PROCEEDINGS OF SYMPOSIUM ON MULTIPLE-SOURCE URBAN DIFFUSION MODELS

U. S. ENVIRONMENTAL PROTECTION AGENCY

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Editor: Arthur C. Stern

Sponsors: National Air Pollution Control Administration
and North Carolina Consortium on Air Pollution

U.S. ENVIRONMENTAL PROTECTION AGENCY
Air Pollution Control Office
Research Triangle Park, North Carolina, 1970

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Air Pollution Control Office Publication No. AP-86

PREFACE

This symposium was conducted under the terms of a contract between the Meteorology Division of the National Air Pollution Control Administration (NAPCA) and the Department of Environmental Sciences and Engineering, School of Public Health, University of North Carolina at Chapel Hill (UNC). The contract officer for the sponsor was Mr. Lawrence E. Niemeyer, Assistant Director, Division of Meteorology, NAPCA. The responsible officer for the University was Arthur C. Stern, Professor of Air Hygiene. The symposium was held from October 27 to 30, 1969, at the Carolina Inn on the University campus. On December 4, 1970, the functions of NAPCA were transferred to the Air Pollution Control Office (APCO) of the Environmental Protection Agency. All references to the former, therefore, now refer to the latter.

Although UNC was the contractor, it was agreed that the symposium would be sponsored by the North Carolina Consortium on Air Pollution, comprising: Duke University; North Carolina State University; the Office of Manpower Development, NAPCA; Research Triangle Institute; and the University of North Carolina at Chapel Hill. The detailed planning for the symposium was done by a steering committee representing the members of the Consortium and the contract officer.

All the papers, both invited and volunteered, that were presented during the symposium, are included in this volume. In addition to the invited participants, some attendees were selected from persons who responded to the public announcement of the symposium. Almost all papers were preprinted and distributed to participants in advance of the meeting. Although there was open discussion after every presentation except the Keynote and Banquet speeches, the only discussions incorporated in the Proceedings are those subsequently submitted in writing.

Questions from the floor and authors' responses do not appear unless those same questions and answers were also included in the written discussion. Every author questioned was given an opportunity to submit a rebuttal. The nature of such an arrangement made it necessary, for the sake of coherence, to incorporate all discussion in a separate chapter, divided into two sections: speaker-directed discussions and discussions submitted by the participants.

Particular thanks are given to the graduate students in Air Pollution in my department at UNC, who acted as floor monitors during the symposium – particularly to Harvey Jeffries and Douglas McKay, who managed the audio-visual arrangements throughout the symposium. The registration of participants and the preparation of the symposium program and information kits were ably handled by the Continuing Education Department of the School of Public Health, UNC. I am especially appreciative of the excellent services of my secretary, Martha Davis, for her help in the preparation and conduct of the symposium and in the coordination of these proceedings.

Arthur C. Stern
Chapel Hill, N. C.
November 1970.

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9. TIME – SPACE MODEL FOR SO_2

ABSTRACT

A multiple-source diffusion model for the simulation and prediction of long-term (climatological) ground-level sulfur dioxide concentrations in urban areas is described. The computer input consists of data from an emission source inventory together with statistics on relevant diffusion parameters.

Because of the capacity of available computers, only a limited number of the largest emission sources (approximately 150) can be treated individually. Smaller industrial emission sources are treated as residential sources. These are represented by a large number of stacks (about 150) of the same dimensions, distributed over areas of 1 square kilometer, for which the mean area emissions have been estimated.

The meteorological input consists of data on wind direction, windspeed, and Pasquill-Turner stability classes.[1, 2] *These parameters are assumed to be spatially homogeneous throughout the metropolitan area. Low-level emissions (residential) are correlated with low-level windspeeds and Pasquill-Gifford diffusion parameters,*[1, 3] *whereas high-level emissions (industrial) are correlated with extrapolated windspeeds and Brookhaven diffusion parameters.*[4] *The program also uses corresponding statistics for urban boundary layer depths and values for parameters affecting absorption at the earth's surface.*

The diffusion model used is basically Gaussian. It is modified, however, such that turbulent diffusion is restricted exclusively to the depth of the urban boundary layer. This is true for all sources having effective emission heights less than the height of the upper limit of the boundary layer. The rate of decay of sulfur dioxide is taken into account, as well as the experimentally determined absorption at the earth's surface.

The model calculates fields of steady-state ground-level concentrations that correspond to a given spatial distribution of emission sources and to any possible combination of relevant meteorological diffusion parameters. Knowledge of frequency distributions of these meteorological diffusion parameters permits the derivation of frequency distributions of ground-level concentrations for any location within or outside of the metropolitan area. The computerized experiments simulate frequency distributions of ground-level concentrations for a great number of regularly arranged grid points (up to 2500 with a mesh size of 500 by 500 meters) and for a variety of time periods (months, heating

period, seasons, year, etc.). The frequency distributions are characterized by a limited number of parameters (mean, percentiles, etc.). Each parameter is plotted as a system of isograms on a map of the metropolitan area.

Experiments to validate the model were conducted during the heating period in 1967-68 at four continuously monitoring stations that had been installed at special locations within the limits of the metropolitan area of Bremen. During the sampling period, the assumption of a sufficiently homogeneous wind field was validated by wind measurements at the same locations. The calculated frequency distributions of half-hourly mean values of concentrations generally agreed fairly well with those derived from observed values. Comparison, however, shows that the model does not simulate ground-level concentration fields in the vicinity of industrialized areas very well, because uncontrollable low-level emissions from industrial plants could not be taken into account in the diffusion model.

AUTHOR

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9. NUMERICAL SIMULATION OF TEMPORAL AND SPATIAL DISTRIBUTIONS OF URBAN AIR POLLUTION CONCENTRATION

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INTRODUCTION

Increasing industrialization in Germany during the 1950's led to great interest in the problem of ascertaining minimum stack heights essential to pollution control. In line, therefore, with its responsibilities in developing air pollution standards and criteria, the *Kommission Reinhaltung der Luft* [Air Pollution Control Commision] within the Association of German Engineers [*Verein Deutscher Ingenieure* (VDI)] established a research group on air pollution meteorology in 1958. The group was expected to develop the scientific basis for an approximate solution to the problem. The results of research during the first period, based mainly on the work of Sutton,[5] led to a simple nomogram for estimating minimum stack heights.[6, 7] The nomogram is widely used for legal and administrative purposes, although, among other shortcomings, very little is known about one of the most important input parameters of the model and therefore of the nomogram. This parameter (in German, *Immissions-Grundbelastung*) characterizes the temporal and spatial distributions (air loadings with time) of ground-level concentrations of pollutants in the area in which the newly built stack is located. In most cases the location is in an urban area already possessing a great number of emission sources. It is extremely difficult to define such a measure. A simple number constant in space and time, as proposed by the VDI,[7] will

not suffice for urban areas. Instead, such a parameter is dependent on horizontal space coordinates and, ultimately, on time (e.g., season).

In view of the crucial dependence of minimum stack heights on this parameter, some means of predicting ground-level concentrations in urban areas must be found before the stack-height problem can be solved.

Based on the work of Frenkiel,[8] the multiple-source urban diffusion model being described in this paper was developed by the author in 1962. It was hoped that this model would be able to solve problems of the kind mentioned above. After financial support for programming and computing time became available, a number of simulation experiments were conducted from 1963 through 1965. A tentative report was published early in 1966.[9] During that time the first papers on urban air pollution modeling by Turner[2] and Clarke,[10] although they aimed at the solution of the real-time prediction problem, were of great help. Especially, the replacement of Pasquill's stability categories[1] by Turner's[2] proved to be quite useful.

The purpose of the diffusion model is perhaps understood best by a discussion of Figure 9-1, which shows the logical structure of some features of the urban air pollution problem. Assuming that sufficient input data are available, a mathematical multiple-source urban air pollution model should yield a set of output data such as that indicated in Figure 9-1.

The most important of these data certainly is a real time short-term prediction of concentrations for the entire urban area. Most authors in the field of urban air pollution modeling were interested primarily in that problem. Following Turner,[2] they applied the well known steady-state theory of transport and dilution to simulate and predict time series of concentrations. Quite recently, Marsh and Withers[11] demonstrated the inadequacy of such a procedure. The model of Davidson[12] that applies a non-steady-state theory should provide a means of solving the short-term prediction problem, as well as the problem of time series simulation, more successfully. If this turns out to be true, the very important feedback circuit, "warning system," can be closed; i.e., appropriate control measures can be applied to the source-emission input in order to reduce the predicted concentrations below a given limit.

The problem of minimum stack heights and, more generally, that of city planning is connected with the problem of simulation and prediction of long-term (climatological) ground-level concentration fields. Here, time series of concentrations are of minor interest; instead, statistics of observed or calculated concentration fields for given long periods of time are important.

There is no doubt that for a given location and a given period of time only the frequency distribution of ground-level concentrations forms the basis of what could be called "air pollution climatology." Generally, these frequency

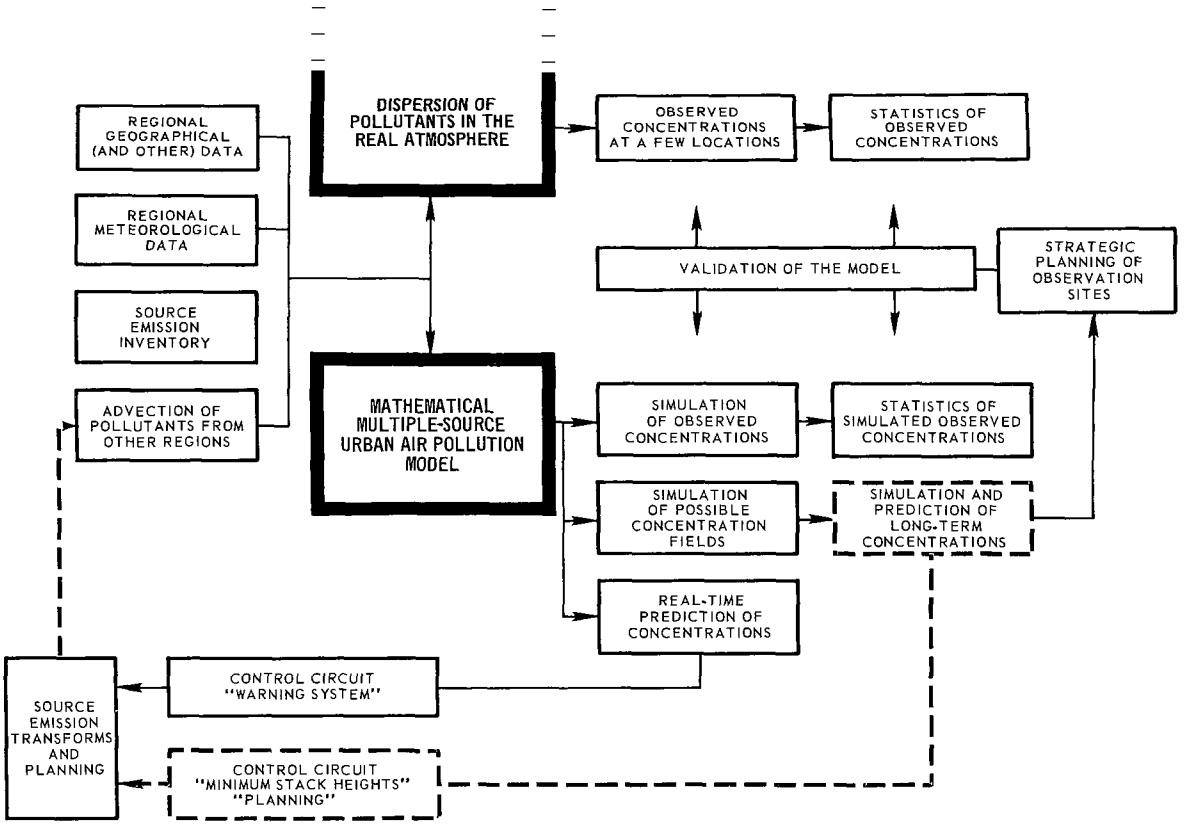

Figure 9-1. Major elements of the urban air pollution problem connected with mathematical modelling.

distributions vary from location to location within the urban area and with time and season. Figure 9-2 shows a typical example of the frequency distribution in winter of measured half-hourly mean values of sulfur dioxide concentrations in Bremen.

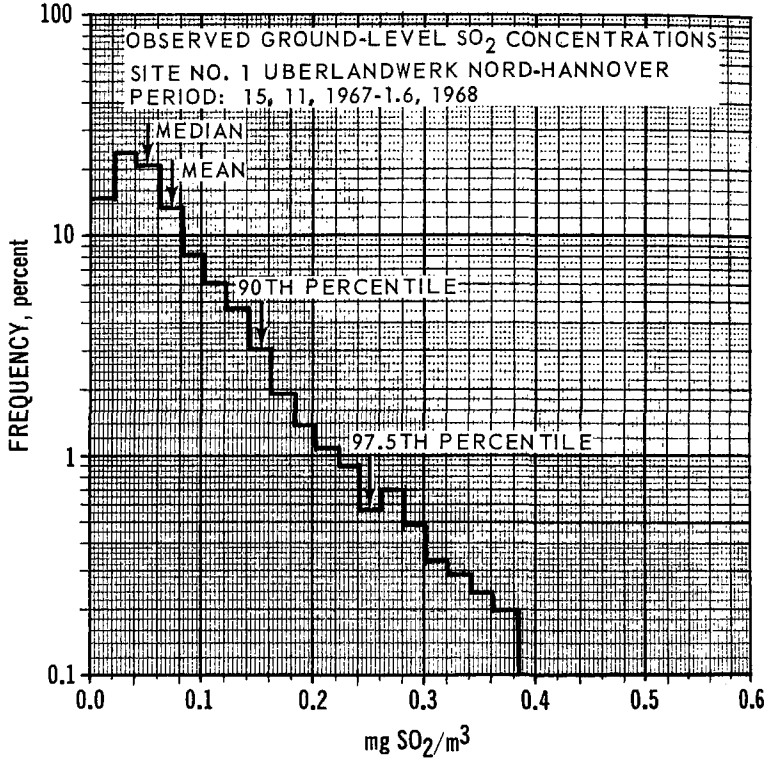

Figure 9-2. Winter time frequency distribution of measured half-hourly mean values of sulphur dioxide concentrations downtown Bremen.

Although it is not believed that a calculated steady-state field of concentration will fit observations at many locations within the urban area very well, it can be expected that statistical evaluation of a great number of such fields may lead to reasonable results in a climatological sense. This expectation forms the basis for this paper. If the expectation is justified, the feedback circuit, "minimum stack heights, city planning," can be closed and, in addition, means for the strategic planning of observation sites will then be available.

The following information is used in calculating pollutant concentrations: period of time (month, heating period, seasons, year, etc.) divided into equal

intervals (for example, hours); data from source emission inventories; relevant meteorological parameters, etc. From these data the model then calculates possible steady-state ground-level concentrations for each interval of time and for a large number of grid points within the urban area. From the stored concentration data, the frequency distribution of concentrations is obtained for each grid point. If the frequency distribution is characterized by a set of parameters (mean percentiles, etc.), these parameters are plotted as a system of isograms on a map of the urban area. Such maps then may be used to define the *Immissions-Grundbelastung* (ground-level concentrations), to solve problems of city planning as well as problems of strategic planning observation sites.

From the very beginning the main concern of the investigation was to apply the model to a real situation and to validate the model by suitable measurements. For several reasons the city of Bremen was chosen for the first mathematical experiments. Local authorities of the city of Bremen were willing and able (in 1963) to collect information on source emissions, which led to a very complete source emission inventory. The location of the city, on flat terrain and only 40 miles from the North Sea, is favorable in many respects: the city is well ventilated throughout the year and, in addition, the relevant meteorological fields are approximately homogeneous horizontally. In addition, advection of pollutants from other regions can be neglected. The input data, therefore, were well defined and relatively simple and allowed the application of a simple model.

MATHEMATICAL MODEL

The steady-state theory of the transport and dilution of pollutants is based on a number of simplifying assumptions: the relevant meteorological fields are stationary and are horizontally homogeneous; dispersion is not limited in the vertical direction; mean windspeed exceeds a certain lower limit; and the earth's surface is flat and not absorbing. The well-known formula for the spatial distribution of a pollutant[1] then is:

$$\chi = \frac{Q}{U} \exp[\gamma\tau] \frac{\exp\left[-\frac{y^2}{2\sigma_y^2}\right]}{\sqrt{2\pi}\,\sigma_y} \left\{ \frac{\exp\left[\frac{(h-z)^2}{2\sigma_z^2}\right]}{\sqrt{2\pi}\,\sigma_z} + \frac{\exp\left[-\frac{(h+Z)^2}{2\sigma_z^2}\right]}{\sqrt{2\pi}\,\sigma_z} \right\} \quad (1)$$

As usual, $h = h_s + \Delta h$ is effective stack height, $\tau = x/U$ is travel time, and $T = 1/\gamma$ is decay time.

Assuming that the plume standard deviations, σ_y and σ_z, are functions of travel time, τ, it can be shown that Equation (1) is a solution of the following[1,3] initial-value and boundary-value problem:

$$\frac{\partial\chi}{\partial\tau} = \frac{d}{d\tau}\left(\frac{\sigma_y^2}{2}\right)\frac{\partial^2\chi}{\partial y^2} + \frac{d}{d\tau}\left(\frac{\sigma_z^2}{2}\right)\frac{\partial^2\chi}{\partial Z^2} - \gamma\chi \quad (2)$$

$$\tau \to 0 : \quad \chi \to \frac{Q}{U} \delta(y) \delta(h-Z) \tag{3}$$

$$Z = 0 : \frac{\partial \chi}{\partial Z} = 0 \tag{4}$$

$$Z \to \infty : \chi \to 0 \tag{5}$$

The initial condition, that is, Equation (3), expresses the fact that a point source of strength, Q, is located at the effective stack height, h. The boundary conditions show that there is reflection of the pollutant at the earth's surface and further that dispersion is not limited in the vertical direction.

It may be noted that Equation (1) has the character of Green's function in the special boundary-value problem, Equations (2), (4), and (5). It seems legitimate, therefore, to apply Equation (2) to problems connected with boundary conditions different from those described by Equations (4) and (5) Two important assumptions are in question; that of a non-absorbing ground and that of unlimited vertical dispersion. Denoting by H the height of a ceiling restricting dispersion to a limited layer of the lower atmosphere (urban boundary layer), and denoting by $a(\tau, y)$ the absorption coefficient of the ground, the boundary conditions, Equations (4) and (5), can be replaced by:

$$Z = 0 : \frac{d}{d\tau}\left(\frac{\sigma_z^2}{2}\right) \frac{\partial \chi}{\partial Z} = a(\tau,y)\chi \tag{6}$$

$$Z = H : \frac{\partial \chi}{\partial Z} = 0 \tag{7}$$

Even if absorption is not a function of location, only mathematical, rather than experimental, methods are suitable for solving Equation (2) together with Equations (3), (6), and (7).[14] In view of the uncertainties connected with absorption at the ground, and with the functional behavior of plume standard deviations for such cases, only experimental calculations were performed with boundary-condition Equation (6).

Important for practical applications, however, is the assumption that dispersion is confined only to the urban boundary layer; i.e., the utilization of boundary condition Equation (7) for the upper ceiling of the layer (Figure 9-3).

Standard methods[15-17] allow the derivation of a modified version of Equation (1) so that it now describes dispersion in a boundary layer of depth H:

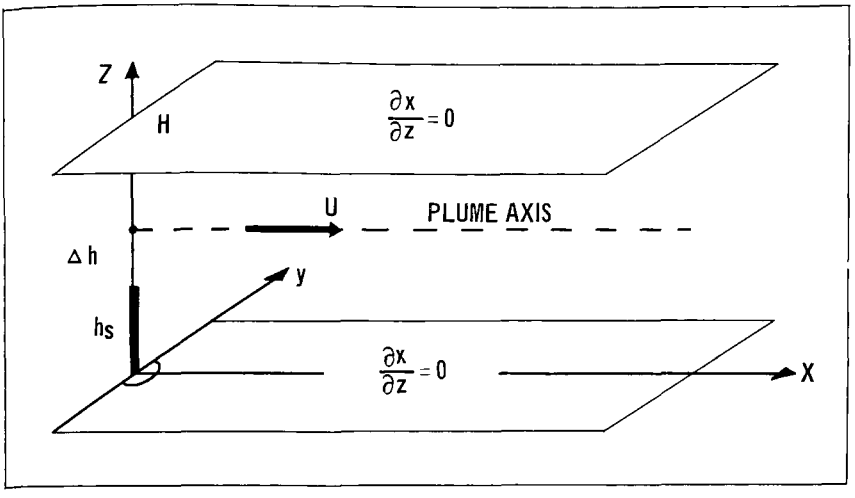

Figure 9-3. Model assumptions.

$$\chi = \frac{Q}{2HU} \exp[-\gamma\tau] \frac{\left[\exp -\frac{y^2}{2\sigma_y^2}\right]}{\sqrt{2\pi}\,\sigma_y} \left\{ \Theta_3 \left(\frac{h-z}{2H} ; \frac{\sigma_z^2}{2H^2} \right) + \Theta_3 \left(\frac{h+z}{2H} ; \frac{\sigma_z^2}{2H^2} \right) \right\} \tag{8}$$

Here

$$\Theta_3(V,W) = \frac{1}{\sqrt{\pi W}} \sum_{\eta=-\infty}^{\infty} \exp\left[-\frac{(V+\eta)^2}{W} \right] \tag{9}$$

is a Jacobian theta-function.

It can be shown that Equation (8) differs only slightly from Equation (1) for $H > 3h$. If, however, the ceiling approaches the effective stack height, i.e., if $H \to h$, then the ground-level concentration increases drastically.

So far only a single source has been considered. In an urban area, a large number of such sources exist. In reality, all of them are point sources as far as emissions are concerned. They may be divided into three groups. Group 1 consists of all industrial stacks, including those of power stations and gasworks; Group 2 consists of stacks of small industries, contributing, say, less than 0.02 percent each to the total output into the city; Group 3 consists of all domestic sources burning fuel for space heating.

Industrial emission sources of Group 1 are treated individually by applying Equation (8). Since they are irregularly distributed over the urban area, and

since Equation (8) applies to a source-oriented coordinate system, the transformation of coordinates shown in Figure 9-4 is performed.

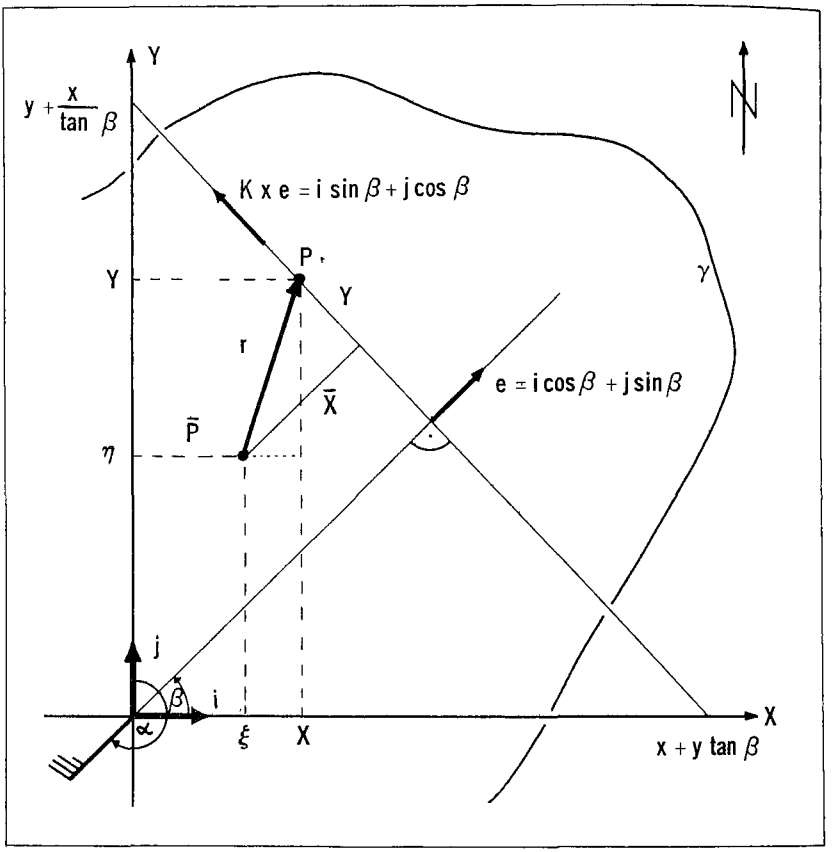

Figure 9-4. Transformation of coordinates from a source-oriented system to a geographically fixed system.

If α denotes wind direction ($\beta = 3\pi/2 - \alpha$), P(x,y) a receptor point, and (ξ_n, η_n) the location of a point source, then the individual source distance in wind direction, $\bar{X}_n$, and the individual crosswind distance, $\bar{Y}_n$, of the receptor point, p(x,y), are given by:

$$\bar{X}_n = e \cdot \gamma = (x-\xi_n)\cos\beta + (Y-\eta_n)\sin\beta \qquad (9)$$

$$\bar{Y}_n = k(e \cdot \gamma) = -(x-\xi_n)\sin\beta + (Y-\eta_n)\cos\beta$$

where

$$\gamma = i(x-\xi_n) + j(Y-\eta_n)$$

Now, source strength, wind speed, travel time, plume standard deviations, and effective stack height are dependent on $(\xi_n \eta_n)$ and $(\bar{X}_n, \bar{Y}_n)$, respectively. Individual source strength is denoted by $Q = Q(\xi_n, \eta_n) = Q_n$ Wind speed relevant for transport and dilution of pollutants originating from the source at (ξ_n, η_n) is given by $U = U(\xi_n, \eta_n)$. Travel time is indicated by τ_n X_n/U_n, plume standard deviations by $\sigma_y = \sigma_y(\tau_n) = \sigma_{y,n}$ and $\sigma_z = \sigma_z(\tau_n) = \sigma_{z,n}$, and local effective stack by $h = h(\xi_n, \eta_n) = h_{s,n} + \Delta h(\xi_n, \eta_n)$ Introducing these new parameters and coordinates into Equation (8), the ground-level concentration originating from emission source "n," i.e., $\chi_n(x,y,z)$, is obtained.

The concentration fields from all individual sources can be superimposed. Contributions to the concentration at receptor point, P, come from all upwind sources having coordinates, $\xi_n \leq x + y \tan \beta$, $\eta_n \leq y + x/\tan \beta$. If N denotes the total number of upwind sources, the concentration P is given by:

(10)

$$\chi = \frac{1}{2H} \sum_{n=1}^{N} \frac{Q_n}{U_n} \exp[-\gamma \bar{\tau}_n] \frac{\exp\left[-\frac{\bar{Y}_n^2}{2\sigma_{y,n}^2}\right]}{\sqrt{2\pi}\,\sigma_{y,n}} \left\{ \Theta_3\left(\frac{h_n - Z}{2H}; \frac{\sigma_{z,n}^2}{2H^2}\right) + \Theta_3\left(\frac{h_n + Z}{2H}; \frac{\sigma_{z,n}^2}{2H^2}\right) \right\}$$

It is obvious that computing time goes up tremendously with an increasing number of individual sources. It is impossible, therefore, to treat all domestic sources of Group 3 individually. In this context one generally talks about area sources. The source strength, Q, is replaced by a local source strength density (source emission per unit area), $q(\xi,\eta)$. Local relevant mean wind speed, $U(\xi,\eta)$, as well as local plume rise, $\Delta h(\xi,\eta)$, are connected with the emission height $h_s(\xi,\eta)$ of the area source. The coordinates, $\bar{X}_n, \bar{Y}_n$, with respect to an individual source are replaced by $\bar{x}, \bar{y}$ which obey the same relations, in Equation (9), as $\bar{X}_n$ and $\bar{Y}_n$ do. If the sum in Equation (10) is replaced by an integral, the contribution of all upwind area sources to the concentration at receptor point, P, is given by:

(11)

$$\chi = \frac{1}{2H} \int_{\xi \leq x + y \tan \beta} d\xi \int_{\eta \leq y + x/\tan \beta} d\eta \, \frac{q(\xi,\eta)}{U(\xi,\eta)} \exp[-\gamma \bar{\tau}] \, \frac{\exp\left[-\frac{\bar{y}^2}{2\sigma_y^2(\bar{\tau})}\right]}{\sqrt{2\pi}\,\sigma_y(\bar{\tau})}$$

$$\left\{ \Theta_3\left(\frac{h(\xi,\eta) - Z}{2H}; \frac{\sigma_z^2(\bar{\tau})}{2H^2}\right) + \Theta_3\left(\frac{h(\xi,\eta) + Z}{2H}; \frac{\sigma_z^2(\bar{\tau})}{2H^2}\right) \right\}$$

Superposition of concentrations, in Equations (10) and (11), gives the steady-state concentration field at any location in space, (X,Y,Z), if individual point sources as well as area sources act together in that urban area.

Apart from the fact that source emission data for area sources, i.e., $q(\xi,\eta)$ are not available, the analytical integration of Equation (11) cannot be performed. Numerical integration replaces the integral by a sum which represents the area source by a dense, regularly spaced system of point sources having source strength, $q(\xi_i,\eta_k)\Delta\xi\Delta\eta$. This, in fact, has been done in the model. The selection of the area element, $\Delta\xi\Delta\eta$, depends upon resolution and scale. In addition, the characteristics of dispersion as well as the conditions of emission (emission heights) are important. In order to find a satisfactory answer to that question, a number of mathematical experiments was performed. An area source, 500 m by 500 m was represented by a successively increasing number of point sources (Figure 9-5).

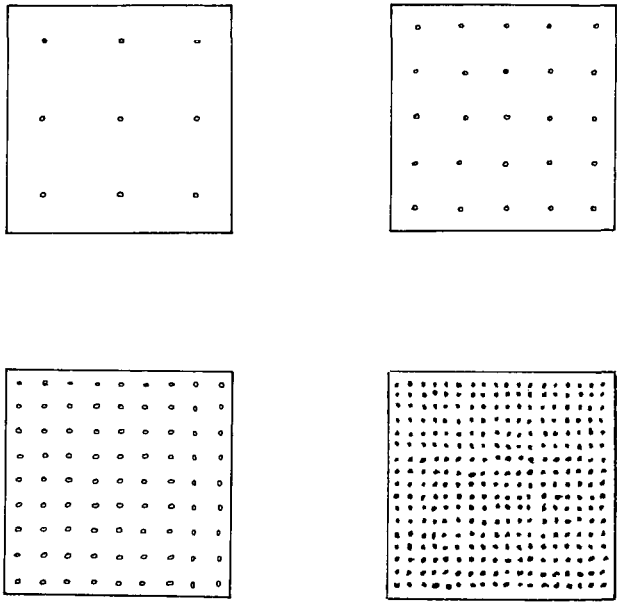

Figure 9-5. Simulation of an area source by the use of increasing number of point sources distributed regularly over an area 500 x 500 meters.

As Figures 9-6 and 9-7 show, an area size of $\Delta = \Delta\xi\Delta\eta$ = 56 m x 56 m should be sufficient for the representation of an area source by a great number of point sources under the conditions indicated in Figures 9-6 and 9-7.

In order to get the same degree of approximation for a wide range of windspeeds and stability categories, the 500 m by 500 m area source must be represented by at least 100 individual sources ($\Delta = \Delta\xi\Delta\eta$ = 50 m x 50

m) or better, by 144 individual sources ($\Delta=\Delta\xi\Delta\eta \approx 42$ m x 42 m). This corresponds roughly to the mean distance between individual stacks from space heating units.

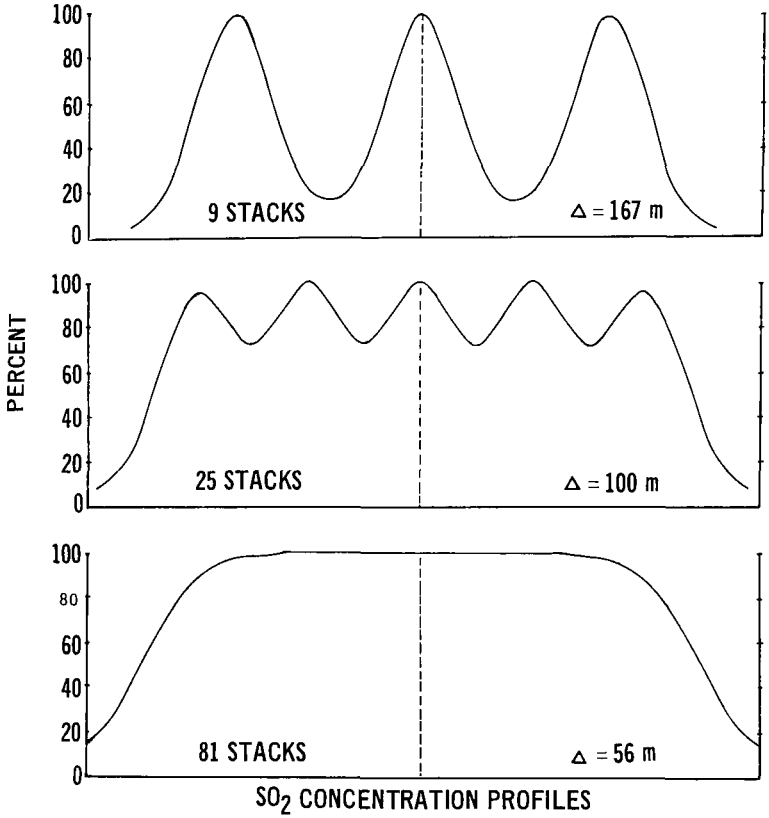

Figure 9-6. Successive approximation of area-source emissions under unstable conditions by the use of an increasing number of point sources. (Relative crosswind SO_2 concentration profiles taken at X_{max} distance from center of area. Uniform emission height is 25 meters; stability class, 2; wind speed, 3 meters per second.)

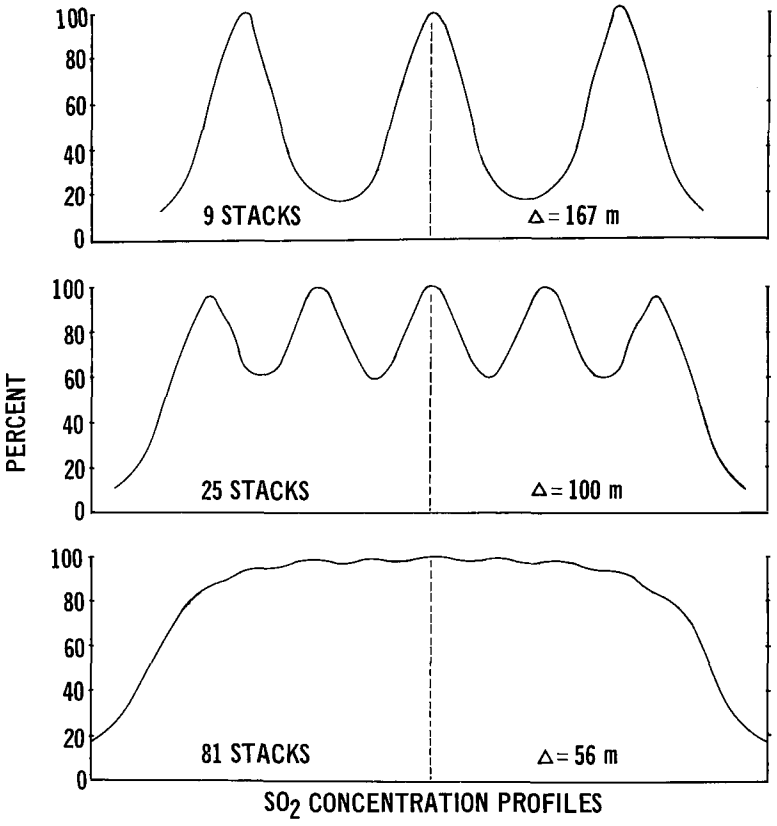

Figure 9-7. Successive approximation of area-source emissions under neutral conditions by the use of an increasing number of point sources. (Relative crosswind SO_2 concentration profiles taken at X_{max} distance from center of area. Uniform emission height is 25 meters; stability class, 2; wind speed, 3 meters per second.)

METEOROLOGICAL DATA INPUT

A set of meteorological data consists of windspeed, wind direction (both taken at anemometer level), and stability category. All three are hourly values taken at the Bremen airport. Observations of windspeed and wind direction at four sites in the city during winter (1967-68) validated the assumption that the airport observations are representative for the urban area of Bremen, at least during winter, which is the most important period with respect to air pollution in Bremen. Stability categories were computed using Turner's scheme.[2]

It was discovered during simulation experiments that 36 wind direction measurements (wind roses divided into 10-degree intervals) are necessary to provide reasonable ground-level concentration fields. Windspeed was divided into seven classes. Including five stability categories, a total number of 1260 combinations exist, of which, however, only about 600 are realized.

Frequency distributions of wind data were calculated for each stability category for a variety of periods (months of the year, seasons, years, and five to ten years). Figure 9-8 shows a typical example of a long-term distribution.

Data on plume standard deviations for urban areas were not available during the years of experimentation. Therefore, the well-known Pasquill-Gifford values[1,3] were used for low emission heights (space heating), whereas the Brookhaven values [4,18] were applied in a slightly modified version to high industrial stacks (Figures 9-9 and 9-10). The results of the St. Louis dispersion study indicate that utilization of those values given in Figures 9-9 and 9-10 inevitably lead to a systematic overestimation of ground-level concentrations.[19] This trend was, in fact, apparent when the results of calculations were compared with those obtained by observations.

Finally, the problem of mean windspeed, U, which is relevant for the transport and dilution of pollutants, was solved in the usual manner. Wind observations were extrapolated from anemometer level to physical stack height for each stack by means of a power-law-profile assumption. This extrapolation was assumed to be a function of stability and was made by the use of parameters taken from the literature (Figures 9-8, 9-9, and 9-10).

EMISSION SOURCE INVENTORY

All emission sources, as mentioned earlier, were classified in three groups. All individual stacks (Group 1) with emission rates greater than 1 kilogram

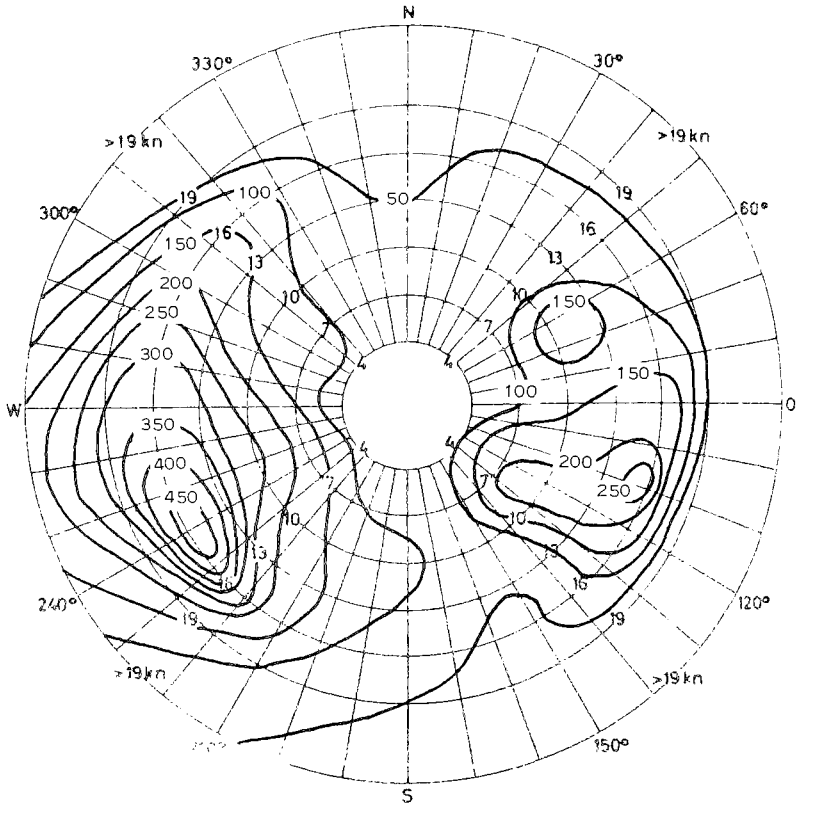

Figure 9-8. Frequency distribution of wind direction and wind-speed for Bremen, 1954 to 1959. Stability class: 4 (neutral). Isopleth numbers represent hours per period.

sulfur dioxide (SO_2) per hour were treated individually. The record contained: geographical location, physical dimensions of the stack, output by volume, exit velocity, exit temperature, and, finally, emission data that included maximum emissions and mean winter and summer emissions. In addition, data were obtained whenever possible on daily variations in emissions and emissions during holidays.

Effective stack heights were calculated by applying Stumke's empirical formula,[20] similar to the well-known CONCAWE-formula, which is applicable to all types of stacks in Bremen.

Group 1 emission sources, consisting of 136 stacks, contributed 75 percent to the total emission rate in Bremen during winter 1965 (Table 9-1). Spatial distribution per square kilometer is given in Figure 9-11 for these sources.

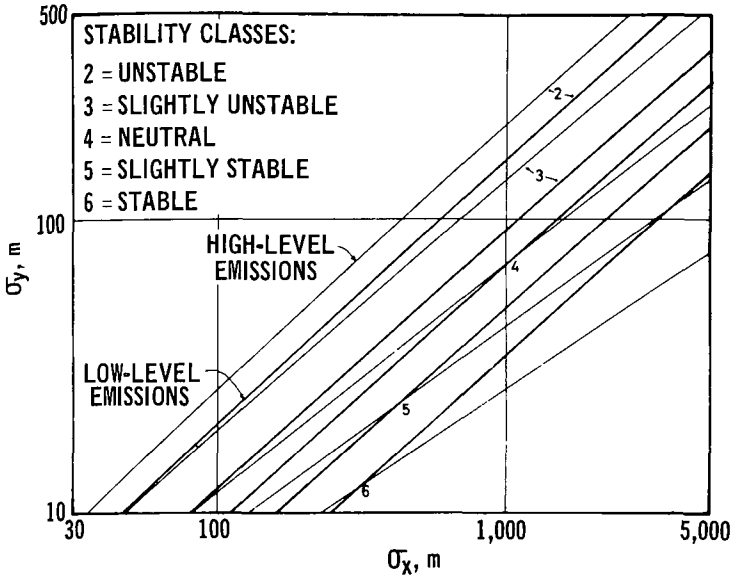

Figure 9-9. Crosswind-plume standard deviations.

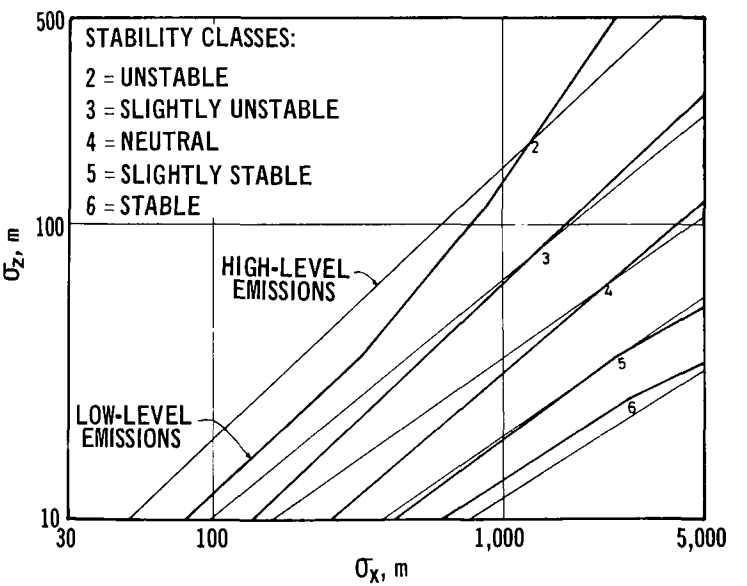

Figure 9-10. Vertical-plume standard deviations.

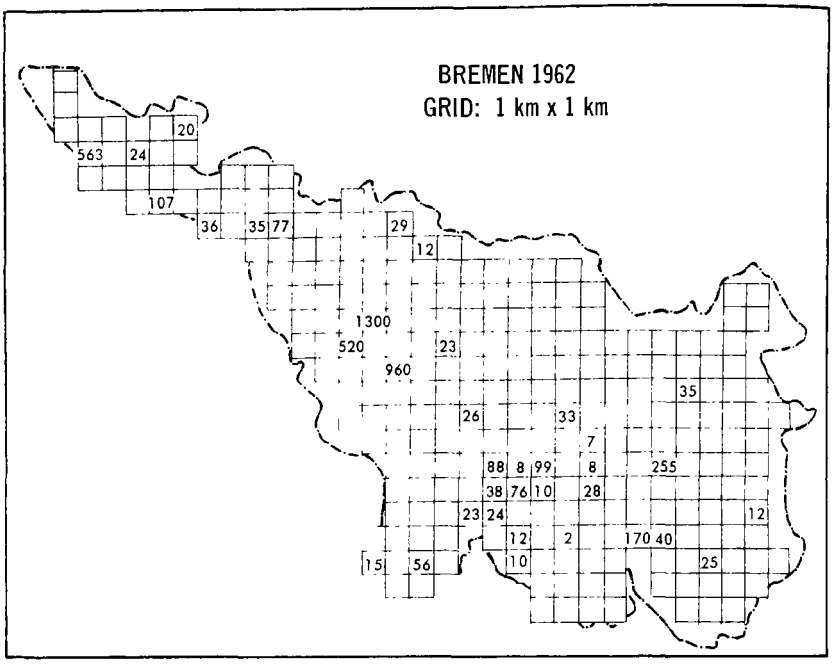

Figure 9-11. Spatial distribution of mean winter time industrial emissions.

Table 9-1. STATISTICS FROM 1965 EMISSION-SOURCE INVENTORY OF BREMEN

Source	Number of stacks	Total emissions, kg SO_2 hr^{-1}		Percent of total emissions	
		Summer	Winter	Summer	Winter
Industries and power plants	136	1,423	4,715	99	75
Small industries	425	46	116	1	2
Space heating	—	—	1,458	—	23
Total	561	3,469	6,289	100	100

A large number of individual stacks from small industries contributed less than 0.02 percent each to the total emission rate, i.e., less than 1 kilogram SO_2 per hour. They contributed only 1 to 2 percent altogether and, therefore, were not treated individually. Instead, the same technique was used as that applied to emissions from space heating (Figure 9-12).

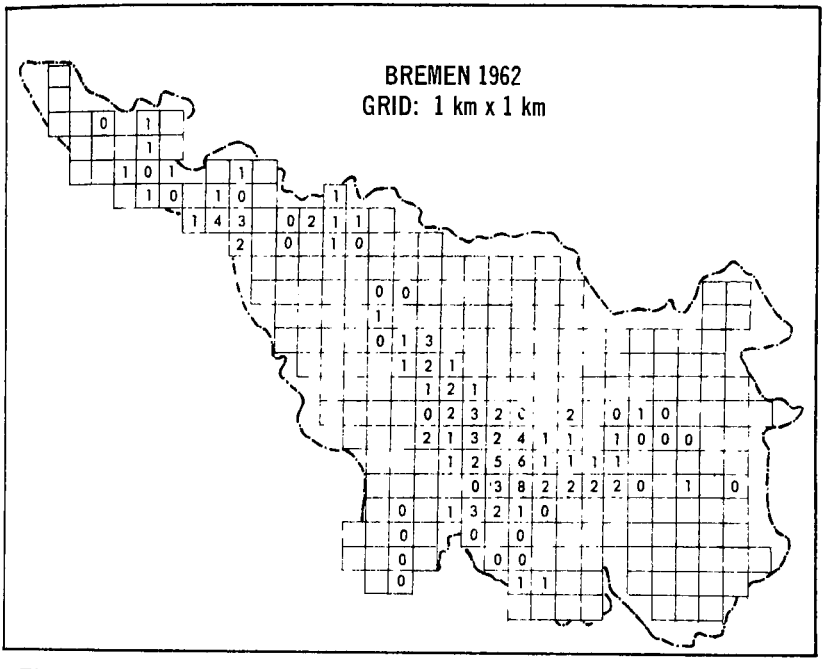

Figure 9-12. Spatial distribution of mean winter time industrial emissions from small industries.

Although it contributed less than 25 percent to the total emission rate, space heating is the dominant factor in air pollution in Bremen because of low emission heights.

Emissions from space heating were obtained in the following way. The spatial distribution of dwelling units in Bremen, which number about 200,000 was known very well. Further, the total amount of coal and fuel oil consumption during heating periods was known. From the sulfur content of the fuels, the total fuel consumption, and the total number of dwelling units, a mean emission rate of 8 grams SO_2 per hour per dwelling unit was obtained. This is the amount that would have been emitted daily during the heating period if the daily mean temperature had remained constant. In several experiments, a relationship between daily mean temperature and daily emission was used to make emissions from space heating a function of time.

A mean emission height of 25 meters was assumed for downtown emissions and 15 meters for suburban emissions. The corresponding effective stack heights were calculated by a simpler method than that used for tall stacks.

Emissions from space heating were treated as "area sources" as described earlier. A grid produced areas 500 m by 500 m. The number of dwelling units in each area was counted. Multiplying by 8 grams SO_2 per hour (or the corresponding, temperature-corrected value) gave the mean emission rate for that area (Figure 9-13). This amount was then divided by the number of individual stacks (from 81 to 144) representing the area source.

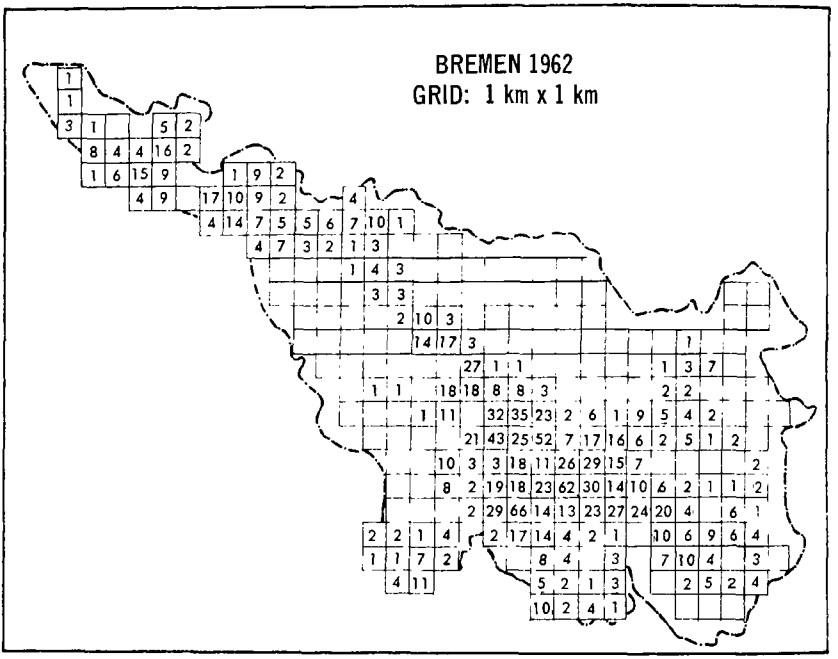

Figure 9-13. Spatial distribution of mean heating period industrial emissions from space heating, kg SO_2/km^2-hr.

The fact that area sources are represented by a large number of individual, equivalent stacks simplifies the calculations a great deal. The distribution of dwelling units in Bremen is such that only about 250 areas, 500 m by 500 m, are covered with dwellings. Since the density of these dwellings varies spatially, the emission rates of the 250 types of stacks, in general, differ from each other. Their physical dimensions and their plume rise values, however, are equal, or are grouped into only two categories (downtown and suburban). With the shift of calculated concentration fields from one point source location to the other within an area of 500 m by 500 m, the computing time is very much reduced.

RESULTS OF SIMULATION EXPERIMENTS

An inventory of all possible steady-state ground-level concentration fields forms the basis of simulation experiments. This inventory was obtained by calculating concentration fields for all possible combinations of meteorological parameters. It has already been noted that about 600 such combinations, representing given weather situations, can occur in Bremen. This number depends, of course, on the classification of windspeed and wind direction used. If one calculates the concentrations at the points of a grid (a grid distance of 500 meters) about 600 numbers have to be stored at each grid point. Since the computer program was written for a grid of 2500 points, a total number of 1.5 million numbers have to be stored. If the source inventory is assumed to be time-dependent (heating period, non-heating period, etc.), the number of concentration values to be stored increases considerably.

The use of concentration field inventory data together with frequency distributions of relevant meteorological parameters permits the derivation of frequency distributions of concentrations for each point on the grid. Other statistics, as well, can be obtained quite simply, such as SO_2 wind roses. Figures 9-14 to 9-17 demonstrate this clearly. Sulfur dioxide wind roses were calculated for the four sites where monitoring stations were later installed. These figures, together with Figures 9-11 to 9-13, show the possibility of identifying large emission sources by means of SO_2 wind roses. It may seem that this is by no means an easy task because emission sources with quite different emission heights work together with meteorological factors having complicated frequency distributions. It may be noted that the simulated SO_2 wind roses coincide considerably well in structure with those obtained by measurement.

Among the many experiments performed, the investigation of the influence of boundary layer thickness on ground-level concentration was the most interesting. The upper ceiling was lowered from 500 m to 25 m. In cases in which the ceiling reached the effective height of an individual stack, this effective height was reduced with the decreasing height of the ceiling until it reached two-thirds its original value. This stack was then thrown out of the inventory on the assumption that the plume would penetrate the ceiling Figures 9-18 and 9-19 show how the isogram patterns change and they also show the tremendously increased concentrations that result if the depth of the mixing layer is approximately equal to the effective height of space heating emissions. Figure 9-20 demonstrates this behavior for a specific location in downtown Bremen. It is obvious that this picture looks different for different locations. Only mathematical experimentation of the kind applied here can simulate the complicated behavior of ground-level concentrations.

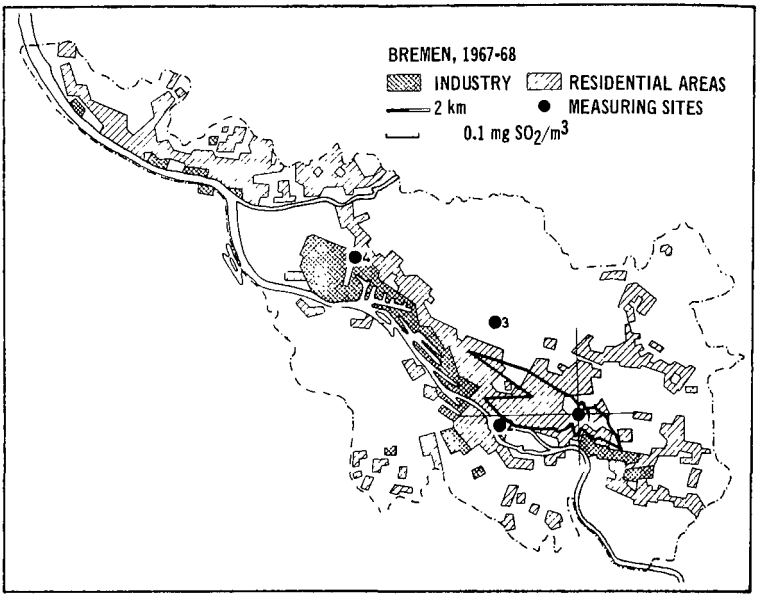

Figure 9-14. Calculated heating-period-SO_2-wind rose for Site 1 in downtown Bremen.

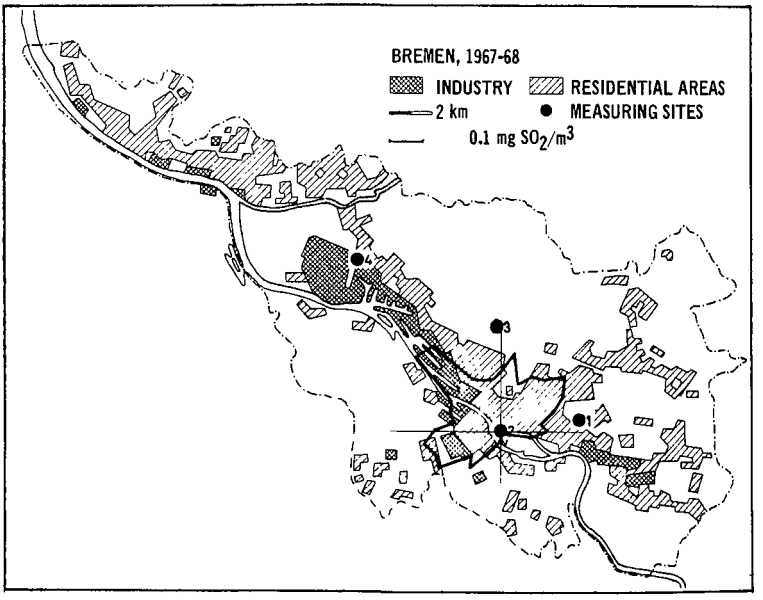

Figure 9-15. Calculated heating-period-SO_2 wind rose for Site 2 in downtown Bremen.

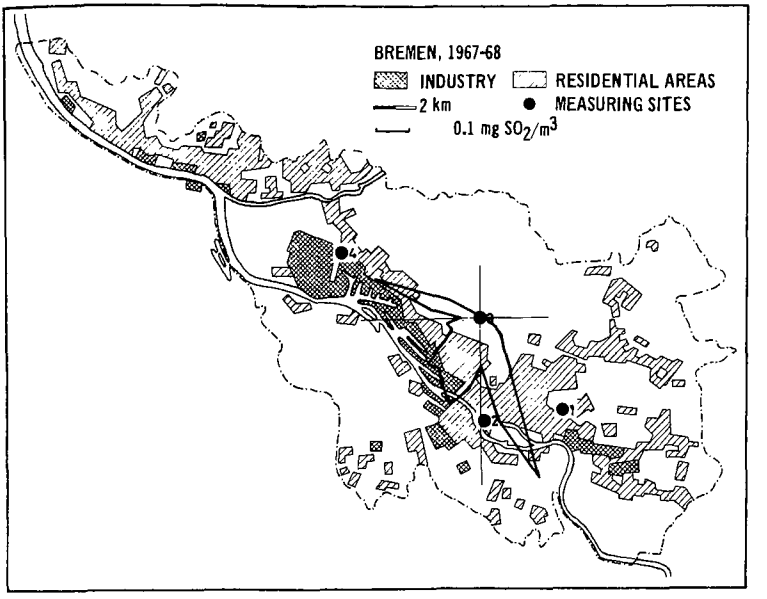

Figure 9-16. Calculated heating-period-SO_2-wind rose for Site 3 on the outskirts of Bremen.

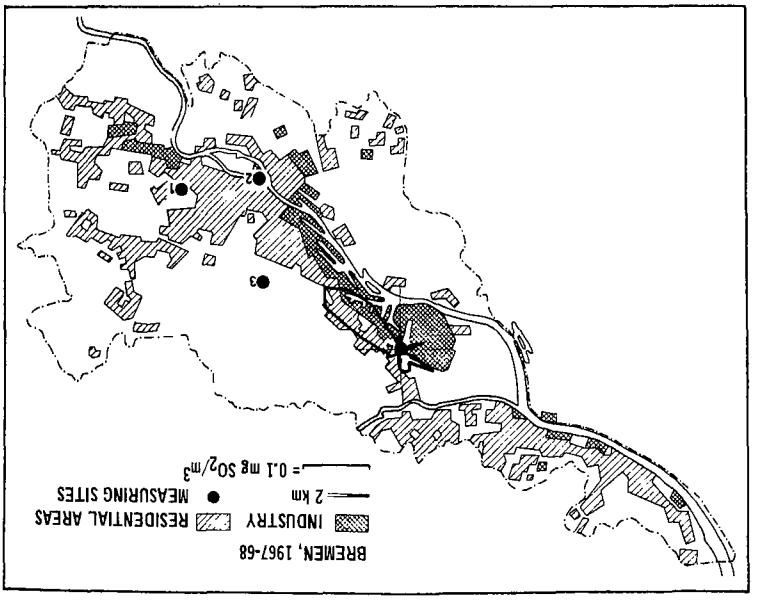

Figure 9-17. Calculated heating-period-SO_2-wind rose for Site 4, in close proximity to an industralized area.

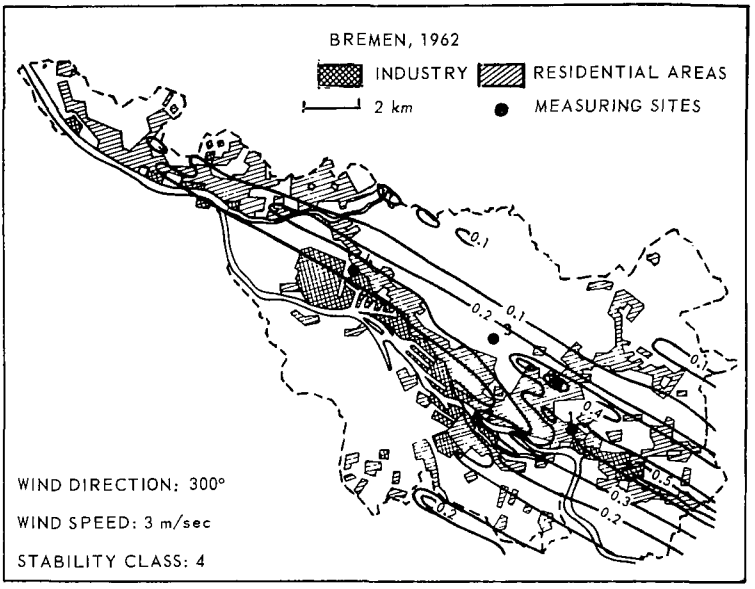

Figure 9-18. Calculated field of ground-level-SO_2 concentration in mg/m^3 for a special meteorological situation and a boundary layer thickness of 100 meters.

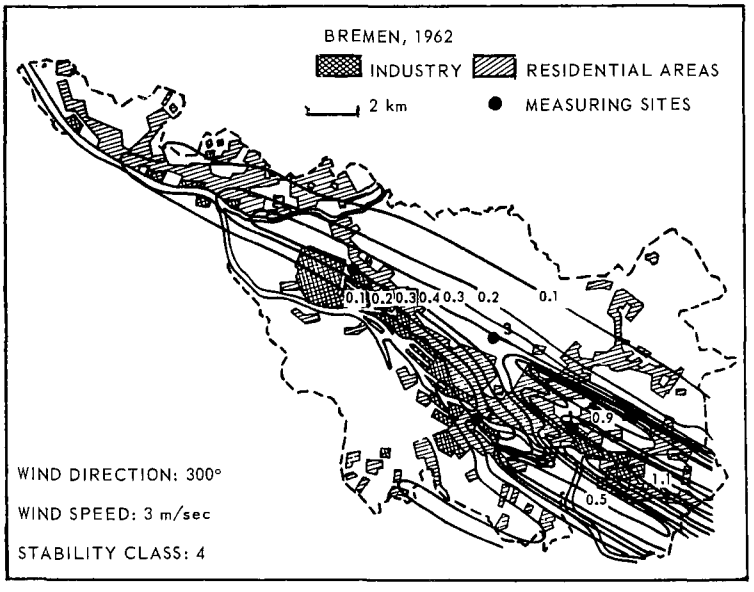

Figure 9-19. Calculated field of ground-level-SO_2 concentration in mg/m^3 for a special meteorological situation and a boundary layer thickness of 25 meters.

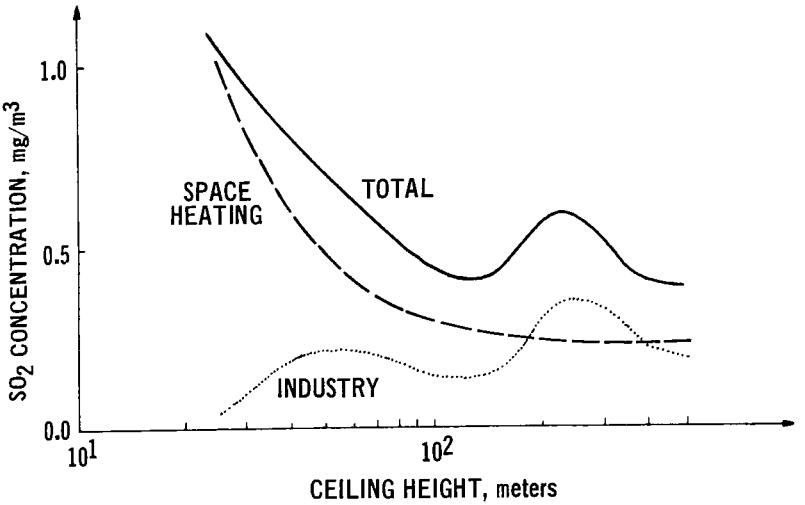

Figure 9-20. Variations in ground-level concentrations of SO_2 in downtown Bremen as a function of boundary layer thickness.

As mentioned in the introduction, frequency distributions of ground-level concentrations were of chief interest from the beginning of this investigation. The method for obtaining these for desired periods of time is straightforward. It must be stated, however, that the derived distributions are not complete because up to now no theory exists for explaining the dilution of pollutants under calm weather conditions. These cases, therefore, were excluded from the statistics as were cases with limited boundary layer depths. Neither source of error, however, plays an important role in Bremen. The frequency of calm conditions as well as the frequency of low-level inversions was small during all periods of time investigated.

Stored data on fields of steady-state concentrations (Figure 9-21) form the basis of statistics of this kind.

Steady-state concentration fields, together with frequency distributions of meteorological parameters, can be used to calculate frequency distributions of concentrations for each grid point. These distributions were characterized by a set of three parameters:

1. The percentage of time (in hours) for which ground-level concentrations exceeded a given value (0.1 milligram SO_2 per cubic meter). Figure 9-22 shows the pattern of this parameter for the heating period of 1962. As seen, only 20 percent of the period concentrations in downtown Bremen were below 0.1 milligram SO_2 per cubic meter.

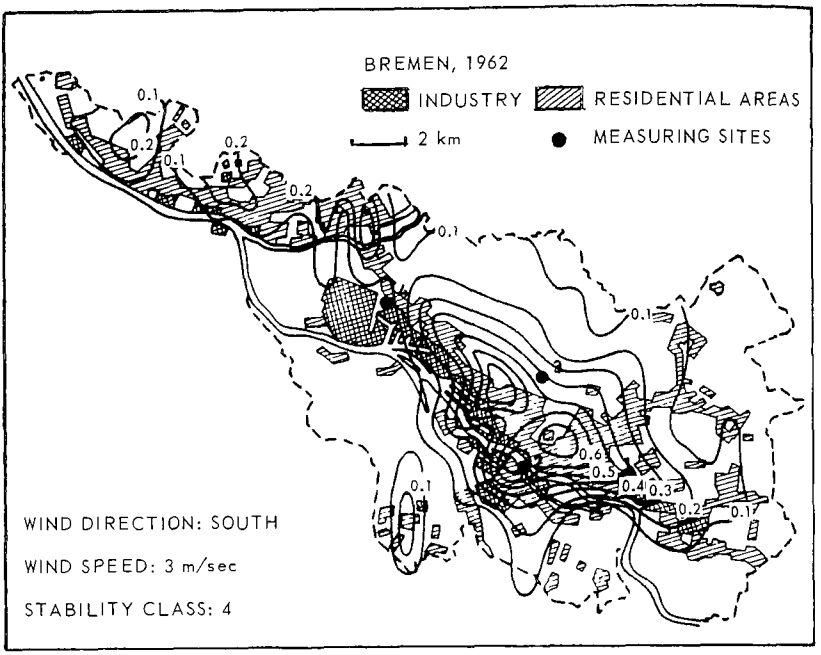

Figure 9-21. Typical possible field of calculated steady-state ground-level SO_2 concentrations in mg/m^3

2. The mean concentration for the period. Figure 9-23 shows the pattern of this parameter. Typically, the pattern of the mean concentration shows little structure and does not contain much information.
3. An upper percentile; for example, the 97.5th percentile. The numbers in Figure 9-24 indicate that for only 2.5 percent of the time (in hours) concentrations exceeded that value given by the respective number.

The following Figures, 9-25 thru 9-27 show the corresponding pattern for a nonheating period in which only industrial sources are contributing emissions.

It might be possible to define *Imissions-Grundbelastung* with the help of these maps of characteristic parameters. This investigation is one step forward in this direction.

VALIDATION OF THE MODEL

During the heating period of 1967-68, four monitoring stations were installed at specially chosen locations. The locations were planned as strategically as possible. First of all, an attempt was made to place all stations on a mean concentration isogram (Figure 9-23). Second, an attempt was

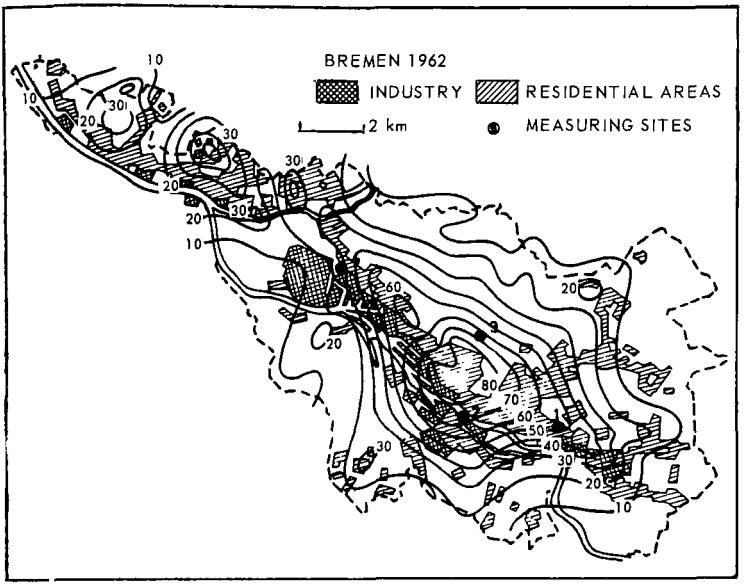

Figure 9-22. Percentage of cases (hours) for which ground-level concentrations exceeded 0.1 mg SO/m^3. Winter 1962.

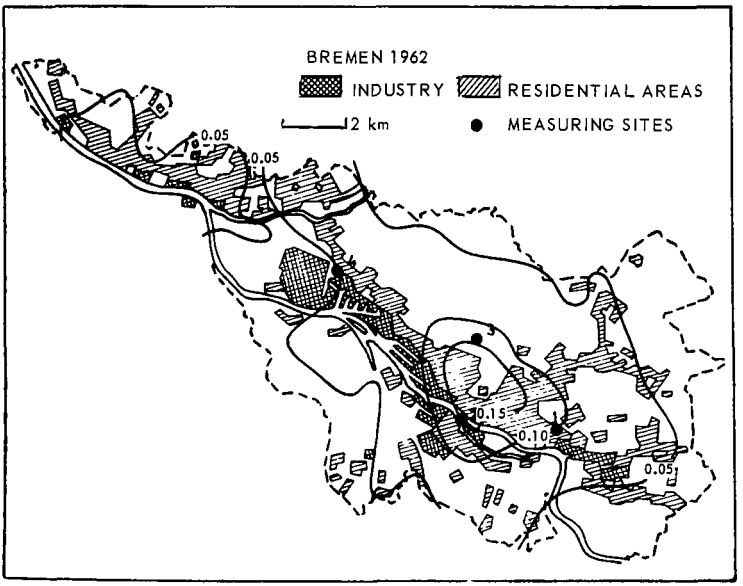

Figure 9-23. Mean ground-level-SO_2 concentration in mg/m^3.

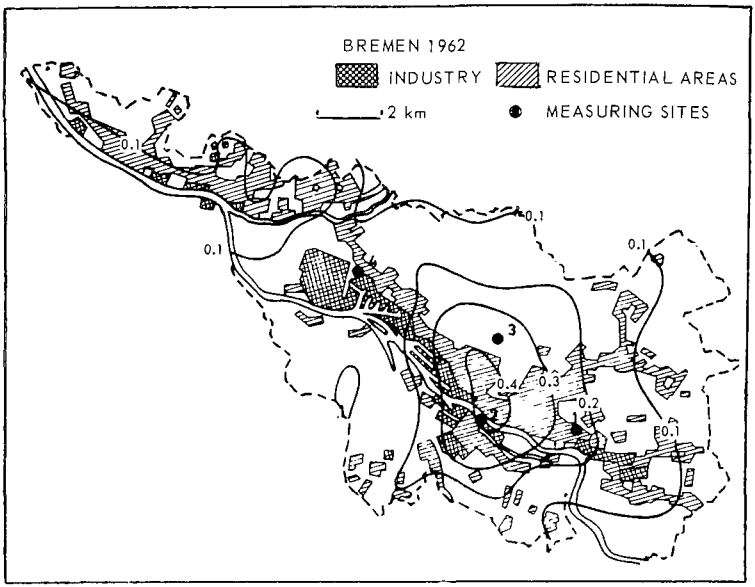

Figure 9-24. 97.5th percentile SO_2 concentrations in mg/m^3. Winter 1962.

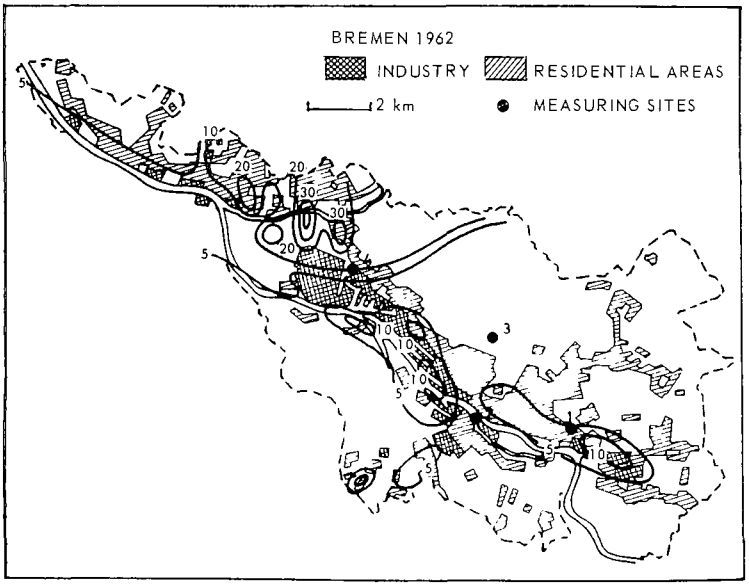

Figure 9-25. Percentage of cases (hours) for which ground-level concentration exceeded 0.1 mg SO_2/m^3. Summer 1962.

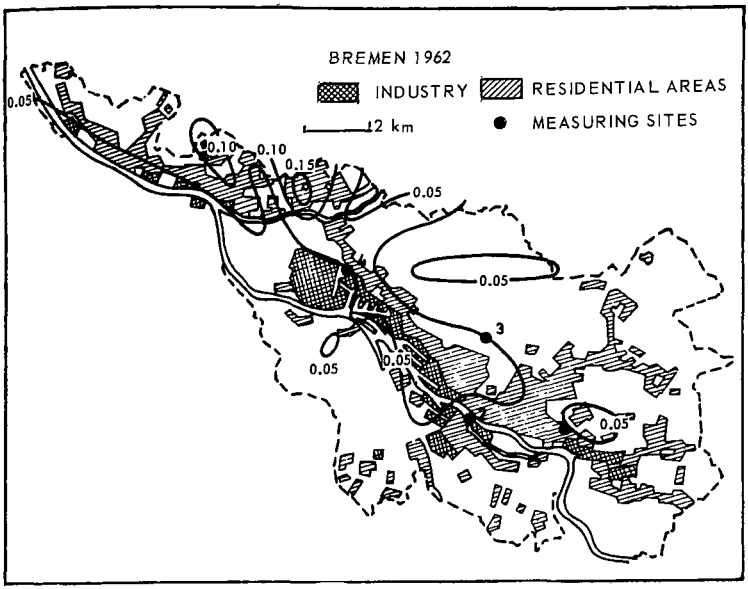

Figure 9-26. Mean ground-level-SO_2 concentration in mg/m^3. Summer 1962.

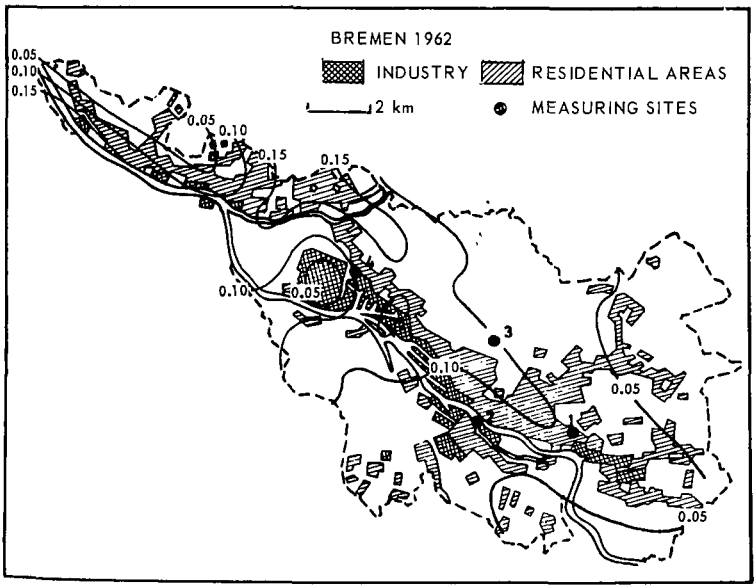

Figure 9-27. 97.5 percentile of ground-level-SO_2 concentrations in mg/m^3. Summer 1962.

made to locate stations in areas as diverse as possible. Station 1 was located in a "normal" downtown area, surrounded mainly by residences. Station 2 was located in the very center of the city on an island. It was surrounded, however, on all sides by the water of the river Weser and of the waterworks. Station 3 was located on the outskirts of the city, separated from downtown Bremen by a large park with tall trees. Station 4 was located in the near vicinity of a large plant.

The monitoring stations measured half-hourly values of SO_2 concentrations. From these values, frequency distributions were derived for every month of the period and for the period as a whole. At the same time, mathematical simulation of the same distributions was performed using the latest version of the emission source inventory and utilizing meteorological statistics for the sampling period. Figures 9-28 through 9-31 show comparisons of observed and calculated frequency distributions. The simulation of Station 1 (downtown "normal" area) is quite satisfactory, as indicated in Table 9-1. For Station 2 (waterworks on the Weser island), the model obviously overestimates the concentrations systematically (Figure 9-29). Overestimation may occur for one or both of two reasons: absorption at the water surfaces, or an insufficient spread as a result of improperly chosen urban plume standard deviations. The same holds for Station 3 (separated from downtown Bremen by a large park), where the filtering effect of the park was not taken into account.

At Station 4 (in the vicinity of a large plant), the reverse is observed. The model systematically underestimates the concentrations. Since emissions from low-level sources of space heating are small in the neighborhood of that station, low concentration values could be expected. The comparatively high concentrations that actually occur have their origin in uncontrollable low-level emissions, which could not be taken into account, from the nearby plant.

Table 9-2 summarizes the observed and calculated mean concentrations for each monitoring station.

Finally, it can be stated that it is worthwhile to invest more effort in diffusion modeling, for simulation may one day be a very important tool in city planning.

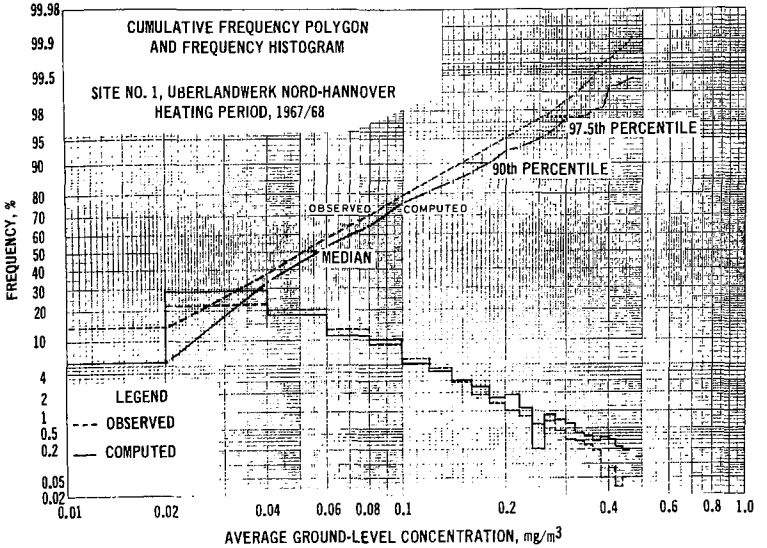

Figure 9-28. Comparison between observed and computed frequency distributions of ground-level concentrations in downtown Bremen.

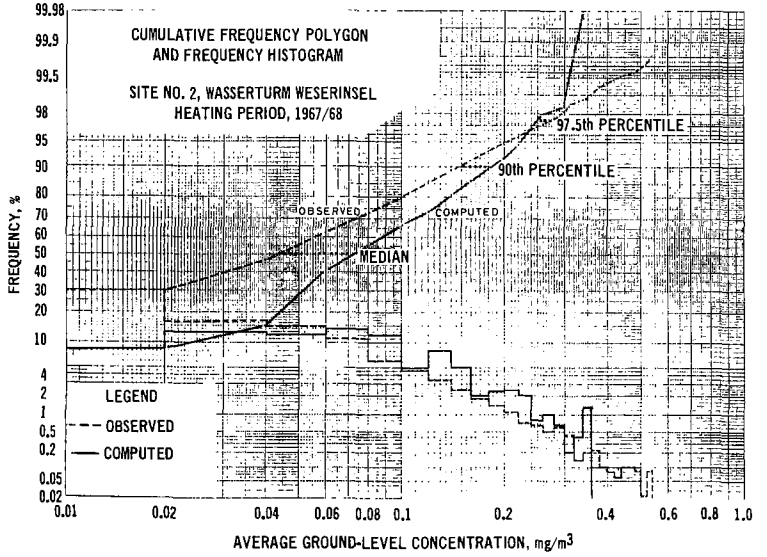

Figure 9-29. Comparison between observed and computed frequency distributions of ground-level concentrations in downtown Bremen.

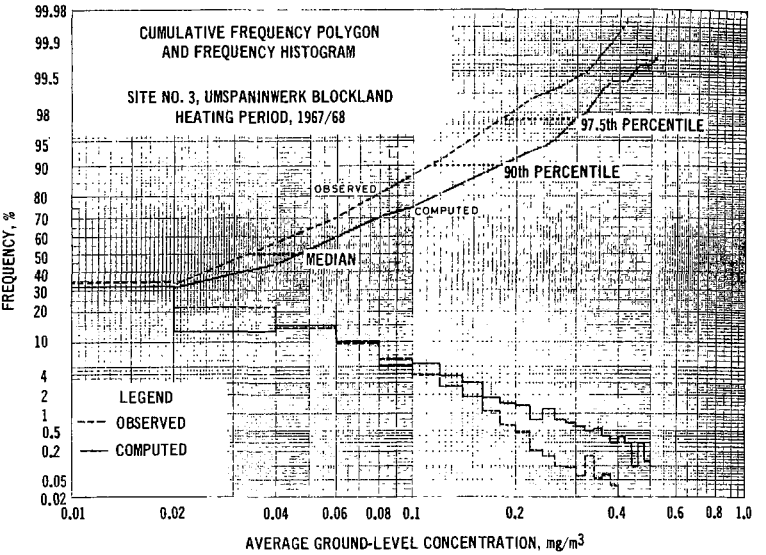

Figure 9-30. Comparison between observed and computed frequency distributions of ground-level concentrations on outskirts of Bremen.

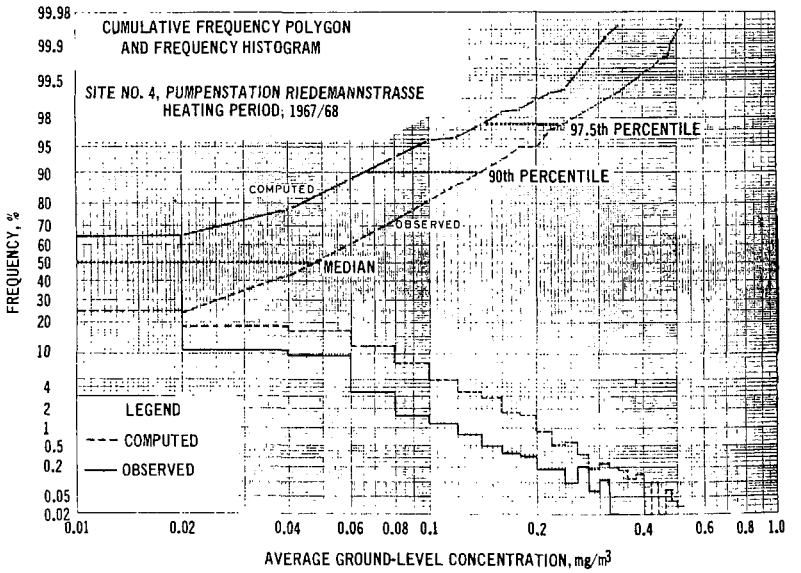

Figure 9-31. Comparison between observed and computed frequency distributions of ground-level concentrations in an industrial district.

Table 9-2. OBSERVED AND CALCULATED MEAN SO_2 CONCENTRATIONS IN BREMEN; HEATING PERIOD, 1967-1968

($mg\ m^{-3}$)

Site	1		2		3		4	
	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.	Calc.	Obs.
November	0.14	0.11	0.15	0.10	0.14	0.08	0.05	0.10
December	0.10	0.08	0.12	0.08	0.10	0.06	0.03	0.07
January	0.10	0.10	0.12	0.13	0.09	0.08	0.04	0.08
February	0.09	0.08	0.12	0.08	0.07	0.06	0.04	0.08
March	0.08	0.07	0.10	0.04	0.07	0.05	0.04	0.07
April	0.09	0.07	0.11	0.05	0.06	0.05	0.05	0.07
May	0.05	0.06	0.07	0.03	0.04	0.03	0.03	0.05
Total	0.09	0.08	0.12	0.08	0.08	0.06	0.04	0.08

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ACKNOWLEDGMENT

In the course of the research, a number of members of the *Institut fur Theoretische Meteorologie der Freien Universitat Berlin* contributed to this work, in many ways, mainly in programming and organizing. Especially, the author wishes to thank the following for the valuable cooperation, without which these experiments could not have been performed: R. Bleck, J. Schwirner, H. Buttner, H. Woick, and P. Lenschow.

APPENDIX – GLOSSARY OF SYMBOLS

$a(\tau,y)$	absorption coefficient of the ground
h	effective stack height
h_s	actual stack height
Δh	plume rise
H	height of dispersion ceiling
N	total number of upwind sources
$P(x,y)$	*receptor point*
$q(\xi,\eta)$	local source-strength density
Q	source strength
T	decay time, $1/\gamma$
U	wind speed
$(\overline{X}_n,\overline{Y}_n)$	source distance in downwind and crosswind directions, respectively
α,β	wind direction angle coefficients
Δ	source area
(ξ_n,η_n)	location of a point source
π	3.14
σ_y,σ_z	standard deviations of plume spread in y and z directions, respectively
γ	*travel time*
χ	concentration

14. DISCUSSIONS

INTRODUCTION

The following discussions were submitted in writing to the editor, subsequent to the Symposium. Attendees were given an open invitation to make comments on the Symposium topic and all of their responses are included in this chapter. Every author whose work was questioned was given an opportunity to read the question and to write a rebuttal if he felt one was needed. The chapter is divided into two sections; the first includes the discussions of Symposium papers and the second contains brief treatments of some additional approaches to multiple-source urban diffusion models.

RESPONSES TO INDIVIDUAL PAPERS

Lettau paper

Frank Pasquill

Regarding the effect on horizontal spread of the turning of wind with height, I would like to refer to a matter that is discussed in more detail in a paper that will shortly appear in the proceedings of a symposium on Recent Research in Air Pollution held by the Royal Society in November, 1968. Evidently, it is necessary to distinguish between the general distortion of a plume and the ultimate contribution of this distortion to enhanced spread at a *given level*. It turns out that there is a substantial time lag between these two phenomena. Examination of field data for stable conditions, available at the time of composing the foregoing paper, indicated that the effect on spread at a given level was unimportant in relation to the spread produced directly by the horizontal component of turbulence within about 5 km from an elevated source and about 12 km from a ground source.

Fortak Paper

Kenneth L. Calder

Dr. Fortak's discussion again emphasizes the point first raised by Dr. Pasquill at this meeting, that while a calculated spatial field of short-period average pollution concentration cannot be expected to agree very closely with that actually observed, the statistics obtained from an ensemble of such calculated concentration fields may well be in close agreement with reality.

As a small but important detail I was interested to see that Dr. Fortak has considered the numerical integration errors associated with the choice of grid size for the area-source specification. His conclusion that an area size of the order of 50 meters by 50 meters may be required for a satisfactory representation of a large number of point sources, is noteworthy, since, I believe, this is much smaller than the size used in some urban models currently being recommended for operational use.

Sheih, Davidson, and Friend Paper

Kenneth L. Calder

One point I found rather confusing in Drs. Sheih, Davidson, and Friend's paper was the initial statement that the model was derived from the statistical theory for turbulent diffusion, although later in the paper they stated that the model was semi-empirical and not derivable from known physical concepts. It would seem that the latter is a more true description since all the adjustable parameters and constants of the model are apparently derived by fitting observational data for sulfur dioxide in New York City. If this is so, then agreement between the model predictions and actual observations may be less impressive than for some other models where the parameter values are estimated independently.

The considerable effort made in this study to develop an adequate method for numerically integrating the emissions from a continuous area source is noteworthy and in strong contrast to the crude procedures used in many other models.

Mahoney, Maddaus, and Goodrich Paper

Harry Moses

One must bear in mind that the concentrations of a given pollutant such as SO_2, at a given station, is a function of several variables. Windspeed is one of these variables. It is possible in a multivariate system to find that several of the individual independent variables correlate poorly with the dependent variable, but when taken together, show a high multiple correlation.

15. APPENDIX
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