailed discussions of this subject can be found in any of the four references at the beginning of this section. Application of these equations has only recently been undertaken, in contrast to the long history of Gaussian solutions.

3.3.2 Aspects of the Conservation of Mass Equations

It is instructive to examine the aspects of these equations which differentiate them from the Gaussian formulations. First, $\sigma_y(x)$ and $\sigma_z(x)$ are replaced by the diffusion coefficients K_x, K_y and K_z. Although the dependence on stability has been eliminated, the problem of estimating the diffusion coefficients remains. There is no completely satisfactory way of doing this. Some investigators appeal to theory, others rely on empirical methods, and still others attempt to compute these coefficients from the data.

The conservation of mass equations, because of their cellular structure, are able to accommodate variable emission rates.

*It should be noted that Donaldson and Hilst[23] use a somewhat different approach. Their equation is based upon the complete Navier-Stokes equations for turbulent fluid motions and includes terms describing the turbulent flux of pollutants. This is an even more general method than the simple conservation of mass approximation, but solution of the complete equations is a formidable computing task.

Typically, the assumption is made that emissions remain constant over a period of one hour or so. Furthermore, through the R_i terms, the equations handle photochemical reactions directly. The functional form and number of these reactions is at the discretion of the modeler and empirical data on the character and speed of such reactions can readily be incorporated in the model.

Another advantage of the grid structure is that a separate wind can be entered for each cell. (How such a three-dimensional distribution of winds is obtained is a subject for another section.) The wind field can be updated at every time step if the data are available. Also, the existence of a stable layer in the atmosphere poses no problem for the conservation of mass model. The mixing level can simply be defined as an impervious boundary condition (i.e., $K_z=0$). A change in the mixing level is handled in the same way at the appropriate time step.

In summary, then, it is clear that the conservation of mass model overcomes many of the limitations of the Gaussian models and hence is potentially a more powerful tool for analyzing air pollution problems.

4.0 IMPLEMENTATION OF THE MODELS

With the exception of the simple problems mentioned earlier where the Gaussian Plume model is used for a few source/receptor combinations (in which case graphs and nomograms can be applied), the solution of dispersion problems requires the use of digital computers. In fact, real-world problems must generally be solved on medium to large-scale computers of the IBM 360/50 class or greater. This section will examine, in detail, how the dispersion equations are solved, starting with the input data needed; proceeding to the software and hardware requirements; and ending with the output data produced.

The process of solving the dispersion equations can best be understood in terms of the simplified block diagram in Figure 3. Note that neither the source emission factors nor the meteorological data are entered directly into the model which computes pollutant dispersion and photochemical reactions. Instead, both are input to preprocessing routines which generate the data required by the dispersion model. The output consists of both listings and graphical representations of the input data; the results of intermediate computations; and the calculated concentrations at specified time intervals.

4.1 INPUT

The required input data are of five kinds: (1) Meteorological data which depict the state of the atmosphere; (2) Emission factors which specify the source characteristics; (3) Geographic and topographic data which delimit the airspace, prescribe the character of the terrain, and specify the locations of sources and receptors; (4) Data on background pollution from sources other than the one being analyzed; and (5) Control instructions which specify how the model is to be run.

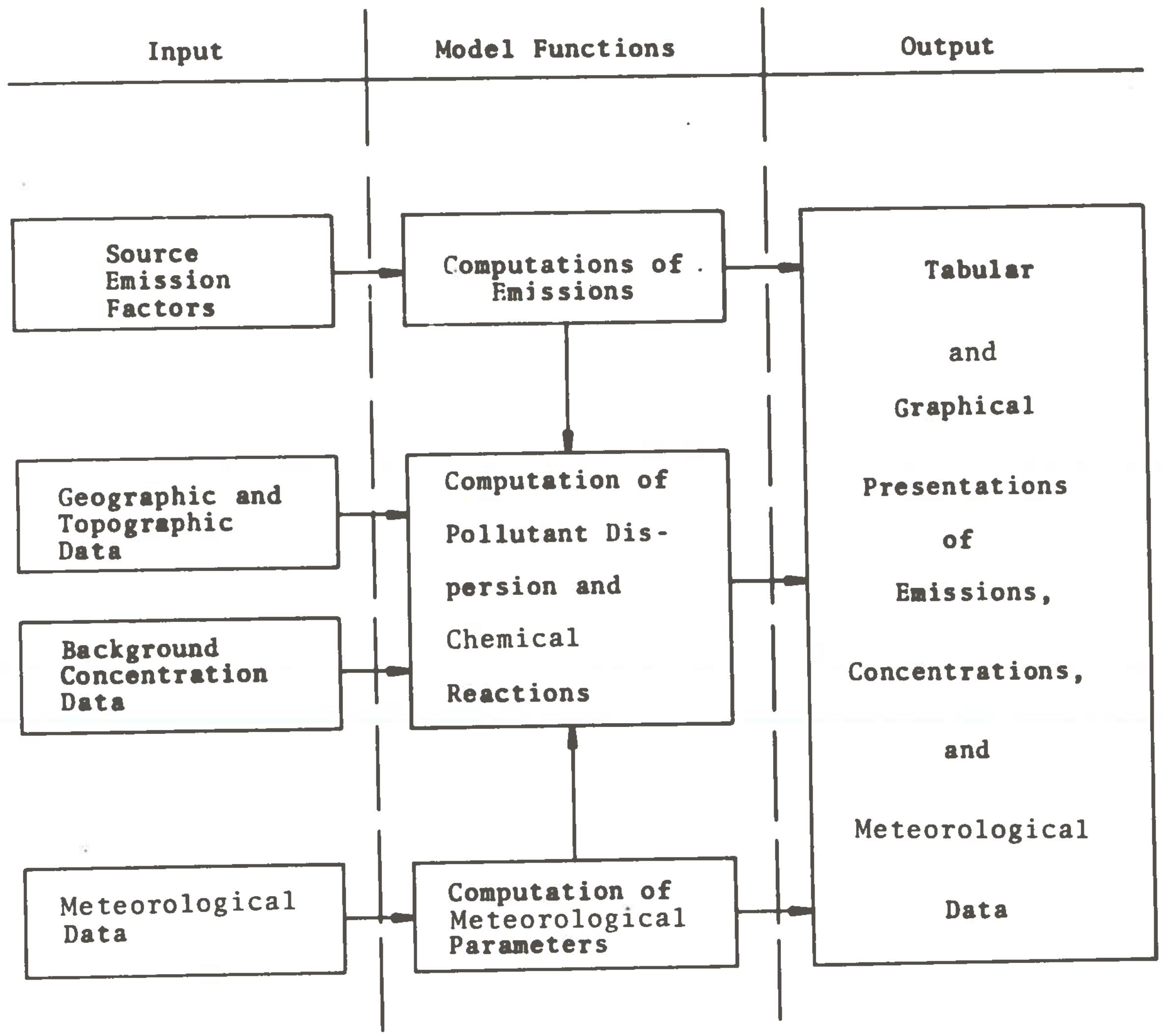


Figure 3. Solution of Dispersion Equations

4.1.1 Meteorological Data

The principal meteorological data needed are: winds, both at the surface and aloft; temperature lapse rates (i.e., variation of temperature with height); and observations of cloudiness. The winds are the mechanism for transporting and dispersing pollutants, while the temperature lapse rate is used to calculate the mixing level. For the Gaussian models the combination of surface wind and incoming solar radiation (or cloudiness) determines the stability class which is required in the solution. The conservation of mass models require meteorological data on a three-dimensional grid.

Surface weather observations of cloudiness, wind, temperature and other variables are routinely made at stations throughout the United States (which are typically separated by tens of miles). Such observations are recorded each hour, or more frequently in times of rapidly changing weather. On the other hand, soundings of the upper atmosphere which measure temperatures and winds, among other variables, are made only twice daily (at 0000z and 1200z; z = Greenwich Meridian Time) at about 50 stations in the United States. Additional data on winds aloft only are provided by weather stations which take PIBALS (Pilot Balloon Soundings). Also, the National Weather Service has assigned an air pollution meteorologist to major cities who makes special wind soundings, strictly for air pollution purposes. For example, in St. Louis two soundings a day are made for this purpose and even more frequent soundings are taken during alert conditions. It is thus apparent that the meteorological data lack the fine scale which is required for dispersion modeling over small areas. This is especially true when the conservation of mass models, which require data for many cells in a 3-dimensional grid, are used; less true when the Gaussian models, which use a single transport wind in many of the equations, are applied.

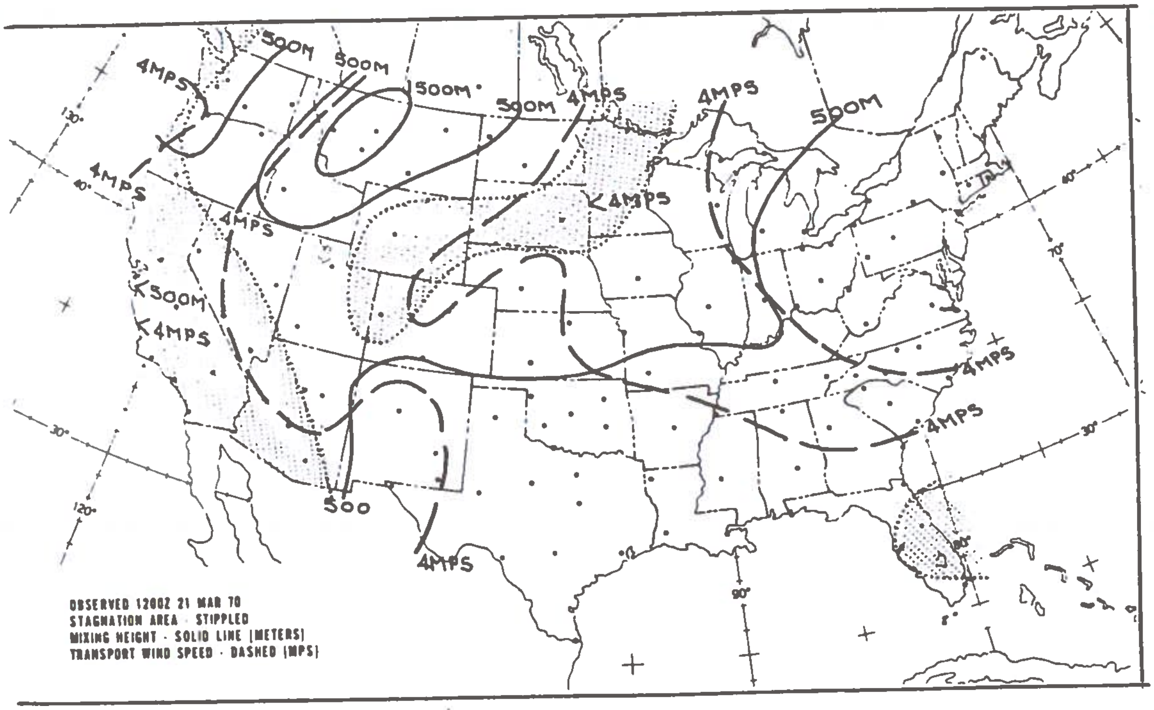
How, then, is the fine-scale wind field obtained in the cases where it is required? Three techniques are reported in the literature, all of which produce a field of streamlines and isopleths (of speed) as an intermediate step to obtaining the winds for individual grid cells. The first[36] is done by a completely manual analysis; the second[37] involves a computer solution of the equations of continuity, momentum, energy and state; the third[38] derives the wind field as a function of local topography and differential heating using the principle of mass conservation. All of these methods produce a two-dimensional wind field at some "representative" level of the atmosphere. The problem of extending the solution to three dimensions has not yet been satisfactorily solved. Various attempts have used: assumed, constant, functions of height, or continuity-derived winds aloft —— none of which can be verified due to the absence of observations. In any event the final step (after the three-dimensional field has somehow been defined) is to obtain winds for each grid cell by interpolation.

When only a single transport wind is required, the existing meteorological data are generally adequate. This is true because time and space averaged winds are known to be slowly varying. The single transport wind is generally used when solutions of the Gaussian Plume equations are desired over a period of one, or a few, hours. This mean wind is usually computed from surface data. Alternatively, when Gaussian solutions are required for a period of several months to a year, the wind rose approach is generally used in which the equations are solved for a representative set of wind direction/wind speed combinations weighted according to frequency of occurrence. The meteorological data is again adequate to support this application since climatological surface wind records dating back 50 years or more are available for most stations in the United States. The question of whether the surface wind is a representative transport wind for the mixing layer remains, however, in both of the above approaches. Some investigators have attempted to overcome this limitation by using an upper level wind field derived from the surface wind by a power function of height.

How, then, is the mixing level determined? Unlike the wind which is a reasonably well behaved function of space and time, the mixing level is very much a local phenomenon which is influenced by cloud cover, time of day, mixing processes in the atmosphere, and other meteorological factors. It is very difficult to predict, mainly because it is not adequately measured due to the wide spacing of sounding stations. The standard approach involves use of the nearest 1200z temperature lapse rate (i.e., the early morning sounding for the United States) in conjunction with a prediction of the maximum surface temperature, under the assumption that the lapse rate above the early morning temperature inversion remains unchanged. The intersection of the dry (or wet, if appropriate) adiabatic lapse rate passing through the predicted maximum temperature, with the morning inversion is the predicted afternoon mixing level. The pitfalls in this procedure are almost too numerous to mention. To name a few: the morning sounding may be too far away from the area of interest to be representative or the sounding may change during the day; the prediction of the maximum temperature may be in error; the improper adiabatic lapse rate may be used in the mixing layer, etc. Dispersion solutions over short periods of a few hours are susceptible to large errors due to these uncertainties in estimating the mixing height, whereas long-term solutions for several months up to a year are less vulnerable since reliable climatological values of mixing height are available for these applications.

The National Weather Service now transmits via facsimile a daily forecast map of air pollution quantities for the United States. An example of this product is shown in Figure 4. The stippled stagnation areas are regions where low winds, stable atmospheric conditions and (often) fog in the mixing layer are all predicted to occur simultaneously. These are the areas most conducive to the occurrence of air pollution. The map also contains isopleths of mixing level and transport wind speed. An analysis of predicted high air pollution days over the United States for a ten-year period is shown in Figure 5. Note that these conditions are concentrated in the Appalachian region and in the far west.

Recognizing the uncertainties in determining the mixing height, a number of investigators are resorting to direct measurements over the area of interest using instrumented aircraft or helicopters. Acoustic sounders and microwave radiometers are also being considered for this application. This approach, while

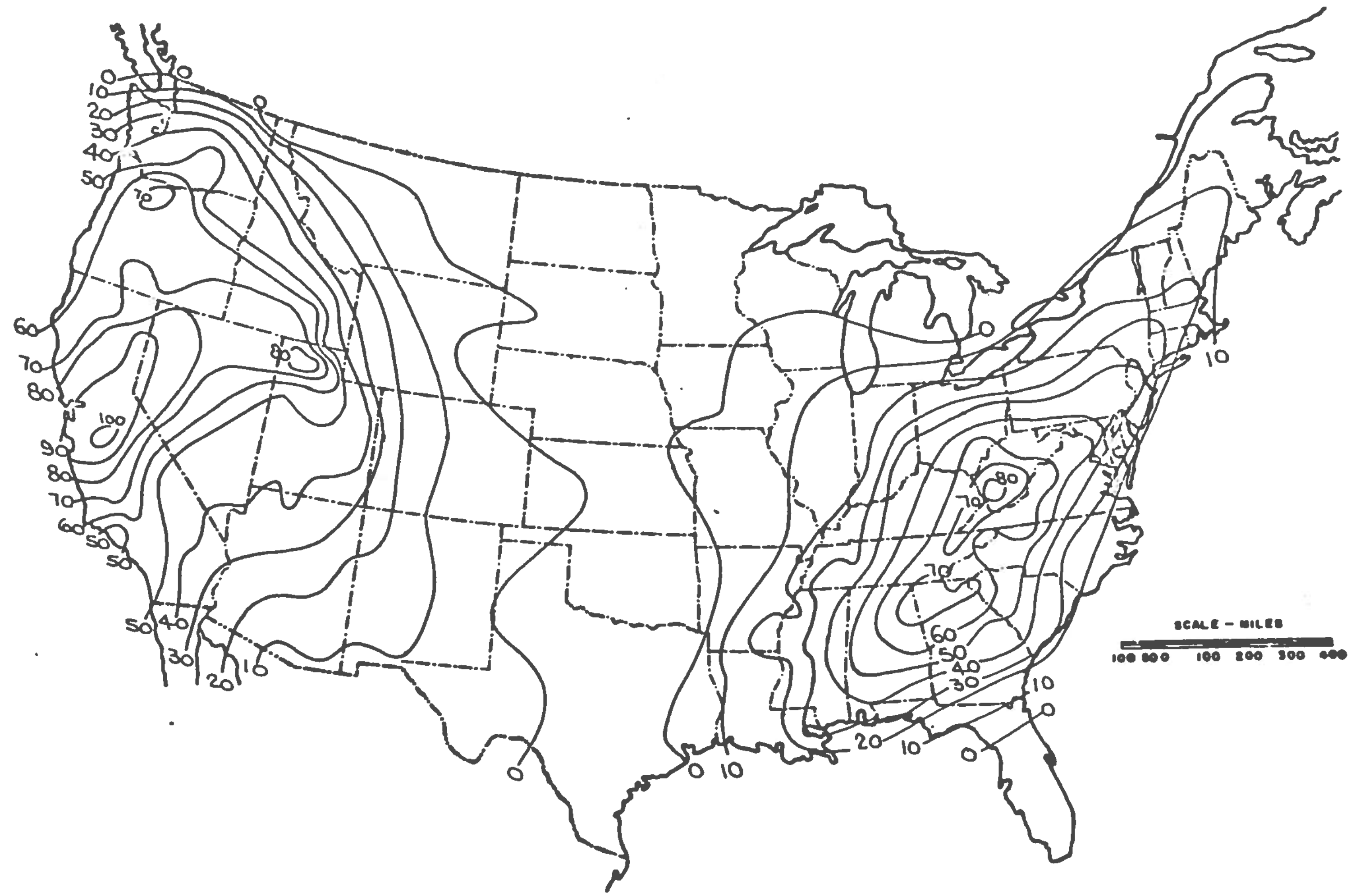


<u>Stippled Area - Stagnation Area</u> - based on observations at 1200Z.

<u>Solid Lines - Urban Morning Mixing Height (meters)</u> - based on observed data for 1200Z in the vicinity of stagnation areas. Only the 500, 1500, 2500, and 3500 (meter) isopleths are depicted.

<u>Dashed Lines - Transport Wind Speed</u> observed in the mixing layer this morning (MPS) in the vicinity of stagnation areas. Only the 4 meter per second isotach is depicted.

Figure 4. Air Pollution Map



39 Episodes West
1 October 1963 - 3 April 1970

75 Episodes East
1 August 1960 - 3 April 1970

Figure 5. Forecast High Air Pollution Potential Days

potentially much more reliable than the standard method, is hampered by the fact that the required vehicles and sensors are not generally available, and when available they tend to be expensive.

4.1.2 Emission Factors

The estimation of emissions from mobile, fixed, or multiple sources is crucial to the successful modeling of their subsequent dispersion. It has been seen that the models themselves are limited in one degree or another by their assumptions and that the meteorological input data are suspect due to inadequate resolution of measurements and other factors. It would be heartening to be able to report that source emissions can be specified with great accuracy for any desired application of the models so that at least the input emission data would not contribute significantly to the error in estimating pollutant concentration distributions. Unfortunately, this is not the case. In fact, emission estimates are as prone to error as any other ingredient in the modeling process.

EPA defines an emission factor as, "a statistical average of the rate at which a pollutant is released to the atmosphere as a result of some activity..."[2]. Emission factors for any transportation source dispersion problem must be calculated from whatever data is available on the transportation system in question. The following kinds of data are required: traffic, vehicle, activity and weather. These data are then coupled with estimates of emissions vs vehicle speed.

The traffic data needed are the total number of vehicles in the system as a function of space and time. These data are recorded at fixed time intervals for grid squares if an area source such as an airport is being analyzed, or for line segments if the source is linear like a road or runway. Also, data on the types of vehicles, as well as the number of each type and the age of each vehicle, are needed in order to make use of emission tables. Furthermore, activity data describing the operating mode of each vehicle is required because this factor governs both the type and amount of pollutants released. Finally, data on temperature and humidity are needed since both affect engine performance which, in turn, influences emissions. It should further be mentioned that fixed sources, intermingled with the mobile sources, may have to be taken into account. This is especially true for airports where fuel storage areas and power plants contribute to the total emissions.

In dealing with mobile sources such as automobiles, trucks, busses, railroad locomotives, and aircraft, emissions must be estimated as a function of space and time for ensembles of moving and stationary vehicles. Basic data on emissions from the three most prevalent types of vehicle engines: internal-combustion, diesel, and gas turbine are available as a starting point.

Automotive emissions occur in the exhaust, in evaporation from the fuel system, and in crankcase blow-by gases (this source was eliminated from U.S. automobiles beginning with the 1963 models). The amounts and kinds of pollutants emitted by a particular car depend on many factors, including the air-fuel ratio in the cylinder, ignition timing, engine speed (as well as temperature and load), engine misfiring, engine compression ratio, engine age, intake air temperature and humidity, composition of the fuel and, of course, the presence or absence of pollution control devices. Because of these many variables, automobile emission factors are generally calculated for a hypothetical driving cycle which typically begins with a cold start, followed by a period of travel at a prescribed average speed. Detailed discussions of this subject and tables of automotive emissions can be found in Volume III of References 39 and 2.

In addition to CO, HC, and NO_x, diesel engines emit particulates in the form of black or white smoke. Diesels also emit odors associated with hydrocarbons.

Emissions from gas turbine engines of jet aircraft have been measured and some results have been tabulated (see Volume III of Reference 39) as a function of engine operating mode (i.e., idle, take off and cruise). HC emissions are two orders of magnitude greater in the idle mode than they are in the other two modes.

On the other hand, NO_x emissions are greatest during cruise, being an order of magnitude larger than during idle or take off. The EPA emission factors for aircraft[2] are calculated for a landing-take off (LTO) cycle which includes all normal operations between the ground and 3500 feet.

Where can the other types of data be obtained which are needed to compute transportation emissions? The best data for analyzing highway emission problems are those which will be routinely recorded for a 42-mile instrumented loop of roads in the Los Angeles area to be operated by the California Division of highways. All the data required for dispersion modeling will be obtainable from this network. These data will be used by Roberts et al[40] as an input to their estimates of contaminant emissions in the Los Angeles basin. The traffic surveillance problem is discussed by Raudseps and Prerau[41] in a paper which describes the use of aircraft and helicopters as aerial platforms for photographing highway traffic. In general, however, highway traffic, vehicle and activity data are not routinely available, but instead are obtained at selected locations for specific purposes. This was the case with Johnson et al[42] who made detailed CO measurements in downtown San Jose, California during November and December 1970 as part of a field test for evaluating their urban diffusion model.

Traffic, vehicle and activity data for airports, while not recorded in a form specifically tailored to modeling, are nonetheless derivable (at some expense) from records which are routinely kept. Aircraft types and the number of each, as well as take off and landing times, are obtainable directly from airline schedules and from controller flight strips. Inbound taxiing time is the difference between gate time, recorded by the airline, and touchdown time recorded by the controller. Outbound taxi and queuing time can be calculated by comparing the actual gate-to-take off time with a known "no delay" time. Letdown and climbout times are also recorded for all arriving and departing aircraft. The time required for take off can be assumed to be the nominal time for each aircraft type. The age of the aircraft engine can be determined from maintenance records.

If pollution concentrations averaged over long periods such as months, seasons, or years are required then the emission data problem becomes much less severe. For highway problems, the average traffic conditions and vehicle distributions are sufficient. For airports, nominal schedules, typical distributions of aircraft and average categories of activity are adequate.

4.1.3 Geographic and Topographic Data

The geographic data specify the coordinates of all salient features to be treated by the model. These include: boundaries of the source area (or location and limits of the source line); location and height of all fixed point sources within the area; location and limits of all line sources in the area; coordinates of all receptors or, alternatively, specifications for a three-dimensional grid covering the entire data of interest. The topographic data depicts the character of terrain as well as the height of major structures in urban areas.

4.1.4 Background Pollution Data

It is necessary to account for the pollution regime in which the transportation system is embedded if one is to accurately measure the contribution of a transportation source. This total pollution concentration from other sources is called the background level. In rural areas the background will generally be low, hence the transportation system may produce most of the pollution. Conversely, in urban areas with high background levels the contribution of some transportation systems may not be so pronounced. In fact, under certain circumstances transportation may act as a local sink for pollution as Rote et al[15] found in their studies of Orange County Airport where pollutant levels were actually less inside the airport than in the vicinity of Palisades Road, a heavily travelled road near the airport boundary. This condition occurred with light and variable winds.

4.1.5 Control Instructions

The modeler uses control instructions to specify the way in which his programs are to be run. Among the instructions at his disposal are those which: specify which programs are to be used and in what sequence; define the time increment for iterative solutions; state the total time interval over which the solution is to be obtained; spell out the input data format and the interval for entry of input data; specify the output parameters, the frequency of outputting data and the form of the output (i.e., tabular or graphical).

4.2 SOFTWARE AND HARDWARE REQUIREMENTS

The characteristics of the computer programs and systems required to run the dispersion models enumerated in Table 7 will now be examined. The bulk of the information on this subject is contained in Tables 8 and 9 which summarize the salient points. All of the material in this section is taken from completed questionnaires returned to T.S.C.

4.2.1 Software Requirements

Table 8 shows the programming language used and the program size for the models developed by the companies listed. All of these models are currently operational on computers which are named in Table 9. The prevalence of FORTRAN IV as the favored language is immediately apparent —— 88% of the programs are written in that language. The significance of this is reflected in responses to the questions on adaptability of the programs, both to another computer and to the same computer at another installation. Because of the universality of FORTRAN, the answer to both of these questions was "yes" in almost every case.

The size of a FORTRAN program is a rough measure of its complexity which, in turn, gives some indication of how readily the program can be modified. Program size can be gauged by the following rule of thumb:

Magnitude	Lines of Code	Number	%
Small	≤ 1000	11	37
Medium	1001-2500	15	50
Large	> 2500	4	13

TABLE 8. SOFTWARE IMPLEMENTATION OF DISPERSION MODELS

Company	Programming Language			Program Size (lines of source code)
	FORTRAN IV	PL/1	Other	
Aeronautical Research Associates of Princeton Inc.	X			6000
Argonne National Lab (1)	X			———
Argonne National Lab (2)	X			———
Argonne National Lab (3)	X			———
Argonne National Lab (4)	X	X		2000 (FORTRAN)
AVCO Systems Division	X			1200
Battelle Columbus Lab	X			850
Boeing Computer Services Inc.	X			450
Center for the Environment and Man Inc. (1)			ANAL70	60
Center for the Environment and Man Inc. (2)			ANAL70	60
Computer Sciences Corp	X			575
Environmental Research and Technology Inc. (1)	X			1800
Environmental Research and Technology Inc. (2)	X			250
ESL Inc.	X			1500
Euclid Research Group	X			3010
General Research Corp. (1)	X			3000
General Research Corp. (2)	X			900
GEOMET INC	X			1500
Grumman Aerospace Corp	X			2700

TABLE 8. SOFTWARE IMPLEMENTATION OF DISPERSION MODELS (CONTINUED)

Company	Programming Language			Program Size
	FORTRAN IV	PL/1	Other	(lines of source code)
IBM-FSD		X		1200
INTERCOMP	X			2200
Kaman Sciences Corp.	X			300
Lockheed, Huntsville			FORTRAN V	700
Mt. Auburn Research Assoc.	X			2000
Northern Research and Engineering Corp.	X			1250
Pacific Environment Services Inc.	X			2500
Systems Applications Inc.	X			800
Systems Control Inc.	X			1500
Systems, Science and Software (1)	X			1200
Systems, Science and Software (2)	X			800
Texas Instruments Inc.	X			2032
TRC	X			1800
Walden Research Corp.	X			1500
Westinghouse Research Lab	X			—

Thus, we see that most of the programs can be classified as small or medium in size. Note that the complete Navier-Stokes solution used by Aeronautical Research Associates of Princeton utilizes a program which is a factor of two longer than the next longest one.

4.2.2 Hardware Requirements

In Table 9 the hardware aspects of the models are catalogued. Sixty-eight percent (68%) of the models were either originally programmed for, or have subsequently been re-programmed for, IBM computers. Among these, the IBM 360 series model 50 or larger is the favored choice in almost all cases. These are computers in the medium to large class which are widely available.

Again, a rule of thumb will be used to categorize the program memory requirements. (Note that the memory requirements listed in Table 9 include FORTRAN plotter routines where appropriate and where this information was supplied by the company.)

Magnitude	Program Memory Requirements (Kbytes)	Number	%
Small	≤100	6	24
Medium	101-200	7	28
Large	>200	12	48

The picture here is somewhat different than was the case for software in that program memory requirements fall into the medium or large categories. This may be due to the fact that the memory requirements for data storage have been included in the figures. These results are not surprising, as one would expect pollution problems to fall into the class of problems characterized by large input, moderate computations and small output.

The list of peripheral equipment in Table 9 contains no surprises. Except for the extensive system used by Aeronautical Research Associates of Princeton, all models require the standard peripherals which one would expect to find in most medium to large batch processing centers. The only non-standard hardware called for is plotters which are needed (or optional) for 32% of the models.

TABLE 9. HARDWARE IMPLEMENTATION OF DISPERSION MODELS

Company	Computer	Program Memory Requirement (Kbytes)	Peripheral Equipment: Card Reader	Card Punch	Line Printer	Disk Drive	Magnetic Tape	Drum	Plotter
Aeronautical Research Associates of Princeton Inc.	UNIVAC 1108	169	X		X		4	12	X
Argonne National Lab (1)	IBM 360/50-75	—	X		X	X	X		X
Argonne National Lab (2)	IBM 360/50-75	—	X		X	X	X		X
Argonne National Lab (3)	IBM 360/50-75	—	X		X				
Argonne National Lab (4)	IBM 360/75	—	X	X			X		
AVCO Systems Division	IBM 360/50	100	X	X	X				
Battelle, Columbus Labs	CDC-6400	215	X		X		X		X
Boeing Computer Services Inc.	≥ IBM 360/50	40	X		X				X
Center for the Environment and Man, Inc.(1)	UNIVAC 1108	—	X		X		X	X	
Center for the Environment and Man, Inc.(2)	UNIVAC 1108	—	X		X		X	X	
Computer Sciences Corp.	CDC-6500	450	X		X	X	X		
Environmental Research and Technology Inc. (1)	≥ IBM 360/65	≤150	X		X	X			

TABLE 9. HARDWARE IMPLEMENTATION OF DISPERSION MODELS (CONTINUED)

Company	Computer	Program Memory Requirement (Kbytes)	Peripheral Equipment						
			Card Reader	Card Punch	Line Printer	Disk Drive	Magnetic Tape	Drum	Plotter
Environmental Research and Technology Inc. (2)	IBM 360/65	—	X		X				
ESL Inc.	IBM 370/145	188	X		X	2	X		
Euclid Research Group	IBM 7040/7094	225	X	X	X		3		
General Research Corp. (1)	CDC-6400	270	X	X	X	X			X
General Research Corp. (2)	CDC-6400	232	X		X	X			
GEOMET Inc.	IBM 360/50	175	X		X	X			
Grumman Aerospace Corp.	IBM 360/67	—			X	X	X		X
IBM-FSD	IBM 360/50	150			X	X			
INTERCOMP	CDC, UNIVAC OR IBM	375	X		X				
Kaman Sciences Corp.	CDC-6400	480	X	X		X			
Lockheed, Huntsville	IBM 7094	169	X		X		2		X
Mt. Auburn Research Assoc.	IBM 360/75	≤480	X		X	2			
Northern Research and Engineering Corp.	CDC-600	195	X		X				

TABLE 9. HARDWARE IMPLEMENTATION OF DISPERSION MODELS (CONTINUED)

Company	Computer	Program Memory Requirement (Kbytes)	Peripheral Equipment						
			Card Reader	Card Punch	Line Printer	Disk Drive	Magnetic Tape	Drum	Plotter
Pacific Environmental Services Inc.	$\geq$IBM 360/50	86	X		X				
Systems Applications Inc.	IBM 360	300	X		X		2		
Systems Control Inc.	IBM 360/65	60	X		X	X	X		X
Systems, Science and Software (1)	IBM 360/75	$\leq$480	X		X	X			X
Systems, Science and Software (2)	UNIVAC 1108	81	X		X				
Texas Instruments Inc.	IBM 360/65	$\leq$100	X		X	X	X		X
TRC	IBM 360/65	$\leq$265	X	X	X	X	X		
Walden Research Corp.	IBM 360/65	202	X	X	X	X			
Westinghouse Research Labs	UNIVAC 1106	—							

4.3 OUTPUT

Two types of computer output are generated: tabular and graphical. All programs described in questionnaires returned to TSC produce tabular output, and about half of them also generate graphical presentations, either routinely or as an option. Examples of typical output products are presented in this section.

4.3.1 Tabular Output

Data which are normally printed out or stored in tabular form at selected times include subsets of the following: the time interval covered by the simulation; all pertinent input data on meteorological variables, emissions, geography, etc.; average and peak ground concentrations of pollutants at selected receptors (Gaussian models) or at grid points (Conservation of Mass models); and distribution of pollutant concentrations in the vertical. Table 10 is an example of tabular data which shows the area covered by the .01, .10, and .20 ppm isopleths for two simulation times. Table 11 is a computer printout of average hourly SO_2 concentrations exceeding certain thresholds for eight monitoring stations in the Chicago area.

4.3.2 Graphical Output

Graphical output can be generated either by a line printer or by an SC4020, or other, CRT plotter. The line printer output data may be presented in the form of a two-dimensional array of concentration predictions superimposed on a geographical map or, alternatively, in a gray-tone format depicting concentration contours. Figure 6 is an example of the array presentation where a two-dimensional grid of SO_2 estimates over Chicago is shown. In Figure 7 we see a typical grey-scale rendering of contours which are produced by using a character set to simulate approximately eight levels of grey.

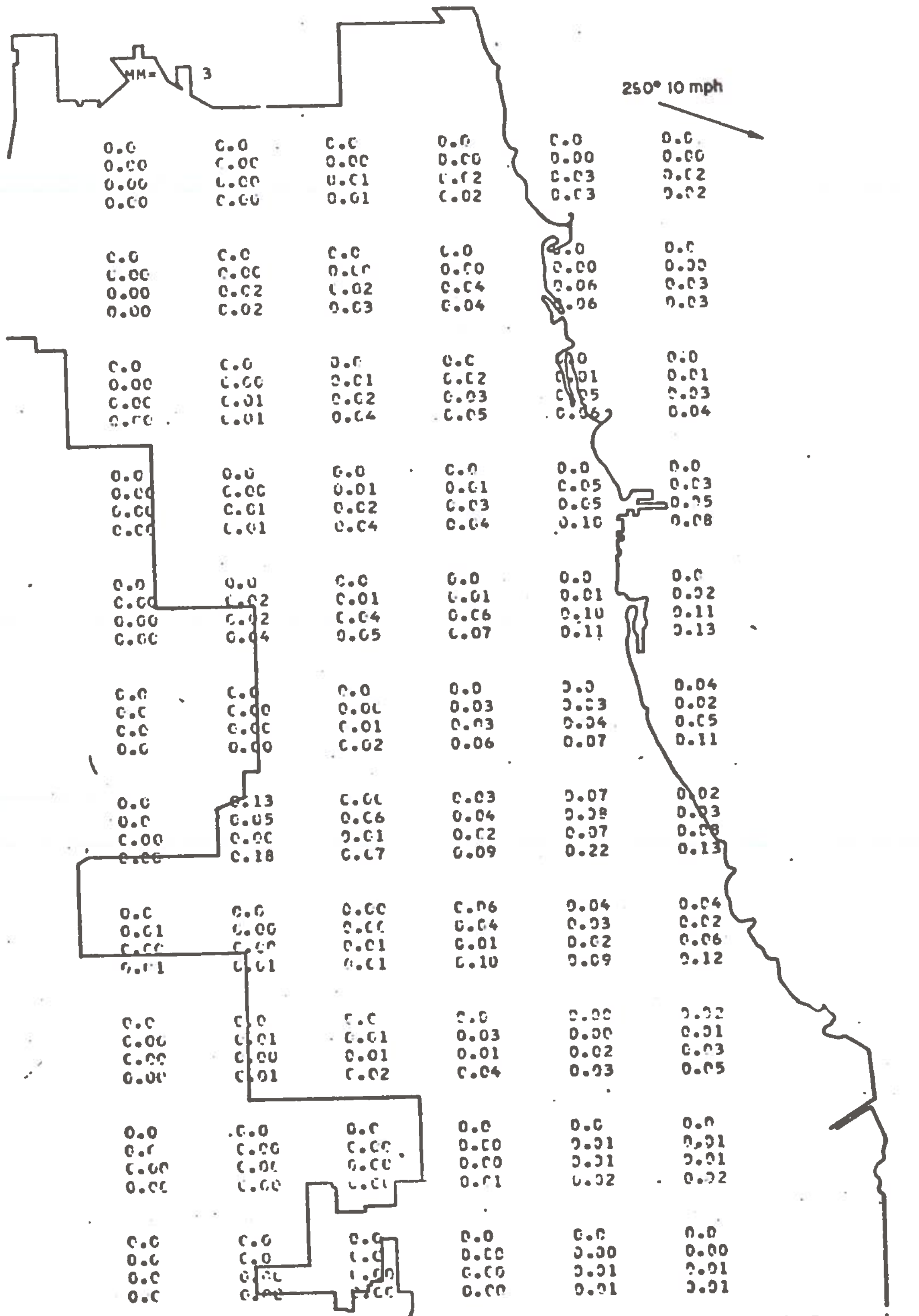


Figure 6. Printout of SO_2 Estimates on a 2x2 Mile Grid Covering Chicago
Argonne National Laboratory, Center for Environmental Studies

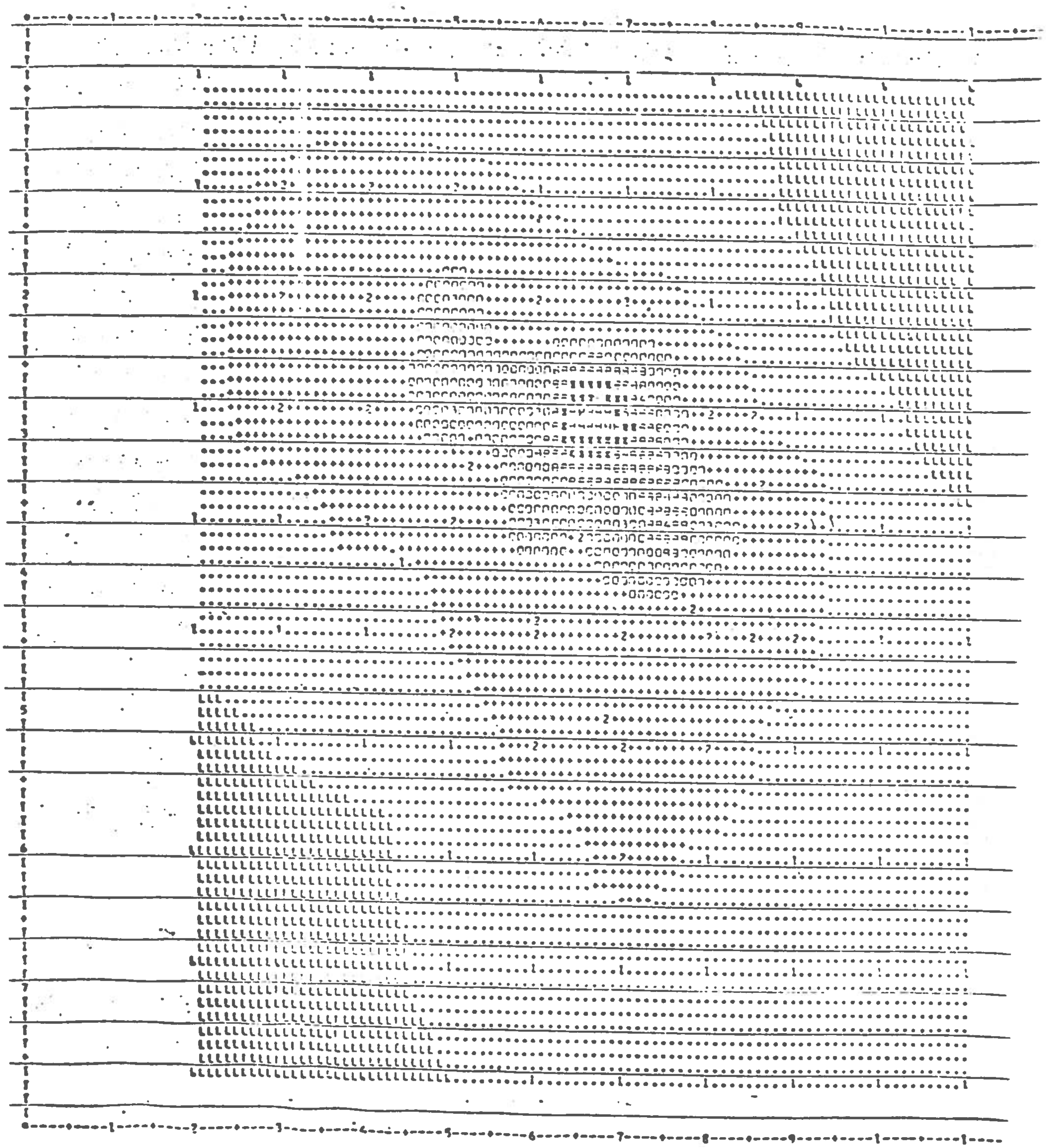


Figure 7. Printer Grey-Scale Rendering of SO_2 Concentration Contours

Argonne National Laboratory, Center for Environmental Studies

TABLE 10. TABULAR OUTPUT OF ISOPLETH LEVELS

Isopleth-area Table

45

PIRING HEIGHT................ 1000.0 FT
WIND SPEED.................... 5.0 MPH
EFFECTIVE STACK HEIGHT....... 1000.0 FT
STABILITY CLASS.............. UNSTABLE-B

--------ISOPLETH LEVEL=.01 PPM--------

QSO2 LB/HR	AREA SQ MI	CLE MI	LGTH MI	WDTH MI	CHIMAX PPM	DCP MI
250	0.5	0.0	1.0	0.5	0.02	1.0
500	2.0	0.3	4.0	0.5	0.04	1.0
750	7.3	0.3	6.5	1.5	0.05	1.0
1000	12.0	0.3	9.0	1.5	0.07	1.0
2500	90.5	0.3	25.0	4.5	0.18	1.0
5000	473.6	0.3	>50.0	6.5	0.36	1.0
15000	1119.4	0.3	>50.0	22.5	1.07	1.0
25000	1368.3	0.3	>50.0	27.5	1.79	1.0
35000	1517.4	0.3	>50.0	30.5	2.51	1.0
50000	1616.9	0.3	>50.0	33.5	3.58	1.0
75000	1764.3	0.3	>50.0	35.5	5.37	1.0
100000	1863.6	0.3	>50.0	37.5	7.16	1.0

--------ISOPLETH LEVEL=.10 PPM--------

QSO2 LB/HR	AREA SQ MI	CLE MI	LGTH MI	WDTH MI	CHIMAX PPM	DCP MI
250	0.0	0.0	0.0	0.0	0.0	0.0
500	0.0	0.0	0.0	0.0	0.0	0.0
750	0.0	0.0	0.0	0.0	0.0	0.0
1000	0.0	0.0	0.0	0.0	0.3	0.0
2500	0.5	0.0	1.0	0.5	0.18	1.0
5000	2.0	0.3	4.0	0.5	0.36	1.0
15000	29.5	0.3	14.0	2.5	1.07	1.0
25000	90.5	0.3	25.0	4.5	1.79	1.0
35000	185.3	0.3	36.5	6.5	2.51	1.0
50000	472.6	0.3	>50.0	9.5	3.58	1.0
75000	721.4	0.3	>50.0	14.5	5.37	1.0
100000	920.4	0.3	>50.0	18.5	7.16	1.0

--------ISOPLETH LEVEL=.20 PPM--------

QSO2 LB/HR	AREA SQ MI	CLE MI	LGTH MI	WDTH MI	CHIMAX PPM	DCP MI
250	0.0	0.0	0.0	0.0	0.0	0.0
500	0.0	0.0	0.0	0.0	0.0	0.0
750	0.0	0.0	0.0	0.0	0.0	0.0
1000	0.0	0.0	0.0	0.0	0.0	0.0
2500	0.0	0.0	0.0	0.0	0.0	0.0
5000	0.5	0.0	1.0	0.5	0.36	1.0
15000	4.3	0.3	6.5	1.5	1.07	1.0
25000	21.0	0.3	11.5	2.5	1.79	1.0
35000	44.0	0.3	17.0	3.5	2.51	1.0
50000	90.5	0.3	25.7	4.5	3.58	1.0
75000	217.5	0.3	39.0	7.5	5.37	1.0
100000	472.6	0.3	>50.0	9.5	7.16	1.0

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PIRING HEIGHT................ 1000.0 FT
WIND SPEED.................... 5.0 MPH
EFFECTIVE STACK HEIGHT....... 1000.0 FT
STABILITY CLASS.............. NEUTRAL-C

--------ISOPLETH LEVEL=.01 PPM--------

QSO2 LB/HR	AREA SQ MI	DLE MI	LGTH MI	WDTH MI	CHIMAX PPM	DCM MI
500	1.3	0.3	2.5	0.5	0.01	0.5
750	12.0	1.0	11.5	1.5	0.02	0.5
1000	22.0	1.3	17.0	1.5	0.02	0.5
2500	214.9	2.3	>50.0	4.5	0.06	0.5
5000	458.4	1.8	>50.0	9.5	0.11	0.5
15000	655.6	1.8	>50.0	14.5	0.34	0.5
25000	755.6	1.3	>50.0	15.5	0.56	0.5
35000	804.4	1.3	>50.0	16.5	0.79	0.5
50000	851.3	1.3	>50.0	17.5	1.13	0.5
75000	950.6	1.3	>50.0	19.5	1.69	0.5
100000	990.6	1.3	>50.0	19.5	2.26	0.5

--------ISOPLETH LEVEL=.10 PPM--------

QSO2 LB/HR	AREA SQ MI	DLE MI	LGTH MI	WDTH MI	CHIMAX PPM	DCM MI
500	0.0	0.0	0.0	0.0	0.0	0.0
750	0.0	0.0	0.0	0.0	0.0	0.0
1000	0.0	0.0	0.0	0.0	0.0	0.0
2500	0.0	0.0	0.0	0.0	0.0	0.0
5000	1.3	0.3	2.5	0.5	0.11	0.5
15000	54.8	2.0	26.5	2.5	0.34	0.5
25000	214.9	2.3	>50.0	4.5	0.56	0.5
35000	310.6	2.3	>50.0	6.5	0.79	0.5
50000	458.4	1.8	>50.0	9.5	1.13	0.5
75000	554.9	1.8	>50.0	11.5	1.69	0.5
100000	603.1	1.8	>50.0	16.5	2.26	0.5

--------ISOPLETH LEVEL=.20 PPM--------

QSO2 LB/HR	AREA SQ MI	DLE MI	LGTH MI	WDTH MI	CHIMAX PPM	DCP MI
500	0.0	0.0	0.0	0.0	0.0	0.0
750	0.0	0.0	0.0	0.0	0.0	0.0
1000	0.0	0.0	0.0	0.0	0.0	0.0
2500	0.0	0.0	0.0	0.0	0.0	0.0
5000	0.0	0.0	0.0	0.0	0.0	0.0
15000	12.0	3.0	11.5	1.5	0.34	0.5
25000	40.5	2.0	22.0	2.5	0.56	0.5
35000	77.8	2.0	30.5	3.5	0.79	0.5
50000	214.9	2.3	>50.0	4.5	1.13	0.5
75000	358.1	2.3	>50.0	7.5	1.69	0.5
100000	458.4	1.8	>50.0	9.5	2.26	0.5

TABLE 11. COMPUTER PRINTOUT OF SO_2 THRESHOLDS

Percent of Hourly SO_2 Concentrations above Indicated Values for Chicago, January 1, 1966 to December 31, 1968

INDICATED VALUES OF SO2 CONC. (PPM)	TAM-1	TAM-2	TAM-3	TAM-4	TAM-5	TAM-6	TAM-7	TAM-8
1.00	0.02	0.0	0.04	0.03	0.02	0.01	0.0	0.00
0.95	0.02	0.0	0.06	0.05	0.03	0.01	0.0	0.00
0.90	0.02	0.00	0.08	0.09	0.05	0.02	0.0	0.00
0.85	0.02	0.01	0.13	0.11	0.06	0.04	0.01	0.00
0.80	0.03	0.01	0.20	0.17	0.07	0.04	0.01	0.00
0.75	0.04	0.01	0.34	0.23	0.08	0.05	0.02	0.01
0.70	0.05	0.01	0.55	0.36	0.09	0.08	0.06	0.01
0.65	0.07	0.04	0.82	0.48	0.10	0.11	0.09	0.01
0.60	0.11	0.07	1.37	0.66	0.11	0.14	0.18	0.01
0.55	0.14	0.11	2.12	1.01	0.14	0.22	0.31	0.03
0.50	0.22	0.25	3.53	1.52	0.21	0.30	0.56	0.04
0.45	0.30	0.39	5.34	2.29	0.27	0.41	0.92	0.08
0.40	0.48	0.63	7.69	3.41	0.44	0.50	1.41	0.11
0.35	0.71	0.93	10.33	4.76	0.67	0.63	2.02	0.19
0.30	1.01	1.73	14.25	7.05	1.05	0.98	3.14	0.39
0.25	1.59	3.24	20.56	11.24	1.88	1.56	5.53	0.92
0.20	2.53	5.63	27.39	17.20	3.08	2.80	9.00	1.94
0.15	4.76	10.57	35.96	26.05	5.94	5.42	14.74	4.12
0.10	8.04	19.01	45.17	35.52	11.22	10.24	23.73	8.46
0.05	17.47	40.43	59.94	53.00	27.32	24.39	44.41	23.95
NO.OF CASES	22290	23762	22663	24140	22723	23320	24424	23371
MAX HRLY VALUES=	1.28	0.90	1.97	1.04	1.24	1.19	0.90	1.14

Argonne National Laboratory, Center for Environmental Studies

CRT plotter output can be viewed either on a computer graphics display or as hard copy in color, or black or white. Samples of plotted output are presented in Figure 8 which shows CO concentration contours over Chicago, and in Figure 9 which depicts contours of CO emissions in the vicinity of roadways.

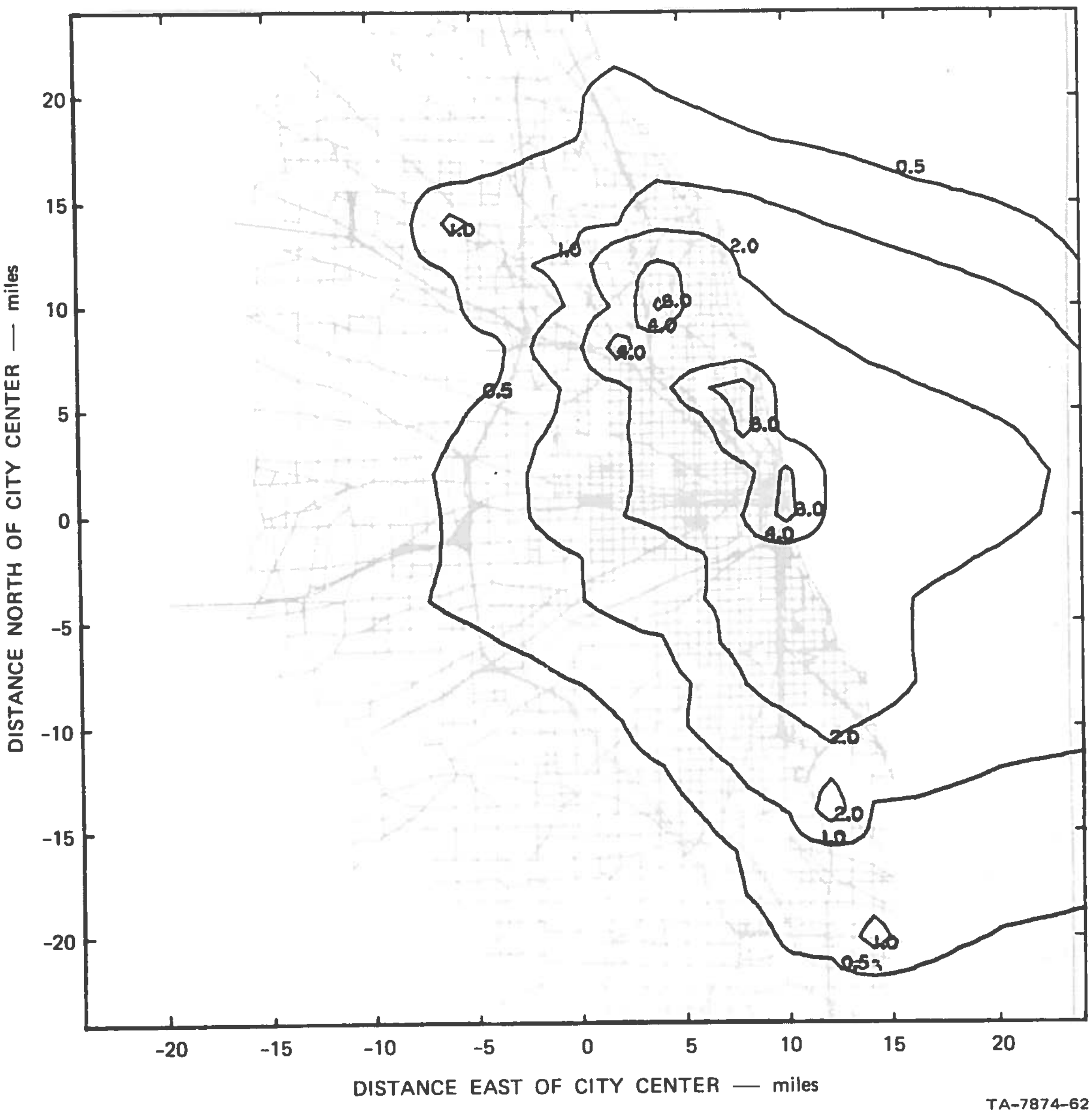
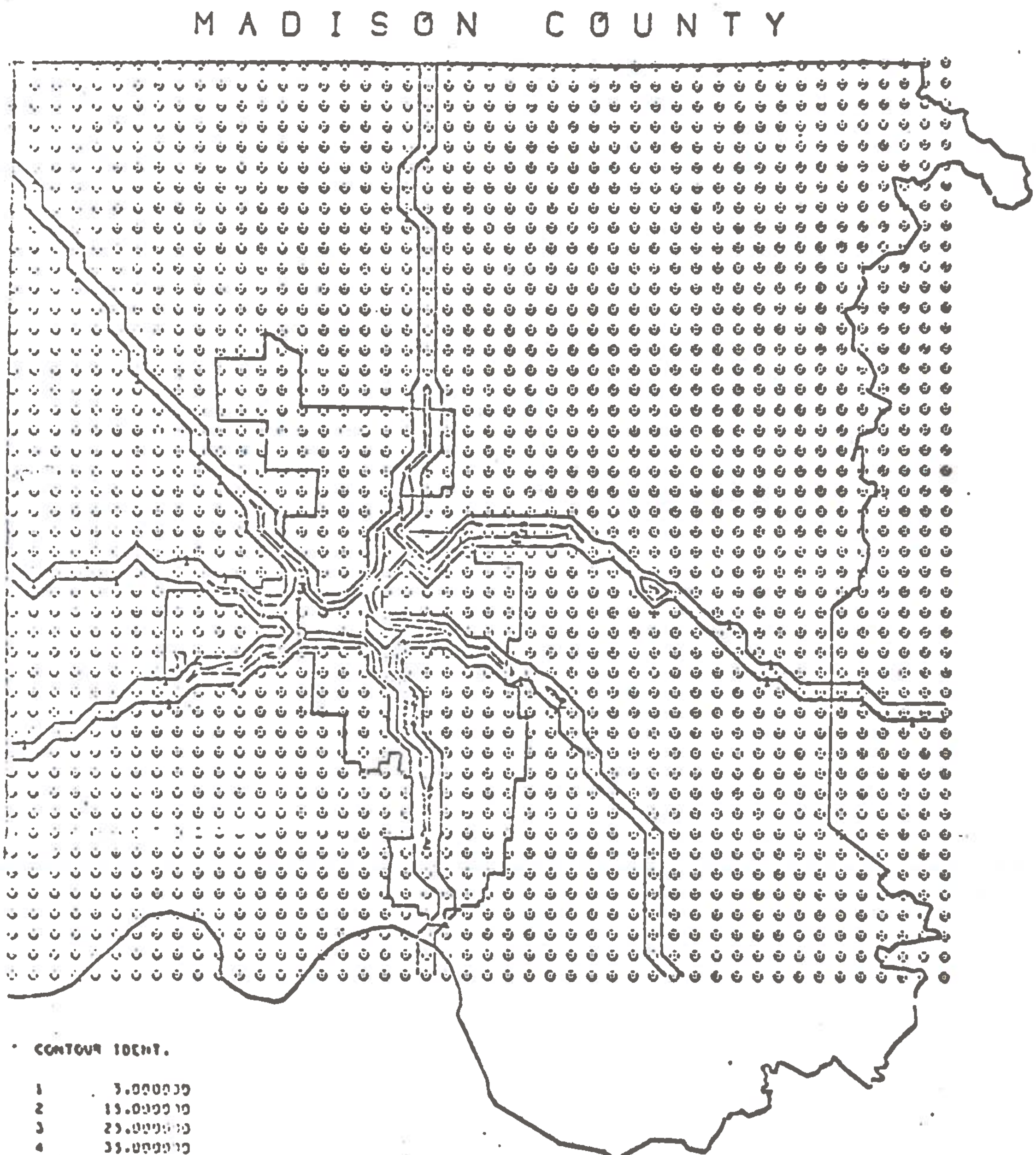


Figure 8. Calculated Carbon Monoxide Concentrations (PPM) For Chicago. (0700-0800 LST; wind 4 ms^{-1}, 270°, mixing depth 200 m; neutral stability)
Stanford Research Institute



CONTOUR IDENT.	
1	5.000000
2	15.000000
3	25.000000
4	35.000000
5	45.000000
6	55.000000
7	65.000000
8	75.000000
9	85.000000
A	95.000000
B	105.000000
C	115.000000
D	125.000000
E	135.000000
F	145.000000
G	155.000000
H	165.000000
I	175.000000
J	185.000000
K	195.000000

Figure 9. SC4020 Plot of CO Concentration Contours over Madison County, Alabama

Lockheed Missiles and Space Company, Inc., Huntsville Research and Engineering Center

5.0 APPLICATIONS OF THE MODELS

The TSC questionnaire requested information on how the models have been used. In particular, each respondent was asked to describe a typical problem to which his model had been applied and to indicate both the time required to solve this problem and the approximate cost. Thirty (30) replies to his question were received of which 18 described transportation problems and 12 non-transportation problems. Since similar models are used for all of these problems, both the transportation (Section 5.1) and non-transportation (Section 5.2) applications are presented here. Each Section contains brief (edited) statements by the modelers on the problems they solved, followed by a table which summarizes the computational aspects.

It should be noted that definitive judgments regarding the relative cost of running these models cannot be made on the basis of the data presented herein. The problems described are diverse, the time periods spanned by the simulations vary widely, and the problems were run on several different machines. The information provided should be regarded as only a sampling of typical running times and costs for a variety of air pollution modeling problems. Precise, comparative performance data for individual models can only be obtained by controlled tests using a common set of input data.

5.1 TRANSPORTATION SOURCE PROBLEMS

1. Northern Research and Engineering, Corp.
   Total emissions and annual-average concentrations were computed for J. F. Kennedy International Airport for 1970. CO, NO_2, SO_2, particulates, lead, and hydrocarbons were the pollutants considered, and fifty (50) receptor locations were specified.

2. IBM-FSD
   A continuous line source was considered with concentrations evaluated at 24 field points for 100 time steps at

one minute intervals.

3. Walden Research Corp.
The average concentration of CO and particulates was calculated at 221 receptor points within a metropolitan area due to emissions from 500 source locations. The results were plotted. Note that this is a typical problem for the study of a large metropolitan region. The program also can be structured for application to the study of a specific traffic link or highway.

4. AVCO Systems Divisions
The space distribution of CO, CO_2, NO, NO_2, etc. behind an aircraft engine was computed for a downstream distance of 2 miles.

5. Systems Applications, Inc.
A simulation of CO concentration throughout the Los Angeles Basin on a 25 x 25 x 10 grid (0500-1600 PST; 11 hrs.) was conducted. The average hourly concentrations were computed at 625 locations for the entire period.

6. Pacific Environmental Services, Inc.
The trajectory of an air parcel (whose position and composition at a given time of day are known), and the concentrations of pollutants within the air parcel, were calculated as a function of time of day, and printouts were furnished for each 15 minute interval over a 3-hour period.

7. The Center for the Environment and Man, Inc.
Sources were specified on an 8000 point grid. The conservation of mass equation was integrated for 150 time steps with 3 changes of meteorological data and emission source factors. 8000 grid point values and/or contoured maps of concentrations were printed out.

8. Lockheed Missiles and Space Company, Inc., Huntsville Research and Engineering Center.
The average daily concentration of CO from motor vehicles on selected major traffic arteries was computed for Madison

County, Alabama, which includes the City of Huntsville. The 46 x 46 point grid used in the program with a grid distance of 1 km completely covers the county. Concentrations of CO in ppm were computed for each grid square. Output was generated in both tabular and graphical formats.

9. ESL, Inc.
The hourly average concentration of NO_x was computed on the windward side of a six lane section of six lane freeway at a total of 72 receptor sites at ground level and at a height of five feet.

10. Systems, Science and Software
   A. The concentration of CO in the Los Angeles air basin was computed over an 18-hour period throughout a grid 22 x 16 by 4 cells high covering 60 miles x 45 miles x 1200 feet. (Model 1, see Table 7)
   B. An at-grade highway is to be replaced by a depressed expressway. The model was used to simulate how this will change local pollution levels. (Model 2, see Table 7)

11. Environmental Research and Technology, Inc.
The 1969 annual average concentrations for particulates, SO_2, CO, Hydrocarbons and NO_x were calculated for a metropolitan source distribution consisting of 143 point sources, 50 line sources and 36 area sources. Twelve (12) receptors were specified, distributed over a region of approximately 50 x 50km.

12. Systems Control Inc.
A dynamic system with 25 unknown parameters was identified using input/output data records, 480 data points in length. This system is equivalent to a freeway system with 8 measurement stations for wind speed, direction, CO, and corresponding stability data. The times noted in Table 12 are for a single run of the type that would be required to reduce model errors to a minimum. Multiple runs are initially required.

13. Grumman Aerospace Corp.
The 24 hour average concentration of CO at 250 points of a grid covering John F. Kennedy Airport was computed.

14. General Research Corp.
   A. The concentration of 11 species at 5 vertical points was calculated. Results were printed out every 10 minutes, for a 3-hour trajectory between two points in the Los Angeles Basin. (Model 1, see Table 7)

   B. The CO concentration was computed at 100 points in a vertical plane normal to a freeway for 8 hours on a stagnant day. Computation interval - .1 min; Output interval for vertical data maps - 30 mins; Output interval for ground concentration profiles - 1 min. (Model 2, See Table 7)

15. Computer Sciences Corp.
Using as inputs the observed meteorological conditions and the traffic data appropriate for an 18-hour period (including a freeway system modeled by 107 line segments, and a surface street system modeled by 198 area sources), a trial run of the model has been made in which hourly concentrations of carbon monoxide were computed for an 18-hour period for 1200 grid points spanning a large airshed.

16. Kaman Sciences Corp.
The annual distribution of pollutants from 1 km of highway was computed. The highway was divided into $3^5 = 243$ segments. Output was generated for 16 directions and 12 distances from the center of the 1 km section. Quadratic interpolation coefficients were used to calculate any distance along any direction for 8 different orientations of the highway N - S, NNE - SSW . . . SSE - NNW.

Table 12 summarizes the computations involved in solving these problems.

TABLE 12. COMPUTATIONS FOR TYPICAL TRANSPORTATION SOURCE AIR POLLUTION MODELING PROBLEMS

Problem Number	Company	CPU Time (minutes)	Running Time (minutes)	Approximate Cost ($)
1	Northern Research and Engineering, Corp.	5	5	80
2	IBM-FSD	2.6	2.6	30
3	Walden Research Corp.	92.8		395
4	AVCO Systems Division	15	30	400
5	Systems Applications, Inc.	10	15	500
6	Pacific Environmental Services, Inc.	4-5	5-20	42-59
7	The Center for the Environment and Man, Inc.	4.5		40
8	Lockheed Missiles and Space Company, Inc., Huntsville Research and Engineering Center	0.5	0.5	10
9	ESL Inc.	0.6	1.7	19
10A	Systems, Science and Software	10	14	150
10B	Systems, Science and Software	0.8	2	10
11	Environmental Research and Technology, Inc.	3.7	9	450
12	Systems Control, Inc.	4.5	5	110
13	Grumman Aerospace Corp.	12	45	300
14A	General Research Corp.	3.8	4.1	30
14B	General Research Corp.	3	6	22
15	Computer Sciences Corp.	60	120	700
16	Kaman Sciences Corp.	0.2	0.3	2

5.2 PROBLEMS NOT INVOLVING TRANSPORTATION SOURCES

1. GEOMET Inc.

   For the winter season, the mean SO_2 concentration and the frequency distribution of hourly concentrations, at each of 10 locations was calculated. Twenty-four hour sampling intervals (i.e., one hour out of 24 selected for input to the diffusion model) were used. There were 51 point sources plus an area source defined by emission rates at 1200 grid points.

2. The Center for the Environment and Man Inc.

   The program has been run for a set of 27 sources. Results were calculated for each point on a 35 x 35 grid.

3. Mt. Auburn Research Associates, Inc.

   The following trajectory problems have been solved:

   A. Transport of 754 parcels of air through a horizontally uniform, time variant atmosphere with low vertical turbulence, and

   B. Transport of 115 parcels of air through a highly turbulent, complex mountain-valley wind system under steady-state wind conditions using a horizontally resolved wind field for one hour of simulated time.

4. INTERCOMP

   Fifteen to thirty minute average concentrations of SO_2 were computed for each block of a 2300 grid-block system. The period of time covered was 10 hours and the ground concentrations were output both as a contour map and as a complete array of the three-dimensional distribution at intervals of 4, 6, and 10 hours. The area described by the grid was 10 x 10 miles in surface area by 4000 feet in vertical height.

5. TRC

   Twenty-four one-hour values of SO_2 concentration were calculated at 100 receptor points at three heights due to 890 area sources, 350 point sources and 125 line source segments. Results were printed out and a deck was punched.

6. Boeing Computer Services Inc.
   SO_2 concentrations in the vicinity of the Tacoma smelter in a synthetic alternating wind field were computed.

7. Environmental Research and Technology Inc.
   The three dimensional dispersion of area source emissions was calculated over a 16 km downwind distance using Blackadar's wind spiral horizontal velocity profile and vertical diffusivity profile.

8. Texas Instruments Inc.
   The average hourly concentration of SO_2 was computed at 144 receptors due to 256 area sources and 24 point sources. Each source had up to four different stack heights. Each source strength was estimated as a function of process and space heating requirements which, in turn, were computed from the current temperature. Electric power generating plants were among the point sources modeled, according to a power demand schedule.

9. Euclid Research Group.
   The cloud rise, particle formation, transport and deposition from a high-yield explosion was calculated.

10. Argonne National Laboratory
    Hourly sulfur dioxide levels were estimated at 66 points on a 2 x 2 mile grid over the City of Chicago for January 15, 1967.

11. Aeronautical Research Associates of Princeton, Inc.
    Using isotropic turbulence and a Gaussian dispersion profile in y and z, output parameters were computed up to 2500 ft. for a 15 x 15 point grid with mesh sizes of 8 ft. and 16 ft.

The computations entailed in these problems are summarized in Table 13. Comparing the data in Tables 12 and 13 we see that the distribution of times and costs are quite similar in both tables.

We may conclude that, at least for the problems described here, the costs of running all these models is low.

TABLE 13. COMPUTATIONS FOR TYPICAL AIR POLLUTION MODELING PROBLEMS NOT INVOLVING TRANSPORTATION SOURCES

Problem Number	Company	CPU Time (minutes)	Running Time (minutes)	Approximate Cost ($)
1	GEOMET Inc.	4	6	30
2	The Center for the Environment and Man	0.5		5
3A	Mt. Auburn Research Associates, Inc.	3		
3B	Mt. Auburn Research Associates, Inc.	21		
4	INTERCOMP	3		75-110
5	TRC	20	37	200
6	Boeing Computer Services, Inc.	1.3	2	30
7	Environmental Research and Technology Inc.	2		20
8	Texas Instrument, Inc.	0.7	3.3	8
9	Euclid Research Group		14	150
10	Argonne National Laboratory	68	80	410
11	Aeronautical Research Associates of Princeton, Inc.	80[1] 40[2]	80 40	633 —

[1] 8 ft. mesh
[2] 16 ft. mesh

6.0 VALIDATION OF THE MODELS

The TSC questionnaire asks the following questions with respect to validation of models:

> "Has the model been validated with real-world data? If so, indicate the period of time, sample size, geographical area, and the results of such validation(s)."

Of the 29 responses to this question, 22 reported that their model had been validated to some extent and 7 stated that validation had not yet been undertaken. Of the 22 positive responses, 12 reported validation on transportation source problems, and 10 on non-transportation problems. As in Section 5, the results will be reported in two sections, one for transportation (Section 6.1) and one for non-transportation (Section 6.2) validations. The material in this chapter consists of edited quotes from individual company statements concerning the validation of their models. (Regretably, the validation results were reported in a number of different units and it has not been practical to reduce them to a common unit.)

6.1 VALIDATION OF TRANSPORTATION-SOURCE MODELS

1. Northern Research and Engineering Corporation
   Although the model has been used to analyze air quality at a number of airports, very little data has been available for validation purposes. Data were taken by EPA personnel at Washington National Airport during July 1971. They consist of carbon monoxide readings for one-hour periods. The monitors, in each case, were clustered near the head of the principal runway being used for take-offs. Results of the comparison are presented below.

Sampling Period	Average Measured Concentration μg/m^3	Average Predicted Concentration μg/m^3	Error (%)
July 20 8:50-9:50 am EDT	523	740	41
July 23 8:38-9:25 am EDT	844	584	31

Discrepancies between the predicted and measured concentrations seem to be caused by uncertainties in the wind speed and wind direction, and inaccuracies in distributing aircraft activity between runways.

2. Walden Research Corporation
The model has been tested for particulates in both the metropolitan Boston and metropolitan Providence areas and yields correlations of 0.85 and 0.90, respectively. The model has not been tested for CO validation.

3. Systems Applications, Inc.
The model is being validated for the Los Angeles airshed for two days -- Sept. 29 and Sept. 30, 1969 -- predicting concentrations of CO, NO, NO_2, Hydrocarbon, ozone simultaneously for each of eleven monitoring sites (over a 50 x 50 mile area). Predictions are averaged at hourly intervals from 6 AM to 4 PM and compared with measured values. CO validation for 9/29/69 is completed (see Table 14); photochemical pollutant validation is in progress.
Errors for CO were not computed, but are in the range of 10-20%, except for morning peaks at some locations near important sources. In these cases, the 2-mile resolution of the model is too coarse to pick up local concentration peaks. We believe that the errors in CO prediction are within the tolerances required for estimation of concentration levels and their variation in space and time within an airshed.

TABLE 14. SUMMARY OF VALIDATION RESULTS FOR CARBON MONOXIDE FOR 29 SEPTEMBER 1969 (IN PPM)*

Station/Time (PST)	5-6	6-7	7-8	8-9	9-10	10-11	11-12	12-13	13-14	14-15	15-16	16-17
1 CAP	3 (5)	7 (12)	17 (17)	18 (20)	- (19)	- (13)	6 (7)	3 (4)	3 (4)	2 (4)	6 (5)	6 (6)
60 AZU	10 (9)	10 (11)	10 (13)	11 (13)	10 (14)	8 (16)	6 (15)	7 (3)	9 (6)	6 (4)	6 (4)	4 (5)
69 BURK	13 (8)	15 (11)	18 (14)	17 (14)	9 (13)	11 (12)	10 (9)	11 (9)	7 (4)	7 (3)	5 (3)	5 (4)
71 WEST	5 (6)	9 (9)	17 (10)	17 (10)	8 (8)	- (8)	5 (7)	4 (5)	4 (4)	4 (4)	4 (5)	5 (5)
72 LONB	7 (4)	9 (5)	13 (7)	11 (7)	9 (4)	6 (4)	6 (4)	6 (4)	5 (4)	5 (4)	5 (4)	5 (4)
74 RESD	10 (9)	12 (10)	16 (12)	11 (10)	8 (10)	6 (11)	4 (8)	5 (4)	3 (3)	3 (4)	5 (4)	5 (4)
75 POMA	7 (6)	8 (6)	9 (5)	9 (5)	- (5)	6 (5)	5 (8)	4 (9)	5 (7)	6 (6)	6 (4)	6 (3)
76 LENX	6 (5)	15 (5)	9 (6)	5 (5)	5 (4)	6 (4)	- (4)	3 (3)	3 (3)	4 (3)	6 (3)	6 (2)
80 WHTR	- (6)	11 (5)	14 (7)	11 (11)	11 (13)	13 (13)	- (10)	2 (2)	1 (4)	1 (4)	1 (4)	1 (4)
(SC) ELM	- (8)	- (11)	- (16)	8 (17)	6 (19)	6 (14)	9 (8)	5 (6)	3 (3)	2 (2)	2 (3)	- (3)
(SC) VER	9 (8)	12 (8)	17 (11)	15 (13)	15 (11)	9 (8)	6 (7)	4 (5)	3 (5)	3 (4)	4 (4)	3 (5)

*The left-hand figure in each square is the measured value; the figure in parenthesis is the predicted value. All values are in parts per million of carbon monoxide, averaged over a period of one hour.

Systems Applications, Inc.[34]

4. Pacific Environmental Services, Inc.
The model has been tested for the Los Angeles Basin using meteorological data for more than twenty stations. Simulations were run for September 29 and 30, 1969, both high smog days. All trajectories terminated at pollutant monitoring stations. A summary of these simulations is shown in Table 15. In addition, the model has been used for control strategies such as the variation of traffic patterns.

5. The Center for the Environment and Man, Inc.
The model has been applied to the state of Connecticut (funded by NAPCA) and also to the Toronto Metropolitan Region (funded by the Canadian government). The grid scale used in Connecticut (5000 ft) and that in Toronto (1000 meters) were much larger than would be applicable to many transportation problems. Each did, however, include several thousand sources of each of five pollutants: CO, hydrocarbons, particulates, nitrogen oxides and SO_2 and each source value included the contribution due to mobile sources (cars, trucks, buses, etc.) with given traffic distribution data.
Each application was extensively tested in a validation phase with dozens of samplers operated in dozens of test periods. Full discussion of validation test results was given in project reports, but basically 2-hour average concentrations for 30 selected stations were within a factor of 2.25 fifty-percent of the time, while only one-percent were in error by a factor of 10.
The work discussed above was with a previous version of the model which limited the calculations to those sources which affected only a few selected receptor points. The present version of the model considers the influence of every source upon the concentration of every grid point.

TABLE 15. COMPARISON OF CALCULATED VS. OBSERVED CONCENTRATION VALUES, MIXING DEPTH*, AND ASSOCIATED DATA**

	MIX/DEP (Meters)	O_3	NO_2 (pphm)	NO	CO
Run #1 9/30 Station: Burbank					
Start at 0715	30	2	11	51	2281
Calc. at 0930	266	10	7	4	698
Observed: Hour 9		6	28	33	1400
Run #2 9/30 Station: Burbank					
Start at 0830	55	6	10	35	2543
Calc. at 1130	571	22	11	3	1882
Observed: Hour 11		20	50	5	1800
Run #3 9/30 Station: Burbank					
Start at 1030	214	4	23	23	502
Calc. at 1330	840	19	12	4	678
Observed: Hour 13		10	-	-	800
Run #4 9/29 Station: Burbank					
Start at 0715	30	3	16	29	1724
Calc. at 0930	30	15	53	22	2600
Observed: Hour 9		7	29	14	900
Run #5 9/29 Station: Burbank					
Start at 0830	30	5	24	23	1602
Calc. at 1130	280	33	18	4	1958
Observed: Hour 11		14	19	3	1000
Run #6 9/29 Station: Burbank					
Start at 1030	157	12	23	5	976
Calc. at 1330	2058	22	7	2	942
Observed: Hour 13		14	-	-	700
Run #7 9/29 Station: Azusa					
Start at 0715	30	3	13	6	1029
Calc. at 0930	106	8	13	10	1186
Observed: Hour 9		16	11	1	1000
Run #8 9/29 Station: Azusa					
Start at 0830	30	8	17	5	1083
Calc. at 1130	418	19	10	4	1172
Observed: Hour 11		24	5	1	600
Run #9 9/29 Station: Azusa					
Start at 1030	250	17	30	4	1036
Calc. at 1330	839	16	4	2	531
Observed: Hour 13		38	-	-	900
Run #10 9/29 Station: Azusa					
Start at 1230	273	10	10	3	3630
Calc. at 1530	444	4	1	1	22
Observed: Hour 15		14	5	1	600
Run #11 9/29 Station: Pasadena					
Start at 0830	30	7	14	12	1302
Calc. at 1130	330	39	29	5	2672
Observed: Hour 11		41	12	1	-
Run #12 9/29 Station: Long Beach					
Start at 0830	30	3	17	17	1021
Calc. at 1130	293	16	12	5	1910
Observed: Hour 11		6	22	8	600
Run #13 9/29 Station: West LA					
Start at 0830	30	3	18	24	1254
Calc. at 1130	220	15	29	13	1605
Observed: Hour 11		12	-	-	500
Run #14 9/29 Station: Downtown LA					
Start at 0715	30	2	8	28	1542
Calc. at 0930	30	38	98	14	5510
Observed: Hour 9		8	19	30	-
Run #15 9/29 Station: Downtown LA					
Start at 0830	30	3	17	24	1190
Calc. at 1130	235	38	52	9	3183
Observed: Hour 11		9	10	5	600

*Start and Final Values Shown.
**Includes Background (Initial) Concentrations.

Pacific Environmental Services, Inc.

6. Lockheed Missile and Space Company, Inc., Huntsville Research and Engineering Center
The model has been evaluated by EPA for the Department of Transportation (FAA) in conjunction with a proposal to simulate airport quality resulting from airport taxiing and airport operations, including vehicular traffic on and adjacent to the airport. The model was considered acceptable. We do not have real-world data with which to validate the model. We have statistically validated other atmospheric models with real-world data and see no reason why this model will not validate at the 90% and 95% error level within the atmospheric and monitoring data accuracies.

7. ESL, Inc.
The model has been tested using simultaneous air quality and meteorological data from the New Jersey Turnpike and from several California high volume freeways. Most of these experiments were conducted during 1971 and are continuing into 1972. The results have confirmed model predictions over a range of wind speeds, directions, traffic volumes, roadway geometries and roadway designs. The model was verified both in absolute magnitude and in predicting the three dimensional air quality levels in the vicinity of the roadways.

8. Systems, Science and Software
The model (i.e., model 1, see Table 7) has been tested by simulating CO concentrations in the Los Angeles Air Basin ($\sim$20x40 miles) on two separate days - September 23, 1966 and September 30, 1969 - for the major part of each day. The day-averaged concentrations predicted at 12 Los Angeles Air Pollution Control District (APCD) sampling sites averaged within 20 percent of the measured data. The correlation coefficient for the simulated and observed concentrations was 0.73 with a mean deviation of 0.67 ppm. Results are shown in Table 16.
The photochemical version of the model has been tested by

TABLE 16. 3 A.M. TO 8 P.M. AVERAGE CARBON MONOXIDE CONCENTRATIONS (CO IN PPM)

STATION	Observed	Simulated by the Present Model	Gaussian Model Simulation
Downtown LA	16	18	22
Azusa	13	11	3
Pasadena	17	21	15
Burbank	16	20	7
East LA	12	18	5
West LA	16	12	13
Long Beach	14	13	8
Hollywood	17	17	7
Pomona	13	10	3
Lennox	13	11	11
Anaheim	9	9	7
La Habra	6	9	3

Systems, Science and Software[43]

simulation of NO, NO_2, O_3 and HC concentrations in the Los Angeles Air Basin, for September 30, 1969. The results were qualitatively correct - showing O_3 build-ups, NO conversion to NO_2, and NO_2 depletion. The sets of photochemical reactions available at the time of the simulation were insufficient to correctly predict the effect of the chemical reactions. Work has been continuing on further development of a good reaction set.

9. Environmental Research and Technology, Inc.
The model has been validated in several studies. Of particular relevance to highway problems, the model predictions were compared with measured concentration levels from six sampling sites along and adjacent to an existing roadway near Seattle, Washington. The measurements were made over a time period of four months. Observed and computed concentrations of carbon monoxide and hydrocarbons were highly correlated with near unity regression analysis slopes.

10. General Research Corporation
    A. Model 1 (see Table 7) is currently undergoing controlled evaluation under contract from the Environmental Protection Agency. Preliminary validation has been reported in Reference 33. Computed carbon monoxide concentrations generally agreed with measured values within $\pm 20\%$. In the case of photochemical products, reasonably good results were obtained by adjusting model parameters. However, the authors state that much more work needs to be done in order to remedy uncertainties in both the data and in the model assumptions.

    B. Thus far, validations of model 2 (Table 7) have consisted of comparisons with various analytical solutions (e.g., for steady state Gaussian plumes and step changes in flux or concentration boundary conditions). In each case, it has been possible to achieve accuracy in the 90% and above range which is certainly within the error of real-world input data.

11. Computer Sciences Corporation
The model output for the 18-hour, September 23, 1966 period for the Los Angeles basin has been compared with actual pollution concentrations as monitored by the L.A. Air Pollution Control District (APCD). Concentrations at 1200 points were tabulated. Most of the computed concentrations fell within a factor of three of the measured values. Currently identified sources of error relate to wind convergence and transport through the boundaries. Technical approaches to resolve these problems have been proposed.

6.2 VALIDATION OF MODELS FOR NON-TRANSPORTATION SOURCES

1. GEOMET, Inc.
Model calculated results have been compared with SO_2 concentrations observed in St. Louis and Chicago. There were 9420 comparisons of two-hour concentrations at 10 stations over an 89 day winter period for St. Louis. There were 5407 comparisons of one-hour concentrations at eight stations over a 31 day January period for Chicago. The following results were achieved.

Comparison of Error Distributions in Percent(%) for Two-Hourly St. Louis and Hourly Chicago Validation Calculations

Range of Predicted Minus Observed Concentration $\mu g/m^3$	St. Louis (Mean Observed Concentration = 154 $\mu g/m^3$)	Chicago (Mean Observed Concentration = 96 $\mu g/m^3$)
$\pm$ 5	8	8
$\pm$ 10	15	17
$\pm$ 20	25	30
$\pm$ 50	46	53
$\pm$ 100	65	73
$\pm$ 150	76	82

The following results were obtained for long term concentrations at individual locations:

Period	Number of Comparisons	Location	Regression of observed on predicted Correlation	Slope	Intercept
Dec. 1964 - Feb. 1965	10	St. Louis	0.675	0.98	-0.56
Jan. 1967	8	Chicago	0.873	0.63	4.9

Averaged over all stations the results were:

Location	Observed mean	Calculated mean
St. Louis	154	151
Chicago	96	145

2. AVCO Systems Division
   No validification has yet been made for the air pollution study. However, a similar computation has been made for the air dissociation behind a hypersonic projectile and the results compared very well with the measured data.

3. The Center for the Environment and Man, Inc.
   Model results have been compared with single point measurements accumulated over many years. Thirty (30) day expected values and thirty (30) day adverse values fell within 20 percent.

4. Mt. Auburn Research Associates, Inc.
   The model has been validated by comparing simulated fall-out data with observed data for a number of nuclear test shots. Atmospheric conditions vary widely. Geographic locations are the Nevada Test Site and the Pacific test islands (Bikini and Eniwetok atolls). Details regarding the observed data are classified, however the agreement of data is excellent.

5. INTERCOMP

The model has been tested in two ways. First, the wind calculation has been compared with flow tests in wind tunnels with complex flow geometry--i.e. simulating both urban buildings and terrain features. Second, calculated SO_2 concentrations have been compared with values measured in a large urban area. Both of these tests were quite satisfactory.

We have also made extensive application of our model to single-plant problems with measured concentrations available at several different points. Among these applications were (1) a copper smelting operation located between a large body of water and an adjacent mountain range, (2) emissions from a hydro-fining operation located in a river valley and affected by the valley winds as well as the predominating regional wind system, and (3) a gas processing plant where brief periods of high concentration were caused by a fumigation effect in breaking up a low-level temperature inversion. In each of these applications the model gave computed concentrations in good agreement with measured concentrations. The areas described ranged from roughly fifteen square miles to over one hundred square miles. The time periods correspond to from one to twenty days taken from the last year and one-half.

We have not validated the model for transportation problems by comparing it with measured traffic emission data. Rather, the model has been validated with a more general class of diffusion problem where other complicating features are present such as terrain and plume rise. We would anticipate no difficulty in applying the model to transportation problems. The increased flexibility of our model should allow a much more complete description of the transportation problem than has previously been considered--e.g. flow and diffusion associated with elevated freeways and other complex flow problems.

6. TRC

The model was validated for the State of Connecticut for SO_2 and particulates for twelve 2-hour average concentrations on each of 24 days. For 555 24-hour mean particulate concentrations 50% were within a factor of 2, 1% were outside a factor of 10. For SO_2 2-hour averages (5651 comparisons of observed and predicted data) 50% were within a factor of 2.25 and 5% outside a factor of 10. When averaged for 24 hours (469 comparisons), 50% were within a factor of 1.75 and 0.5% were outside a factor of 10.

The model was validated in Toronto for SO_2 for one-hour concentrations (over 5000 comparisons). Fifty percent of the comparisons observed/calculated were within a factor of 1.7 and 0.2% were outside a factor of 10. Overall, about 60% of the comparisons were within a factor of 2. The improved validation at Toronto arises from the smaller geographic region considered and the smaller variability in source distribution.

7. Environmental Research and Technology, Inc.

The model results have been compared with results of other (Gaussian plume type) models, some theoretical (analytic) solutions to the governing equation, and tested with data taken from a study of fumigation of upper level emissions.

A major problem in 'real-world' validation of numerical models is the lack of detailed observation of wind and diffusivity fields, together with air pollution measurements. The results of the comparisons made to date show that the model predicts concentration values in agreement with measurements and with theory.

8. Systems Control, Inc.

Numerous models have been developed and verified based on actual process data. The program updates parameters in the model iteratively until the best possible model is found, i.e., the model with the smallest error. The models have been validated with the well known Box and Jenkins Q test for model acceptability. Recent models developed by SCI have passed the Q test for model acceptability at the 95% level in the petrochemical and aeronautical industries.

9. Euclid Research Group
   The model has been validated for military applications with data from Pacific nuclear-explosion tests. The maximum period of time was about 24 hours.

10. Argonne National Laboratory
    Calculations for the Chicago region growth models compare satisfactorily with observations.

6.3 CONCLUSIONS

From the foregoing, it is apparent that the validation of models is far from satisfactory, primarily due to the fact that data for validation has been very scarce. This is especially evident when one notes that all of the results for the Los Angeles basin are based upon two particular days for which data happens to be available. Presumably, this state of affairs has now been partially rectified by the installation of a 42 mile instrumented highway loop in the vicinity of Los Angeles. Also, if present plans are implemented, a similar instrumented test bed will be installed in St. Louis in 1972[44]. These two sites should furnish adequate data for the comparative evaluation of models which deal with the dispersion of highway pollutants.

Validation of photochemical models has barely begun. Again, a major problem is data. However, problems of model resolution are also present as demonstrated by the fact that the models fail in the same way when handling laboratory data, as they do when applied to real-world data.

The results to date are too skimpy to conclusively demonstrate that the conservation of mass approach is superior to the Gaussian methods, although the former has a decisive theoretical advantage. It may be that, in practice, this advantage cannot be realized because of the difficulty in estimating the eddy transport terms. This points to the fact that inadequate resolution in the meteorological data is a major factor in modeling inadequacies, both for the Gaussian and the conservation of mass formulations. It is the universal practice of investigators to point to this source of error when their models fail - and with good reason. Nor are prospects good for solving this problem. The modeler will generally have to be content with routine meteorological data except in the vicinity of large cities where special soundings are available. This is due to the fact that the conventional meteorological network was designed to provide observations on the meso (10's of miles) and macro (100's of miles) scales, whereas many pollution problems must be dealt with on the micro (miles) scale. Of course, this deficiency could be overcome (at considerable expense in computer time) by laboriously solving the complete Navier-Stokes equations to obtain the turbulence field.

The difficulty in estimating source emissions is another impediment to model performance. Again, this is an area where progress cannot soon be expected, both because of the complexity of the problem and because of the near impossibility of making the required measurements.

Finally, it must be stated that the best hope for advancement in the field of air pollution modeling is controlled experimentation. Test beds are becoming available, as noted above, and hence the opportune time has arrived to competitively evaluate the best available models in order to quantitatively assess the strengths and weaknesses of each. This testing phase should be supported by a research and development program aimed at improving, refining and extending the most promising models.

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APPENDIX A

LIST OF REQUESTERS AND RESPONDERS
THE TSC QUESTIONNAIRE
THE SAMPLE COMPLETED QUESTIONNAIRE

List of Companies Requesting and Returning the TSC Questionnaire

Name	Address	TSC Questionnaire Requested	TSC Questionnaire Returned
Aeronautical Research Associates Of Princeton	50 Washington Road Princeton, N.J. 08540	X	X
Aerophysics Research Corp.	Box 187 Bellevue, Wash. 98009	X	
Aerospace Systems Inc.	One Vine Brook Park Burlington, MA 01803	X	
Air Resources, Inc.	800 E. Northwest Highway - Palatine Illinois 60067	X	
Anderson-Nichols Company Inc.	150 Causeway Street Boston, Mass. 02114	X	
Arthur D. Little Inc.	Acorn Park Cambridge, MA 02140	X	
AVCO Everett Research Lab.	2385 Revere Beach Pkwy. Everett, Ma 02149	X	
AVCO Systems Division	Wilmington, MA 01887	X	X
Battelle Columbus Labs	505 King Avenue Columbus, Ohio 43201	X	X
Boeing Computer Serv.	P.O. Box 24346 Seattle, Wash.	X	X
Carnegie-Mellon University, Environ-mental Studies Institute	Schenley Park Pittsburgh, Pa 15213	X	
Center for Air Environment Studies Pennsylvania State University	204 Chemical Engineering University Park, Penn. 16802	X	
Center for Environ-mental Studies Argonne National Laboratory	9700 So. Cass Ave. Argonne, Illinois 60439	X	12

List of Companies Requesting and Returning the TSC Questionnaire (Continued)

Name	Address	TSC Questionnaire Requested	TSC Questionnaire Returned
Chairman, Meteorology Dept. UCLA	Los Angeles, Calif.	*	
Community Sciences Inc., Engineering & Planning	1835 K Street Suite 502 Washington, D.C. 20006	X	
Computer Sciences Corp.	8728 Colesville Rd. Silver Spring, MD 20910	X	X
CONSAD Research Corp.	121 No. Highland Avenue Pittsburgh, Penn. 15206	X	
Control Data Corp.	60 Hickory Drive Waltham, MA 02154	X	
Cornell Aeronautical Laboratory	4455 Genesse Street Buffalo, New York 14221	X	
CSC Computer Systems Engineering, Inc.	Republic Road Treble Cove Industrial Park North Billerica, MA 01862	X	
Datatronic Systems Corp.	8155 Van Nuys Blvd. Panorama City, Cal. 91402	X	
Dept. of Mechanical Engr. M.I.T.	Cambridge, MA	*	
Diversified Technology Inc.	339 W. Broadway San Diego, CA 92112	X	
Donald Arnstein	10920 Rose Avenue Los Angeles, Calif. 90034	X	
Engineering Numerics Corp.	P.O. Box 637 Dallas, Texas 75207	X	

*Questionnaire was mailed without request to these organizations.

List of Companies Requesting and Returning the TSC Questionnaire (Continued)

Name	Address	TSC Questionnaire Requested	TSC Questionnaire Returned
Environmental Engineering	2324 S.W. 34th Street Gainesville, Florida 32601	X	
Environmental Research & Technology	429 Marrett Road Lexington, MA	*	2
ESL Inc.	495 Java Drive Sunnyvale, Calif. 94086	X	X
Euclid Research Group	1760 Solano Avenue Berkeley, Calif. 94707	X	X
Gas Dynamics Analysis & Test Aero-Thermo-dynamics, Lockheed Missile & Space Co.	Sunnyvale, Calif.	*	X
General Electric Lexington, MA 02173	114 Waltham Street	X	
General Electric Company Reentry and Environmental Systems Division	P.O. Box 855 Philadelphia, Penn. 19101	X	
General Electric Co. Transportation Systems Div.	2901 East Lake Road Erie, Pa 16501	X	
General Research Corp. Systems Research Div.	P.O. Box 3587 Santa Barbara, Calif. 93105	X	2
GEOMET, Inc.	50 Monroe Street Rockville, MD 20850	X	X
Gibbs & Hill, Inc.	393 Seventh Avenue New York,New York 10001	X	

*Questionnaire was mailed without request to these organizations.

List of Companies Requesting and Returning the
TSC Questionnaire (Continued)

Name	Address	TSC Questionnaire Requested	TSC Questionnaire Returned
Grumman Aerospace Corp.	Bethpage, N.Y. 11714	X	X
Head, Dept. of Meteorology, M.I.T.	Cambridge, MA	*	
ITRI IIT Research Institute	10 W. 35 Street Chicago, Illinois 60616	X	
Information & Communication Applications, Inc.	Suite 805, The World Bldg. 8121 Georgia Avenue Silver Spring, Maryland 20910	X	
INTERCOMP	200 West Loop South Suite 1480 Houston, Texas 77027	X	X
I. V. Computer Consultants Inc.	55 Northern Blvd. Greenvale, N.Y. 11548	X	
Jackson & Moreland Publications	438 Park Square Bldg. Boston, Mass. 02116	X	
John D. Kettelle Corp.	1770 Lancaster Pike Paoli, Penn. 19301	X	
Kaman Sciences Corp.	1700 Garden of the Gods Road Colorado Springs, Col. 80907	X	X
Lockheed Aircraft Corp.	3127 McDowell Avenue N.W., Huntsville, Alabama 35805	X	X
Lockheed Electronics Co., Inc.	Plainfield, N.J. 07061	X	
Meteorology Dept. University of Wisconsin	Madison, Wisconsin	*	

*Questionnaire was mailed without request to these organizations.

List of Companies Requesting and Returning the TSC Questionnaire (continued)

Name	Address	TSC Questionnaire Requested	TSC Questionnaire Returned
Meteorology Research Inc.	P.O. Box 637 Altandena, Cal. 91001	X	
Methonics Inc.	6239 Edgewater Drive Orlando, Florida 32810	X	
Michigan Techno-logical University	Houghton, Michigan 49931	X	
Midwest Research Institute	425 Volker Blvd Kansas City, Missouri 64110	X	
MSA Research Corp.	Laboratory & Plant Evans City, Penn. 16033	X	X
Mt. Auburn Research Associates, Inc.	385 Elliot Street Newton, MA 02164	X	X
North American Weather Consultants	Santa Barbara Municipal Airport Goleta, Cal. 93017	X	
Northern Research & Engineering Corp.	219 Vassar Street Cambridge, MA	X	X
NUS Corporation	4 Research Place Rockville, Md. 20850	X	
Pacific Environmental Services Inc.	P.O. Box 25925 W. Los Angeles, Calif. 90025	X	X
Research Institute Oklahoma University	Norman, Oklahoma 73069	X	
Riverside Research Institute	80 West End Avenue N.Y., N.Y. 10023	X	
Ryckman-Edgerley-Tomlinson & Assoc	500 Coronet Building 225 So. Meramec Ave. St. Louis, Missouri 63105	X	
Scott Research Laboratories, Inc.	P. O. Box D-11 Plumsteadville, Penn. 18949	X	

List of Companies Requesting and Returning the TSC Questionnaire (Continued)

Name	Address	TSC Questionnaire Requested	Returned
Sierra Research Corp.	P. O. Box 3007 Boulder, Colorado 80303	X	
Space & Planetary Science Department Wolf Research & Development Corp.	6801 Kenilworth Ave. Riverdale, MD 20840	*	
Stanford Research Institute	Menlo Park Calif. 94025	X	X
Systems Applications Inc.	9418 Wilshire Blvd. Beverly Hills, Calif. 90212	X	X
Systems Control Inc.	260 Sheridan Avenue Palo Alto, Calif. 94306	X	X
Systems Science & Software	P.O. Box 1620 LaJolla, Calif.	X	2
Texas Instruments Inc.	13500 No. Central Expressway, Dallas, Texas	X	X
The Center for the Environment & Man Inc.	275 Windsor Street Hartford, Conn.	X	2
The MITRE Corp.	Westgate Research Park, McLean Va. 27101	X	
TRC/The Research Corporation of New England	210 Washington Street Hartford, Conn. 06106	X	X
TRW Inc, Mail Stop W1/6385 Washington Operations	Westgate Park 7600 Colshire Drive McLean, Virginia 22101	X	
Tulane University	New Orleans, La.	X	

*Questionnaire was mailed without request to these organizations.

List of Companies Requesting and Returning the TSC Questionnaire (Continued)

Name	Address	TSC Questionnaire Requested	TSC Questionnaire Returned
UCC	11480 Sunset Hills Road Reston, Va. 22070	X	
Walden Research Corp.	359 Allston Street Cambridge, MA 02139	X	2
Westinghouse Electric Corp. Research & Development Center	Beulah Road Pittsburg, Penn. 15235	X	X
Westinghouse Electric Co.	1801 K St. N.W. Washington, D.C.	X	

U.S. DEPARTMENT OF TRANSPORTATION

TRANSPORTATION SYSTEMS CENTER
55 BROADWAY
CAMBRIDGE, MASSACHUSETTS 02142

December 28, 1971

Dear

The questionnaire, MAP-01, which you requested in response to our Commerce Business Daily announcement of December 21, 1971 is enclosed. Thank you for your interest in furnishing the Government with information about your capabilities in the field of transportation source air pollution modeling.

Please return the completed questionnaire to me at code TCD no later than January 14, 1972.

Sincerely,

Eugene M. Darling, Jr.

Eugene M. Darling, Jr.
Chief, Software Implementation Branch

Enclosures:
  1 questionnaire
  1 sample completed questionnaire

Department of Transportation
Transportation Systems Center
Cambridge, Massachusetts

Transportation Source Air Pollution Modeling Questionnaire, MAP-01

Firm Name:

Firm Address:

Principal Investigator(s): Phone:

INSTRUCTIONS

Please type your answers directly on the attached questionnaire, MAP-01. A sample completed questionnaire for a hypothetical model is supplied for your guidance. The responses in the sample are at the desired level of detail; hence the space provided for your answers should be sufficient. Please fill out a separate questionnaire for each transportation source air pollution model which you wish to have the Government consider. At the top of each page of each questionnaire enter the firm name and the model name. Supplemental material is not required, but may be submitted at your option. However such material will not be considered unless it is accompanied by a completed questionnaire. No formal results of the evaluation of questionnaires will be furnished by the Government. The closing date for submission of questionnaires is January 14, 1972.

DISCLAIMER

____ hereby states that
Firm Name
the information submitted in the attached questionnaire(s), MAP-01 is not proprietary and further agrees that the Government is free to make any use of said information it deems appropriate, including publication with proper acknowledgements in Government technical reports.

____
Signature Date

____
Title

Firm Name:
Model Name:

DOT/TSC MAP-01/1

I. GENERAL DESCRIPTION OF THE MODEL

Briefly discuss the aspects of the model indicated below.

A. MODEL NAME:

B. PURPOSE:

C. TYPE:

D. BASIC EQUATION:

Firm Name:
Model Name:

I. (Continued)

E. SPECIFICATIONS:

Diffusion Coefficient:

Winds:

Mixing Level:

Stability Classes:

Other:

F. POLLUTANTS:

G. MISCELLANEOUS:

Firm Name:
Model Name:

DOT/TSC MAP-01/3

II. FLOW DIAGRAM OF THE MODEL

Draw a rough flow diagram showing inputs, model functions, and outputs.

Firm Name:
Model Name:

III. IMPLEMENTATION OF THE MODEL

A. STATUS

Is the model implemented in a working computer program? If not, is the program currently being written?

Can the program be directly used for modeling air pollution from transportation sources? If not, what level of effort (dollars and/or manpower) would be required to adapt the model to such applications?

III. (Continued)

B. HARDWARE REQUIREMENTS

Briefly describe the computer system required to run the program.

Computer:

Computer Word Size:

Program Memory Requirement (bytes or words):

Operating System Memory Requirements:

Peripheral Equipment Requirements:

Non-Standard Hardware:

III. (Continued)

C. SOFTWARE REQUIREMENTS

Discuss the following software aspects of the program.

Operating System:

Operating System Modifications:

Operating System Functions Used:

Programming Language:

Program Size (lines of code):

Program Adaptability:

Can the program be run on a similar computer at another installation?

Can the program be run on another computer?

IV. PROGRAM OPERATION

A. CHARACTERISTICS

Discuss the following factors relating to the manner in which the program runs.

Flexibility:

Is the input extensively parameterized, or is major reprogramming required for different input conditions?

Structure:

Does the program consist of several distinct parts which are run separately, or does it consist of unified parts which interface and run automatically?

Other:

Are there other special characteristics which affect program operation? Explain:

Firm Name:
Model Name:

IV. (Continued)

B. INPUT

For each type of input data describe the source, frequency, distribution, units, format and other pertinent aspects.

Meteorological Data:

Emission Data:

Other Data:

Firm Name:
Model Name:

IV. (Continued)

C. COMPUTATIONS

In order to provide a rough indication of the operating speed and the cost of running the model, describe a typical problem that has previously been run and supply the information requested.

Typical Problem:

Computation Specifications for this Problem:

CPU time:

Running time:

Channel usage:

Cost of the run:

Firm Name:
Model Name:

IV. (Continued)

D. OUTPUT

Describe the output. Give units, frequency, distribution, format and other pertinent information.

Tabular Data:

Graphical Data:

V. <u>VALIDATION</u>

Has the model been validated with real-world data? If so, indicate the period of time, sample size, geographical area, and the results of such validation(s).

SAMPLE

Firm Name: AXY Inc.
Model Name: HIPO

DOT/TSC MAP-01/1

I. GENERAL DESCRIPTION OF THE MODEL

Briefly discuss the aspects of the model indicated below.

A. Model Name:

HIway POllution (HIPO) Model

B. Purpose:

HIPO computes the concentration of pollutants in the vicinity of highways. It is intended as a flexible analytic tool which can be used by planners, designers, and builders of highways to assess the impact of highway emissions on ambient air quality.

C. Type:

Gaussian plume generalized to the case of a continuous line source.

D. Basic Equation(s):

$$C = \frac{\sqrt{2}\,Q}{\sqrt{\pi}\,u\sigma_z}$$

Firm Name: AXY
Model Name: HIPO

I. (Continued)

E. Specifications:

Diffusion Coefficient: an empirical σ_z

Winds: horizontal and vertical winds are assumed constant over a period of 1 hour.

Mixing Level: computed from an adjacent 12Z sounding.

Stability Classes: 3

Other:

F. Pollutants:

CO, particulates. Cannot accommodate photochemical reactions.

G. Miscellaneous:

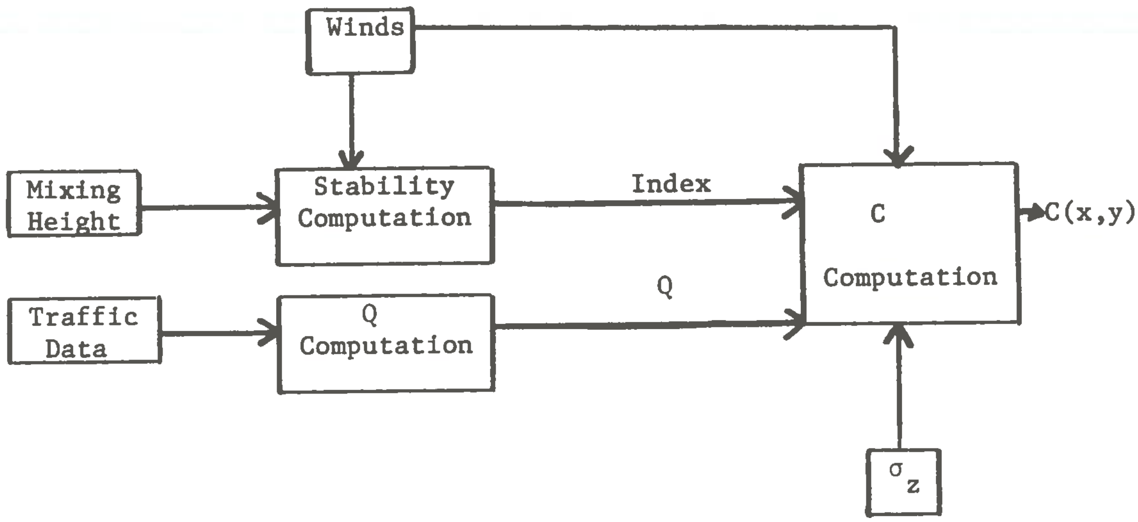
This model is one of a family which is being developed to analyze the impact of transportation emissions on air quality.

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/3

II. FLOW DIAGRAM OF THE MODEL

Draw a rough flow diagram showing inputs, model functions, and outputs.



SAMPLE

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/4

III. IMPLEMENTATION OF THE MODEL

A. Status

Is the model implemented in a working computer program? If not, is the program currently being written?

The model is fully operational for non-reactive pollutants. It is currently being modified to handle photochemical reactions. Modifications are expected to be completed by March 1972.

Can the program be directly used for modeling air pollution from transportation sources? If not, what level of effort (dollars and/or manpower) would be required to adapt the model to such applications?

The program has been specifically designed to calculate the diffusion of highway pollutants. The modification mentioned above is being carried out with Company funds at an estimated cost of $5K.

SAMPLE

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/5

III. (Continued)

B. Hardware Requirements

Briefly describe the computer system required to run the program.

Computer:

IBM 360/50

Computer Word Size:

8 bit bytes, 4 bytes per word. Computations are done in single precision.

Program Memory Requirement (bytes or words):

40,000 bytes

Operating System Memory Requirements:

60,000 bytes

Peripheral Equipment Requirements:

One 2311 disk drive, two 9-track magnetic tape drives, one card reader, one printer.

Non-Standard Hardware:

One CALCOMP plotter.

C. Software Requirements

Discuss the following software aspects of the program.

Operating System:

OS-360

Operating System Modifications:

Priority scheduling for real-time data entry.

Operating System Functions Used:

FORTRAN I/O
Data management MACROS for CALCOMP output
Special MACROS for real-time data entry.

Programming Language:

FORTRAN IV. CALCOMP interface routines written in BAL.

Program Size (lines of code):

1200 lines FORTRAN, 200 lines BAL.

Program Adaptability:

Can the program be run on a similar computer at another installation?

Yes, with operating system modifications indicated above. CALCOMP interface required for graphical output.

Can the program be run on another computer?

Yes, provided that the BAL/CALCOMP interface is rewritten for the other computer.

Firm Name: AXY
Model Name: HIPO

IV. PROGRAM OPERATION

A. Characteristics

Discuss the following factors relating to the manner in which the program runs.

Flexibility:

Is the input extensively parameterized, or is major reprogramming required for different input conditions?

The program is completely general and can accommodate any winds, mixing height and traffic data as input. The program need be modified only if the basic diffusion equation is changed.

Structure:

Does the program consist of several distinct parts which are run separately, or does it consist of unified parts which interface and run automatically?

A separate program, used for real-time collection of traffic data, generates an input tape for the simulation. The simulation, itself, runs automatically.

Other:

Are there other special characteristics which affect program operation? Explain:

There are two options for CALCOMP output. Normally a tape is produced by the simulation and run off-line to generate graphical output. However, the simulation can also be made to interface directly with the plotter.

SAMPLE

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/8

IV. (Continued)

B. Input

For each type of input data describe the source, frequency, distribution, units, format and other pertinent aspects.

Meteorological Data:

Winds: Surface winds in degrees and knots for up to 10 measurement stations are entered each hour. Upper level winds at 1000 ft. intervals up to 10,000 ft. for 5 stations or less are entered twice daily. These data are input on cards.

Soundings: Temperature soundings to 700 mb, both mandatory and special levels, for up to 3 stations are entered twice daily on cards.

Emission Data:

Emissions are computed by standard methods from the instantaneous traffic data. The data required is the number of each type of vehicle (e.g. car, bus, truck etc.) within each one mile segment of road at five minutes intervals during the simulation period. These data are input to the main simulation via magnetic tape.

Other data:

Diffusion Coefficient: Single empirical value of σ_z in feet is entered each hour via cards.

Stability Index: computed every hour from wind and mixing height data and entered via cards.

SAMPLE

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/9

IV. (Continued)

C. Computations

In order to provide a rough indication of the operating speed and the cost of running the model, describe a typical problem that has previously been run and supply the information requested.

Typical Problem:

The average hourly concentration of CO and particulates at 100 points adjacent to a 20 mile stretch of highway was computed for a 24 hour period.

Computation Specifications for this Problem:

CPU time: 10 minutes

Running time: 30 minutes

Channel usage:

Unit	Number of Accesses
Magnetic tape	100,000*
Disk	1,000
Card Reader	100
Line Printer	2,000

*Normal CALCOMP mode used

Cost of the run: $500

SAMPLE

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/10

IV. (Continued)

D. Output

Describe the output. Give units, frequency, distribution, format and other pertinent information.

Tabular Data:

The average hourly concentration of CO and particulates in ppm is listed for up to 100 points adjacent to the highway. Average six hour, twelve hour and twenty four hour concentrations are listed for the same points. These data are output via line printer.

Graphical Data:

CALCOMP plots of average CO and particulate concentration isopleths for the area adjacent to the highway are generated for each hour.

Firm Name: AXY
Model Name: HIPO

DOT/TSC MAP-01/11

V. VALIDATION

Has the model been validated with real-world data? If so, indicate the period of time, sample size, geographical area, and the results of such validation(s).

The model has been extensively tested using data from an instrumented section of the Santa Monica Freeway. During the past year the model has been run and verified for 6 separate 10 day periods which spanned the four seasons and included a wide variety of meteorological conditions. The mean error and 95% error level for these 6 periods is shown below:

Errors (ppm)

Averaging Interval (Hrs)	CO Mean	CO 95%	Particulates Mean	Particulates 95%
1	.08	.25	.17	.41
6	.06	.21	.14	.37
12	.05	.16	.10	.25
24	.02	.10	.06	.19

AXY Inc. believes that these errors are within the tolerances required for effective assessment of the impact of highway emissions on air quality.