P-3

6th NATO/CCMS
International Technical Meeting
on Air Pollution Modeling

# SIMULATION OF $SO_2$-DISPERSION IN THE VENETIAN AREA

by

Runca, E. - Melli, P. - Zannetti, P.

Centro Ricerca IBM, Venezia, Italy

BATTELLE - INSTITUT E.V., Frankfurt/Main
Germany, FR

24-26 September, 1975

Abstract

This study tests the possibility of describing the dispersion of atmospheric pollutants, in a complex coastal zone such as the Venetian area, by means of a diffusion model. The simulation of $SO_2$ - dispersion is carried out by developing two different models. One is a Gaussian type diffusion model, the other one is based on the numerical -integration of the diffusion equation written according to the K-theory. The Gaussian model is based on the assumption that the pollutant has a Gaussian distribution along the vertical and is uniformly distributed crosswind in each sector of the wind rose.

With the use of meteorological data recorded on an hourly-basis and average evaluations of urban and industrial emissions, $SO_2$ three-monthly average concentrations were computed for the period Feb.'73-Feb. '74. The results were compared with the concentration values recorded at ten monitoring stations during the same period. In this comparison a correlation coefficient equal to 0,718 for the year '73 and to 0,798 for the year '74 were obtained. The general agreement between the model results and the measured data proved the validity of the applied technique for simulating long term average concentrations in the Venetian area and its applicability for land planning purposes.

The model based on K-theory integrates the time dependent diffusion-concentration equation according to the method of fractional-steps. The implemented numerical technique allows for variable grid spacing and time steps. Comparison between numerical and analytical solutions proved satisfactory. The model has not, as yet, been applied to the real phenomena because of unsatisfactory input data. It has been designed with the purpose of simulating short term $SO_2$ - average concentrations and complementing the Gaussian model.

## Introduction

Many attempts have been made in the last two decades to simulate $SO_2$ concentration fields in areas affected both by industrial and urban emissions (Pooler 1961, Turner 1964, Shieh 1971, Calder 1971, Martin 1971, etc.). The models developed for such a purpose have proved to work well in situations in which the parameters affecting the dispersion were rather uniform over the whole area. In more complicated areas, on the contrary, further implementations of diffusion models up to now realized are needed in order to formulate a satisfactorily precise idea of their reliability as well as of their limits.

Venice and its surroundings are a typical example of an area in which the dispersion of the atmospheric pollutants is greatly affected by the non-uniformity of its geographic characteristics. In this area the presence of different types of adjacent surfaces (land, lagoon and Adriatic Sea, see fig.1) induces a local circulation which interacts with the synoptic wind making it very difficult to identify the dispersion patterns of a pollutant.

On the other side the study of Air Pollution problem in Venice is made urgent by the damages that pollution causes to its priceless artistic patrimony.

In order to give a practical contribution to this problem an application of diffusion models is being carried out.

The problem was tackled by applying, as a preliminary attempt, a Gaussian type model, by which three montly average concentrations as well as the annual ones were simulated for the years 1973 and 1974. The discussion of the obtained results constitutes the essential part of this article. Later, a diffusion model based on numerical integration of the diffusion equation, written according to the K-theory, will be briefly analyzed. Such a model was built in order to take into account the local characteristics which cannot be included in the previous model.

## Application of the Gaussian model

Since the region under investigation shows the presence of a large industrial area (situated in the mainland) as well as three densely populated urban areas (Marghera and Mestre on the mainland, Venice on the islands at the center of the Lagoon, see fig. 1) both industrial and urban pollution must be taken into account in the model.

Data concerning industrial sources were taken from an inventory carried out by the Local Government in 1972 according to the National Law about Pollution promulgated in April 15th, 1971. Such an inventory showed the presence of 74 stacks with a total emission rate of 160000 tons/year and a range of heights from 10 to 120 m.

The knowledge of the average strength of sources introduces in the model computations a certain inaccuracy, which otherwise is somewhat reduced by the fact that long term averages are calculated.

The evaluation of the spatial distribution of domestic heating emissions was made on the basis of the last national general census, taken in 1972, which furnished a great mass of information not only about the distribution of the population but also about the state of buildings and their facilities (e.g. domestic heating plants).

For the 272 sections, in which the urban districts of the Venetian Area were subdivided, the consumptions of polluting fuels and therefore the yearly emissions of $SO_2$ were computed.

As for the definition of the emission rates (variable throughout the different periods of the year), it was achieved by using the concept of day/degree, defined as:

$$dd = T_b - \frac{\sum_{i}^{24} T_{h,i}}{24}$$

where $T_b$ is the temperature at which heating starts and $T_{h,i}$ is the average hourly temperature at i-th hour of the day.

In Venice $T_b$ is equal to 15,5 C. The total yearly emission was distributed over the whole "cold period", proportionally to the days/degree, as shown in fig. 2.

The above calculated fractions of the total yearly emission were then used to calculate the emission rates for each of the 272 above mentioned sections. Every area emissions was finally introduced in the model as an equivalent constant strength point source, located in the barycenter of the corresponding section.

The height of the urban emissions, including plume rise, was estimated to be about 30 m in the historical center of Venice (whose buildings are generally old and low) and around 45 m. in the urban areas of the mainland, which have developed in the last three decades and show taller buildings. Meteorological data as well as $SO_2$-concentration data were supplied by the network that Tecneco installed in Venice by appointment of the Istituto Superiore di Sanità (Superior Institut for Health). It consists of one meteorological station situated in the historical center of Venice and of 24 monitoring sensors (fig. 1).
The meteorological station records on an hourly basis wind speed, wind direction according to the eight sectors of the wind rose, temperature, pressure, rainfall, humidity, cloudiness and fog. Concentration data recorded by the 24 monitoring sensors are transmitted to a small computer which elaborates the data and prints the hourly average values as well as daily statistics. Besides that, every time the 30 minutes average $SO_2$- concentration "standard" (.30 ppm) imposed by the Italian law is exceeded in a station the computer gives an alert. Since only 10 stations were regularly operating from February 1973, the model has been tested on the data recorded by them in the period February 1973 - January 1975. Anyway some results will also be given for the other operating sensors in the year 1974.

## Diffusion equation

The equation used for the computation is the classical Gaussian plume formula (Pasquill 1962), written according to the modifications introduced by Martin (1971) and Calder (1971). For a single point source the concentration at a receptor point P is given by:

$$C_P = \frac{n}{\Pi^{3/2}} \frac{Q}{\sqrt{2}} \cdot \sum_{\substack{iw=1\\ is=1\\ it=1}}^{6,6,4} \frac{F(id,iw,is,it)}{U_{iw}\, D_P\, S_z(D_P,is)} \exp\left[\frac{-h^2(iw,is,it)}{2S_z^2(D_P,is)}\right]$$

where:

| | |
|---|---|
| n | number of wind rose sectors (n=8, in our computation) |
| Q | source emission rate (Kg/s) |
| F (id,iw,is,it) | denotes the relative frequency of winds blowing into the given 45 - wind direction sector (id), for a given wind speed class (iw), atmospheric stability class (is) and temperature class (it). |
| $U_{iw}$ | average wind speed for the iw - class at source height (m/s) |
| $D_P$ | projection along the wind direction of the distance between the receptor point P and the point source |
| $S_z$ | vertical standard deviation obtained from Gifford's plots (Slade, 1968) (m) |
| h | source effective height (m) |

The above mentioned hourly meteorological data were used to determine the joint frequency distribution of meteorological conditions. As to wind speed the following six classes were used:
0⟶1,57, 1,57⟶3,14, 3,14⟶5,24, 5,24⟶8,38, 8,38⟶11 and greater than 11 m/s; the representative speed $U_{iw}$ was computed as the arithmetic mean of the measured values belonging to the iw-class. In order to take into account the variation of the wind speed with the height an esponential law was used, whose exponent was assumed equal to .25 for unstable and neutral classes and .5 for stable ones. Though low wind speed were the most frequent ones, frequencies of calms were so low that it was decided to disregard them. Wind directions were grouped into 8 classes corresponding to the standard 8 compass directions (N,NE,....,NW).
Atmospheric stabilities were grouped into 6 classes, according to Pasquill's criteria. Finally, in order to take into account the influence of temperature on the plume rise, the following classes were intro-

duced: less than 0, 0→10, 10→20, and greater than 20 C; the representative temperature has been evaluated as the arithmetic mean of the measured values belonging to the it class.
The plume rise has been evaluated according to the Concawe formula (Détrie, 1969). Since no suitable information was available neither the height of the inversion layer nor the decay of $SO_2$ were introduced in the model.

## Results

The monitoring stations were divided into three groups according to their geographical location. Figs. 3-4-5 show measured three-monthly average concentration as well as the calculated one for two stations chosen out of each group. Fig. 3 refers to sensors 6 - 30, located at the southern edge of the Industrial Area, while stations 10-29 (fig.4) are situated between the Industrial Area and the urban centers of Mestre and Marghera and finally fig. 5 shows the results for sensors 16 - 22 located in Mestre and in Venice respectively.
The model simulates fairly well the observed values for all the stations but 10 and 29. This is an expected result since the areas in which they are located show discontinuities (i.e. variations in surface roughness, and land-lagoon transition) greater than elsewhere. To this it must be added that they are very close to the strongest point sources and therefore much more affected by possible inaccuracies in the evaluation of their mutual locations.
All the results have been summarized in figs. 6-7, which also show the regression lines for 1973 and 1974 respectively. The correlation coefficients are .72 for the year 1973 and .8 for the year 1974.
The model was also used to calculate $SO_2$ - annual average concentration for the years 1973 and 1974; the relative results are plotted with the experimental ones in figs. 8-9. As it was expected, the model proved to give better results if the period of calculation was extended. The encouraging results obtained by applying the model

led to extend the calculations over the whole area of interest in order to get a visible description of the spatial distribution of the pollutant. This made it possible to draw the isolines of concentration, shown in figs. 10-11, for the periods June-August 1973 and December 1973-February 1974 respectively. By comparing the two maps a conclusion can easily be drawn that because of the local meteorological conditions (Runca and Zannetti, 1973), in summer $SO_2$ "keeps away" from the historical center, and concentrates itself near the industrial sources. In the winter, the different meteorology prevailing over the area as well as the presence of urban emissions causes a wider spread of the $SO_2$ and consequently raises the pollution level in the urban center of Venice.

## Description of the numerical model

The application of a model based on Gaussian plume formula has a few severe limitations. This approach can give erroneous results in low wind conditions. In addition it cannot incorporate the complex effects induced by the local geography and their influence on the distribution of pollutants. Though the Gaussian formulation has the above limitations it is nevertheless widely used. First, because it offers a practical method for calculation and secondly, because the present availability and accuracy of input data is generally inadequate to develop a more sophisticated model. On the other hand if the diffusion of atmospheric pollutants has to be described in detail the model must accomodate temporal and spatial variations of meteorological parameters, effects of the inhomogeneous surface conditions and other features. Since models based on the numerical integration of the diffusion concentration equation, such as those developed by Randerson 1970, Sklarew 1970, Lamb 1971, Shir and Shieh 1973, proved capable of dealing with the previosly mentioned features, the study which is being carried out tests the application of a model of this kind for simulating short term $SO_2$ - average concentration in the Venetian area.

The basic assumption of the model is that the equation governing local changes in $SO_2$ in the atmosphere can be written, disregarding the decay term, as follows:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + S \qquad (1)$$

where:

| | |
|---|---|
| C | mean concentration of $SO_2$ in $Kg/m^3$; |
| u,v,w | horizontal and vertical components of the wind velocity in m/s; |
| Kx,Ky,Kz | coefficients for eddy diffusion along the x,y,z, directions in $m^2/s$; |
| S | source of $SO_2$ in $Kg/m^3$ sec. |

Equation (1) is numerically solved with the method of fractional steps (Yanenko, 1971) in a three dimensional grid system with the x-axis oriented S-N, the y-axis oriented W-E and the z-axis extended vertically to the height of the mixing layer.
At present the grid system consists of 21x21x15 points.
Along the x-and y-axes the grid points are spaced 100 m.apart. The vertical grid sizes depend on the height of the mixing layer. As yet a final decision on the vertical subdivision has not yet been taken. In this preliminary and testing phase the model runs with a mixing height of 280 m. and a constant vertical grid size of 20 m. The orientation of the grid system is such that the industrial emissions as well as the

urban emissions are as far as possible from the edges of the grid framework. Boundary conditions for the vertical diffusion range are specified, assuming that ground and mixing layer base are impermeable to the $SO_2$, as follows:

$$K_z \frac{\partial C}{\partial z} = 0 \qquad z = 0, H(t)$$

where H (t) is the mixing height. The lateral boundary conditions cannot be well posed. At present the model is testing a few different boundary conditions which are not discussed here; the simplest one assumes that inflow and outflow of $SO_2$ due to horizontal diffusion can be neglected. Anyway it results that if the grid framework is large enough computation is not affected by the lateral boundary conditions. As far as the initial conditions are concerned, since the computation shows (Shir and Shieh 1973) that the observed concentration values are reached within two hours under average wind speed conditions, the concentration field at the beginning of the simulation can be set to zero over the whole region.

Numerical scheme

According to the method of fractional steps the concentration field at the time $t+\Delta t$ is obtained from that at the time t by separating the contribution due to the source, convection and diffusion terms ef equation (1). Hence at every time step the equation $\frac{\partial c}{\partial t} = S$ and the remaining six one-dimensional time dependent equations

(3 for the convection and 3 for the diffusion) are solved separately by a finite-difference technique. The numerical scheme applied to the convection equations is the one devised by B. Carlson (Richtmyer and Morton 1967) and it is illustrated for convection along the x-axis, in fig. 12. The diffusion equations are solved with an implicit space-centered difference scheme allowing for a variable grid spacing. With respect to the x-axis the difference equation is:

$$\frac{C_i^{t+\Delta t} - C_i^{t}}{\Delta t} = \frac{2}{\Delta x_i (\Delta x_i + \Delta x_{i-1})} \left\{ \theta D[C_i^{t+\Delta t}] + (1-\theta) D[C_i^{t}] \right\}$$

with

$$D[C_i] = \frac{\Delta x_i}{\Delta x_{i-1}} K_{x_{i-1/2}} C_{i-1} - \left( \frac{\Delta x_i}{\Delta x_{i-1}} K_{x_{i-1/2}} + K_{x_{i+1/2}} \right) C_i + K_{x_{i+1/2}} C_{i+1}$$

where $\Delta X_i$ is the interval between the i and i+1 grid point and $\theta$ is a parametric constant. This method is always stable for $\frac{1}{2} \leq \theta \leq 1$. Since Carlson's scheme is unconditionally stable, assuming $\frac{1}{2} \leq \theta \leq 1$, the choice of the time step and grid spacing in solving equation (1) is limited only by accuracy. With the application of Carlson's scheme it is not necessary to observe the stability condition $u \Delta t \leq \Delta x$, therefore allowing for a time step such that $u \Delta t = \Delta x$ in the area of maximum concentration gradients. The numerical scheme has been tested by comparing analytical with numerical solutions of equation (1), obtained respectively from the explicit relation used by Roberts to represent the diffusion of a puff of smoke (Sutton, 1953) and from calculations with the proposed method. Fig. 13 shows some of the obtained results.

(3 for the convection and 3 for the diffusion) are solved separately by a finite-difference technique. The numerical scheme applied to the convection equations is the one devised by B. Carlson (Richtmyer and Morton 1967) and it is illustrated for convection along the x-axis, in fig. 12. The diffusion equations are solved with an implicit space-centered difference scheme allowing for a variable grid spacing. With respect to the x-axis the difference equation is:

$$\frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} = \frac{2}{\Delta x_i (\Delta x_i + \Delta x_{i-1})} \left\{ \theta D[C_i^{t+\Delta t}] + (1-\theta) D[C_i^t] \right\}$$

with

$$D[C_i] = \frac{\Delta x_i}{\Delta x_{i-1}} K_{x_{i-1/2}} C_{i-1} - \left( \frac{\Delta x_i}{\Delta x_{i-1}} K_{x_{i-1/2}} + K_{x_{i+1/2}} \right) C_i + K_{x_{i+1/2}} C_{i+1}$$

where $\Delta x_i$ is the interval between the i and i+1 grid point and $\theta$ is a parametric constant. This method is always stable for $\frac{1}{2} \leq \theta \leq 1$. Since Carlson's scheme is unconditionally stable, assuming $\frac{1}{2} \leq \theta \leq 1$, the choice of the time step and grid spacing in solving equation (1) is limited only by accuracy. With the application of Carlson's scheme it is not necessary to observe the stability condition $u \Delta t \leq \Delta x$, therefore allowing for a time step such that $u \Delta t = \Delta x$ in the area of maximum concentration gradients. The numerical scheme has been tested by comparing analytical with numerical solutions of equation (1), obtained respectively from the explicit relation used by Roberts to represent the diffusion of a puff of smoke (Sutton, 1953) and from calculations with the proposed method. Fig. 13 shows some of the obtained results.

## Application of the numerical model

As a preliminary investigation the model has been applied with the same input data used in the Gaussian model and with rough assumptions such as constant mixing height, no surface discontinuities, vertical exchange coefficient expressed by a power law and constant emission rate (urban sources enter the model as point sources, see the Gaussian model ). This application showed some agreement between the observed and the computed hourly values as far as their orders of magnitude were concerned. As expected the agreement between the time evolution of observed and expected values was very unsatisfactory.

Since the model was not built to be applied with the input data used in the Gaussian model, the obtained results are not worth being discussed here. An application of the model is being developed in which the meteorological factors affecting $SO_2$ - dispersion are described by experiments carried out by CNR (Italian National Research Council). This application will be the subject of a future article.

## Conclusions

The application of a Gaussian-type model to compute long term $SO_2$ - average concentration in Venice and its surroundings has been presented. Although it is difficult to describe the local meteorology, the choice of characterizing the atmospheric stabilities according to Pasquill's categories as well as the assumptions concerning height variation of the wind and the plume rise proved to be satisfactory. Since the obtained results showed that the seasonal patterns of $SO_2$ - concentration can be described by the model, it has been used to illustrate the influence of seasonal climate on the $SO_2$ dispersion over the area and the contributions of urban and industrial emissions to the pollution level in the historical center of Venice.

Improvements can be brought to the model by introducing in it a proper definition of the atmospheric stabilities on the basis of a more detailed knowledge of the local meteorology as well as by better defining the industrial emissions rates and locations.
In such a way the model could become a valid tool for land planning purposes and for optimizing the monitoring network.
In addition, a model based on the diffusion concentration equation has been briefly described. The devised numerical scheme allows for variable grid spacing and time step. Since the model's spatial resolution can be increased in the areas where the emissions are located and the advection distance per time steps can be made equal to the grid spacing in the region of maximum concentration gradient, a substantial reduction in numerical errors should result. The application of this model with the same data used in the Gaussian model showed their adequacy in describing the average aspects of the phenomena, but not its time evolution. Better results are expected from an application which is being developed with a set of more appropriate data.

Acknowledgements

The authors are indebted to Tecneco, Regione Veneta, Coses and Veneziana Gas which supplied the basic data in this study.

## References


Calder, K.L. — A climatological model for multiple source urban air pollution - Nato Committee on the Challenges of Modern Society, Air pollution n. 5, 1971

Detrie, J.P. — La Pollution Atmosphérique - Dunod, 1969

Gifford, F.A. — Atmospheric diffusion in an urban area - II IRPA Conference, Brighton, England, 1970

Martin, D.O. — An urban diffusion model for estimating long term average values of air quality - Journal of Air Pollution Control Association, january, 1971

Pasquill, F. — Atmospheric diffusion - D. Van Nostrand, 1962

Pooler, F. — A prediction model of mean urban pollution for use with standard wind roses - Intern. J. Air and Water Pollution, 4, 199-211, 1961

Runca, E. and Zannetti, P - A Preliminary Investigation of the Air Pollution Problem in the Venetian Area - IBM Technical Report CRV007/513-3524, December 1973, Venice Scientific Center, Italy

Shieh, L.J. et al. — The IBM air quality diffusion model with an application to New York City - Palo Alto Scientific Center IBM, 1971

Slade, D.H. — Air Pollution - Academic Press vol. 1, 1968

Turner, D.B. — A diffusion model for an urban area - Journ. of Applied Meteorology, 3, 1964

Lamb, R.G. and Neiburger, M. - An interim version of a generalized urban air pollution model. Atmospheric Environment, 5, 239-264, 1971;

Randerson, D. A numerical experiment in simulating the transport of sulfur dioxide through the atmosphere. Atmospheric Environment, 4, 615-632, 1970;

Richtmyer, R.D. and Morton, K.W. - Difference methods for initial value problems - Interscience Publishers, New York, 1967;

Shir, C.C. and Shieh, L.J. - A generalized urban air pollution model and its application to the study of $SO_2$ distributions in the St. Louis metropolitan area. Tech.Rep. RJ 1227, IBM San Jose Res. Cent., Cal., 1973;

Sklarew, R.C. Preliminary report of the $S^3$ urban air pollution model simulation of carbon monoxide in Los Angeles. Systems, Science and Software Inc., La Jolla, Cal., 1970;

Sutton, O.G. Micrometeorology. Mc Graw-Hill, New York, 1953;

Yanenko, N.N. The method of fractional steps. Springer Verlag, Berlin Heidelberg New York, 1971.

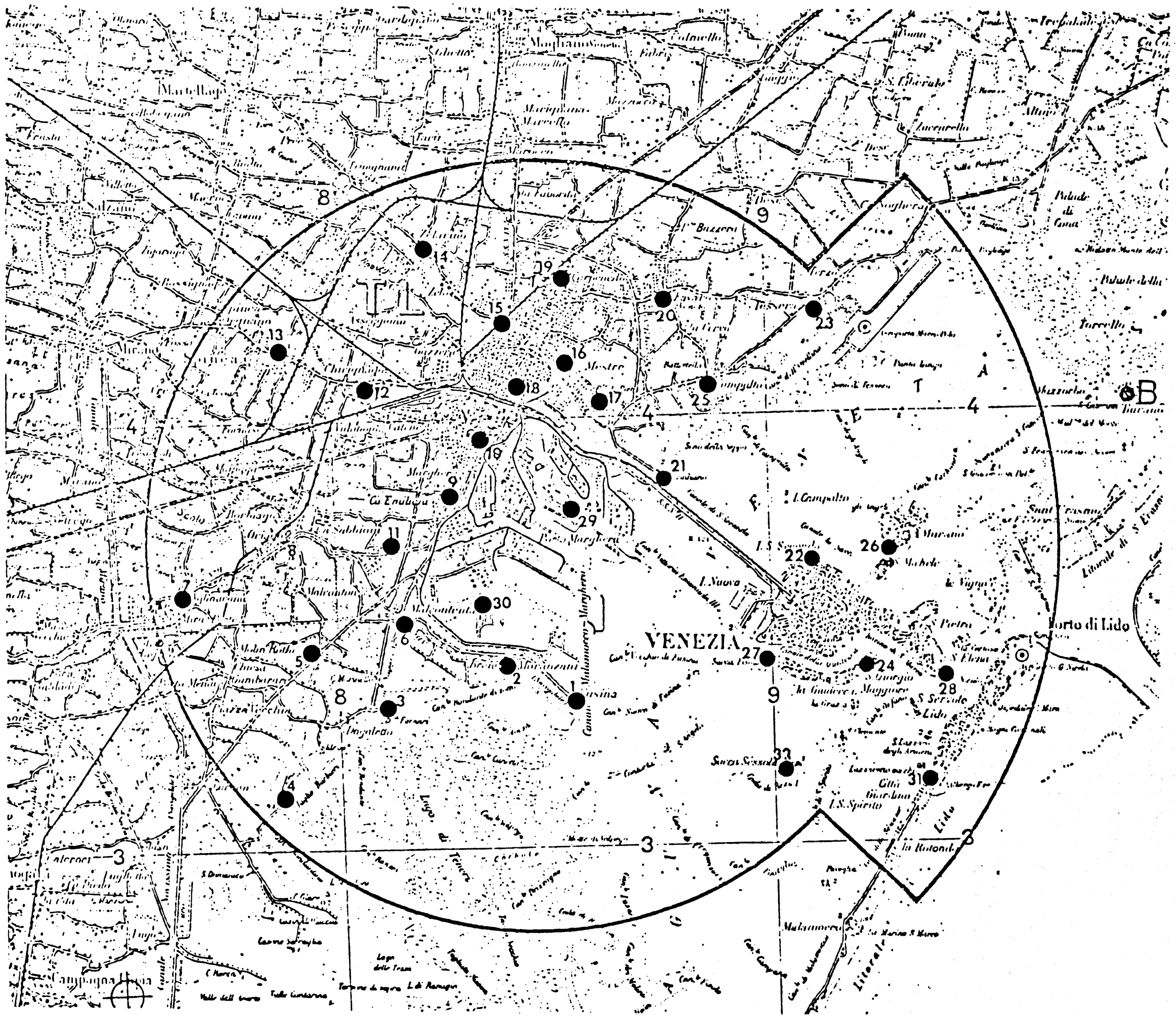



Fig. 1 Venetian Area - Dots indicate the location of the $SO_2$ monitoring stations ( 2,6,9,10,16,17,22,24,29,30 were operating since Feb. '73 )

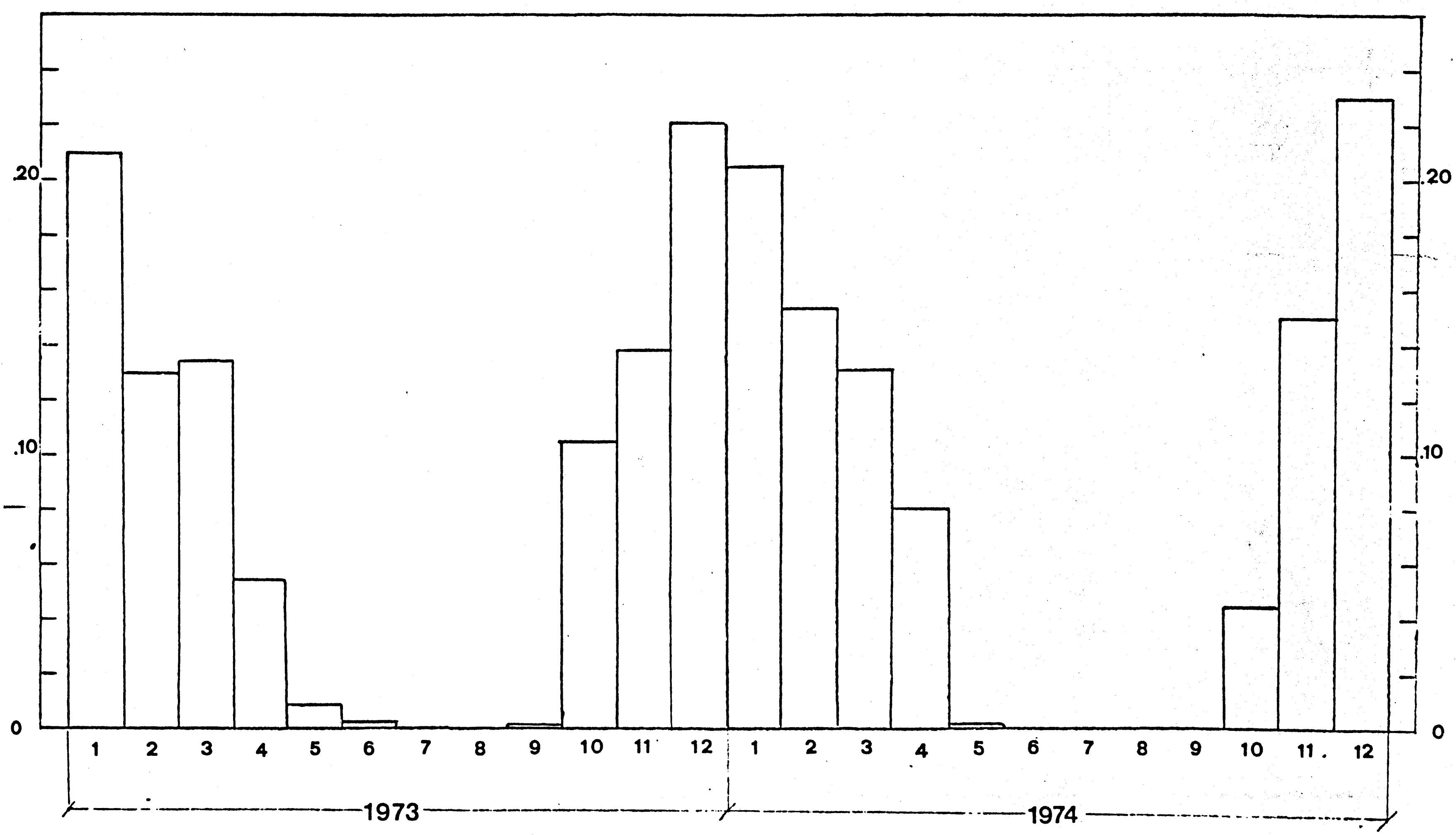
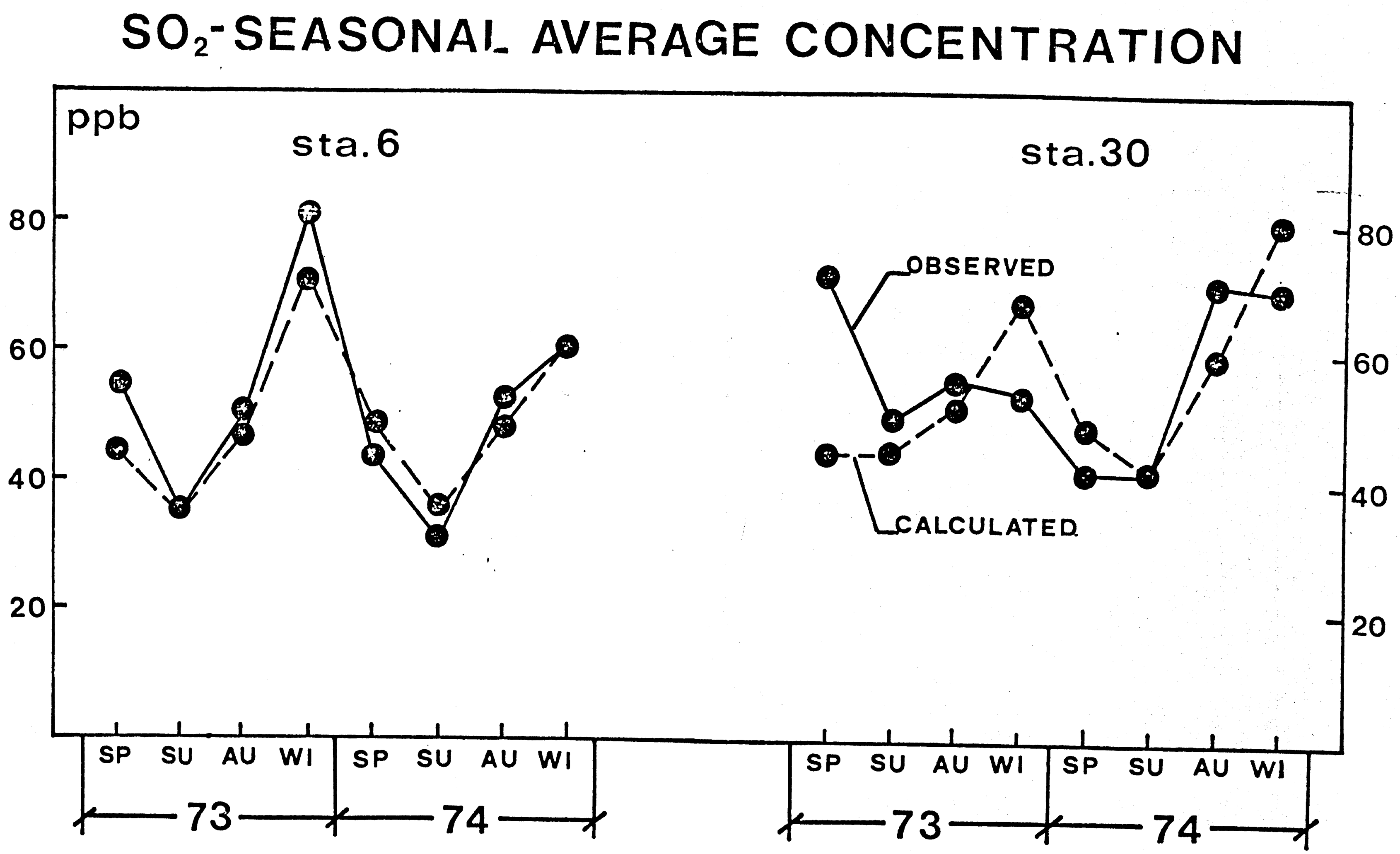


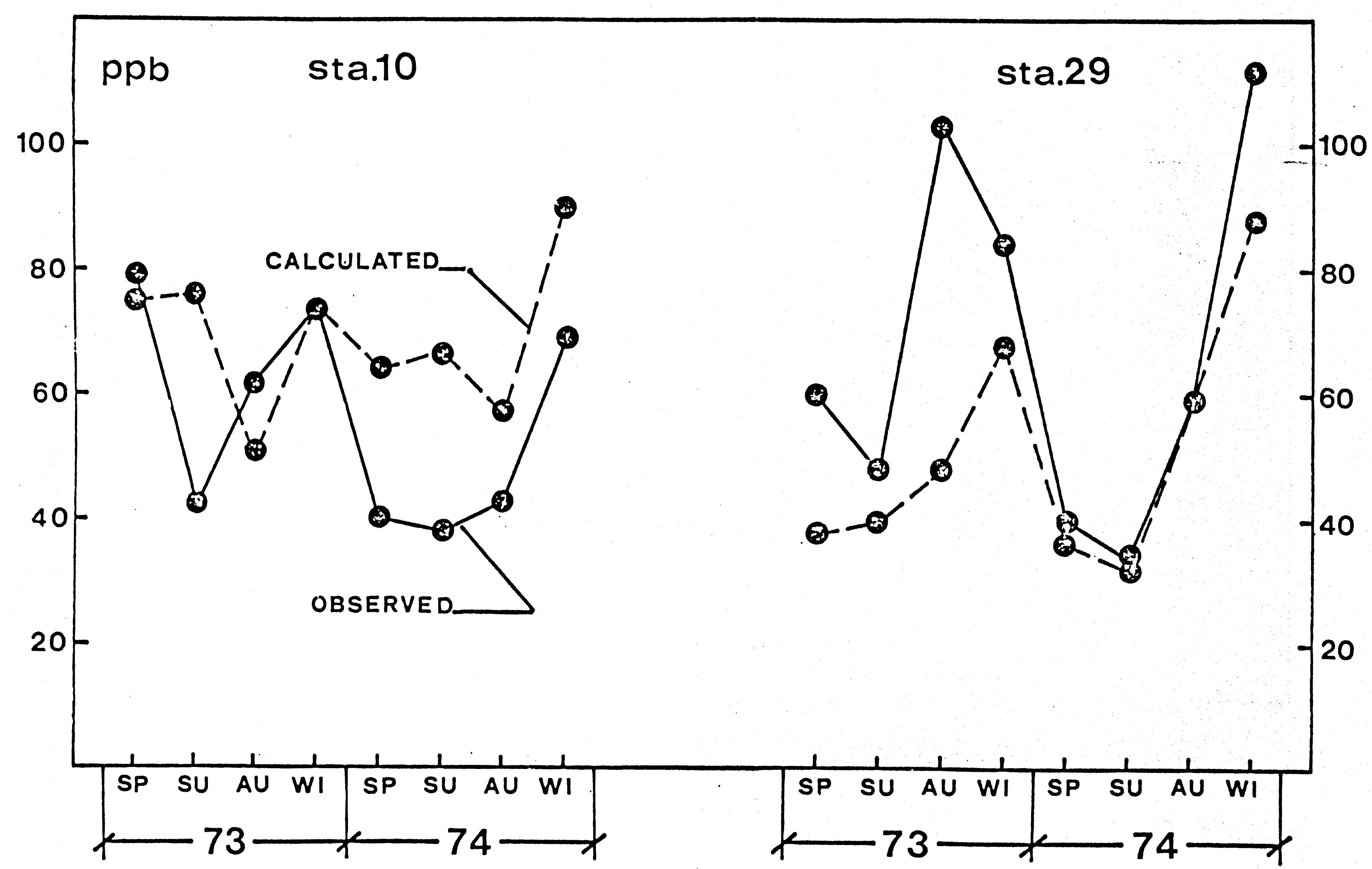

Fig. 2 Histogram of domestic heating emissions distribution throughout the years 1973 and 1974.



SO2-SEASONAL AVERAGE CONCENTRATION
ppb
sta.6
sta.30
OBSERVED
CALCULATED
80
60
40
20
SP SU AU WI SP SU AU WI
73
74


Fig.3

# $SO_2$-SEASONAL AVERAGE CONCENTRATION



# $SO_2$-SEASONAL AVERAGE CONCENTRATION

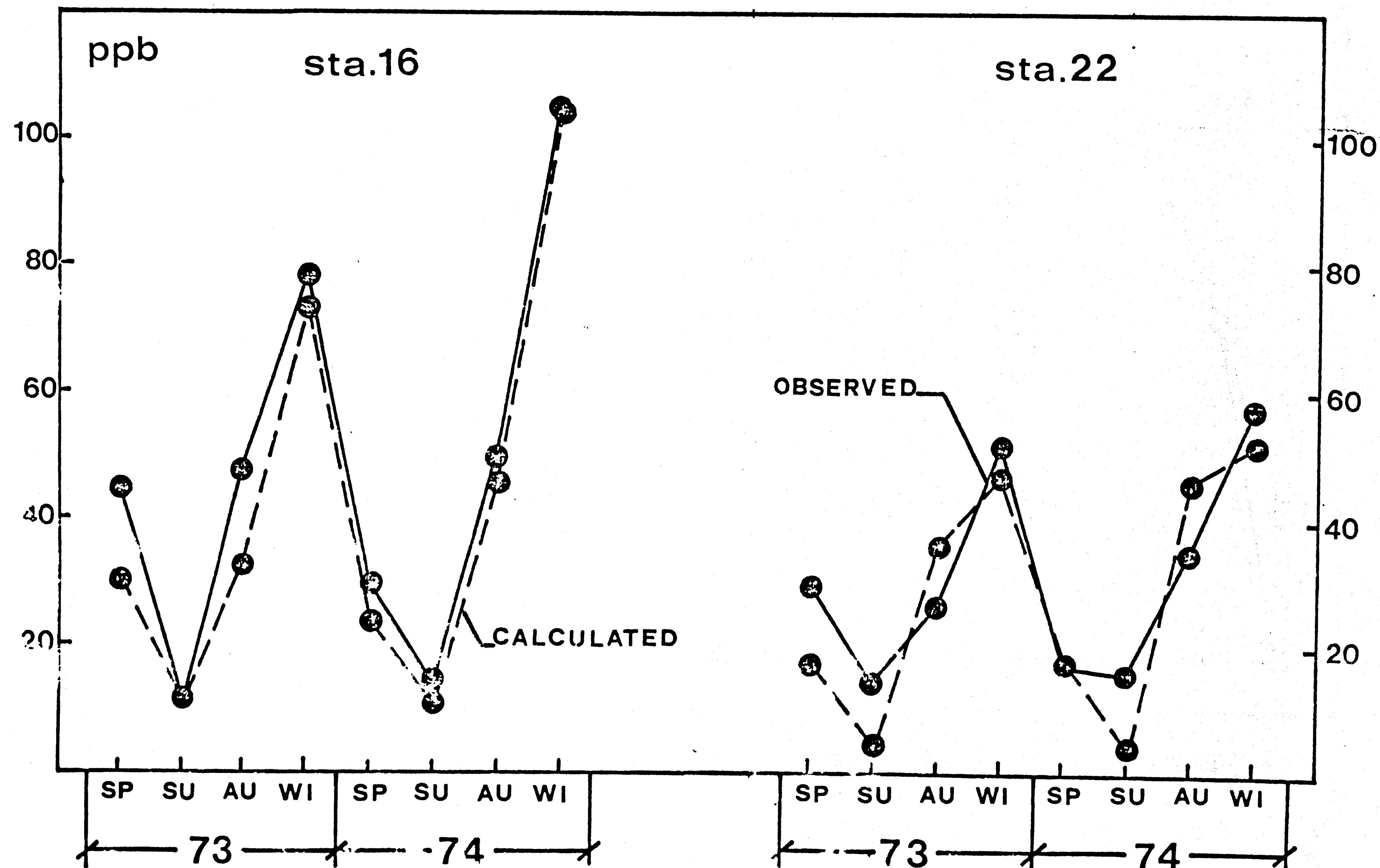



Fig.5

Fig. 6 Regression line of observed versus calculated average $SO_2$ concentration ( ppb ) for three-monthly periods from Feb. '73 to Jan. '74.

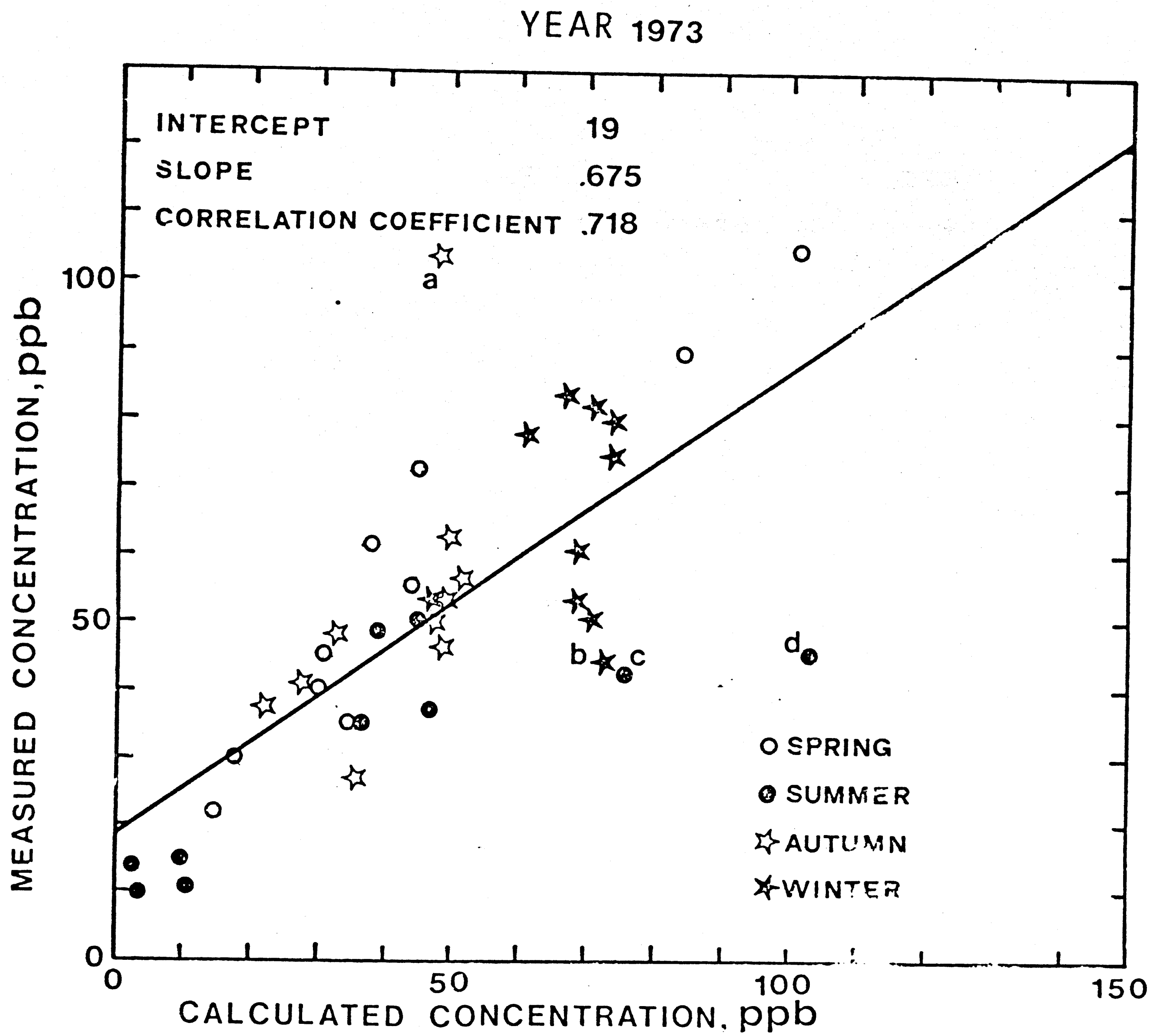
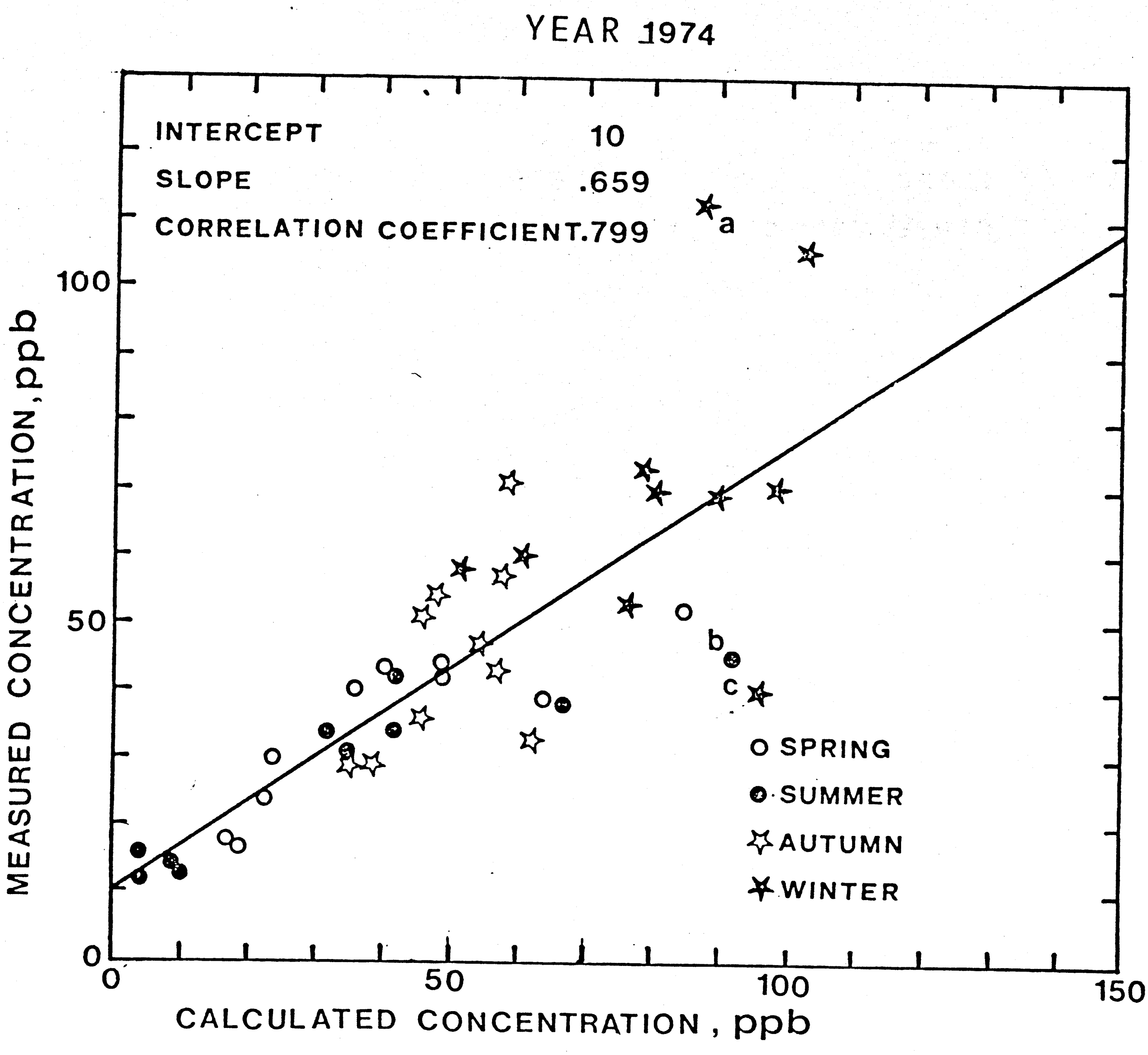


Fig. 7 Regression line of observed versus calculated average $SO_2$ concentration ( ppb ) for three-monthly periods from Feb. '74 to Jan. '75.



## $SO_2$ - ANNUAL
## AVERAGE CONCENTRATION
## 1973

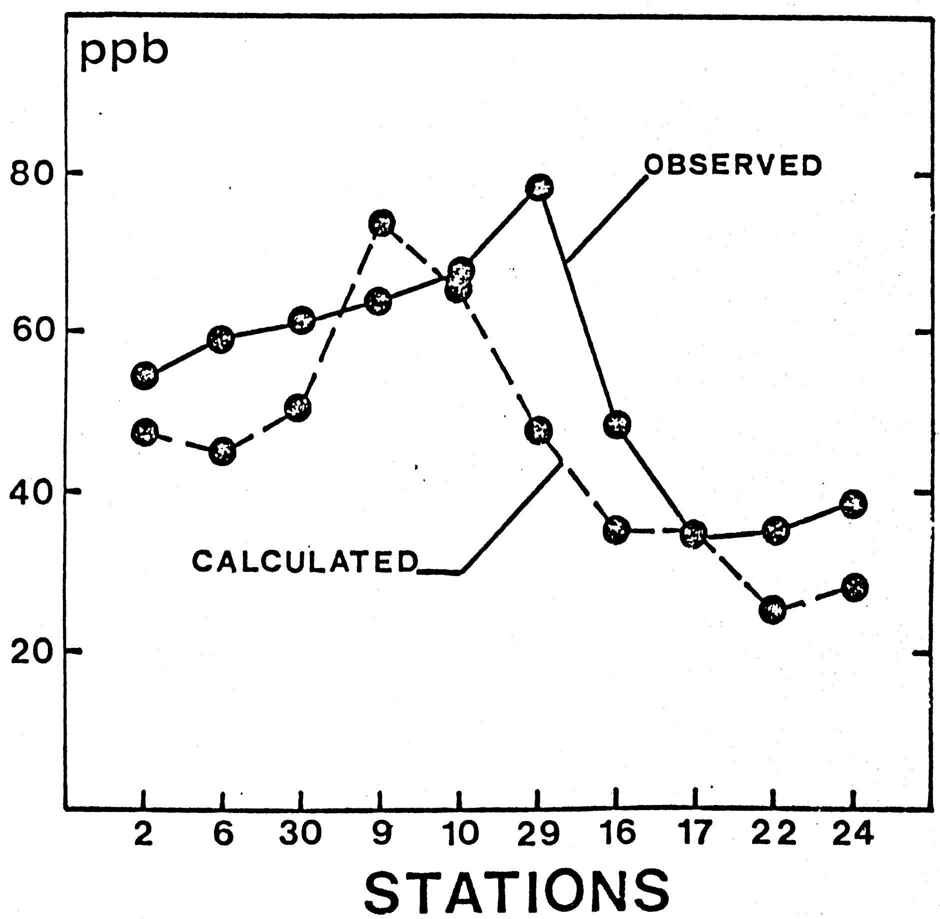



Fig.8

# $SO_2$ - ANNUAL AVERAGE CONCENTRATION 1974

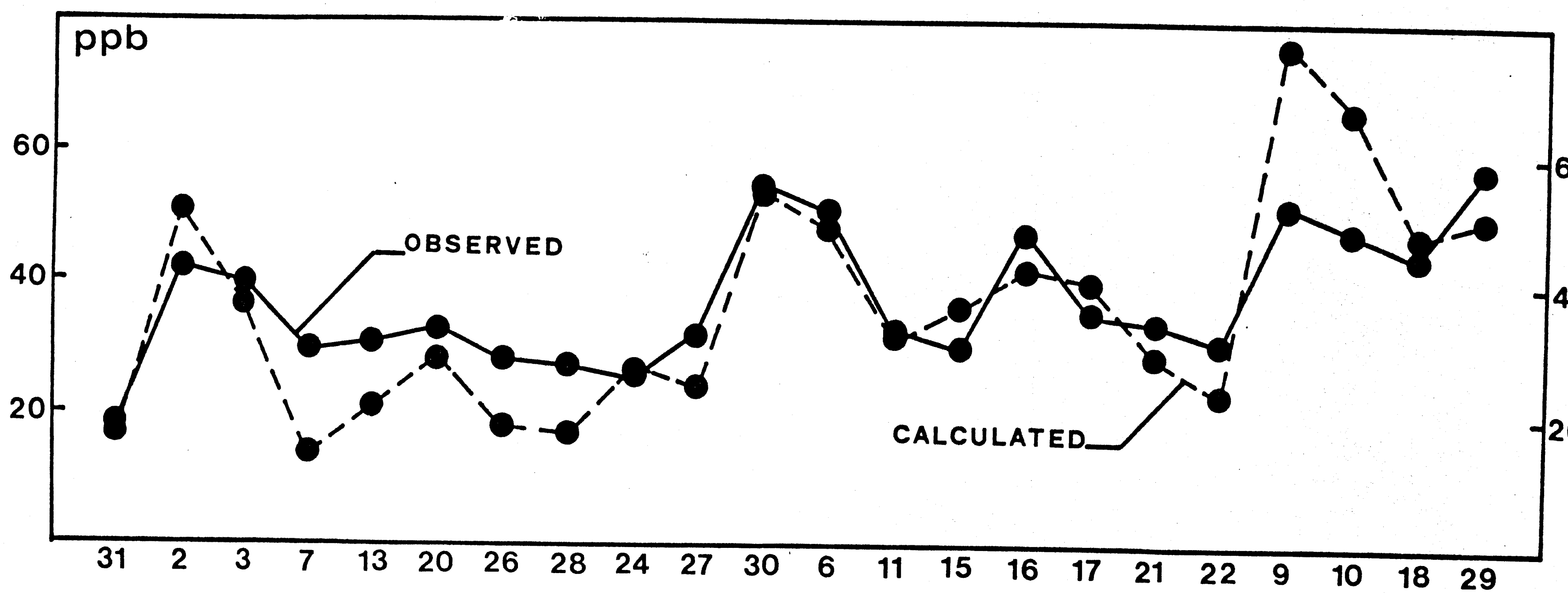



Fig.9

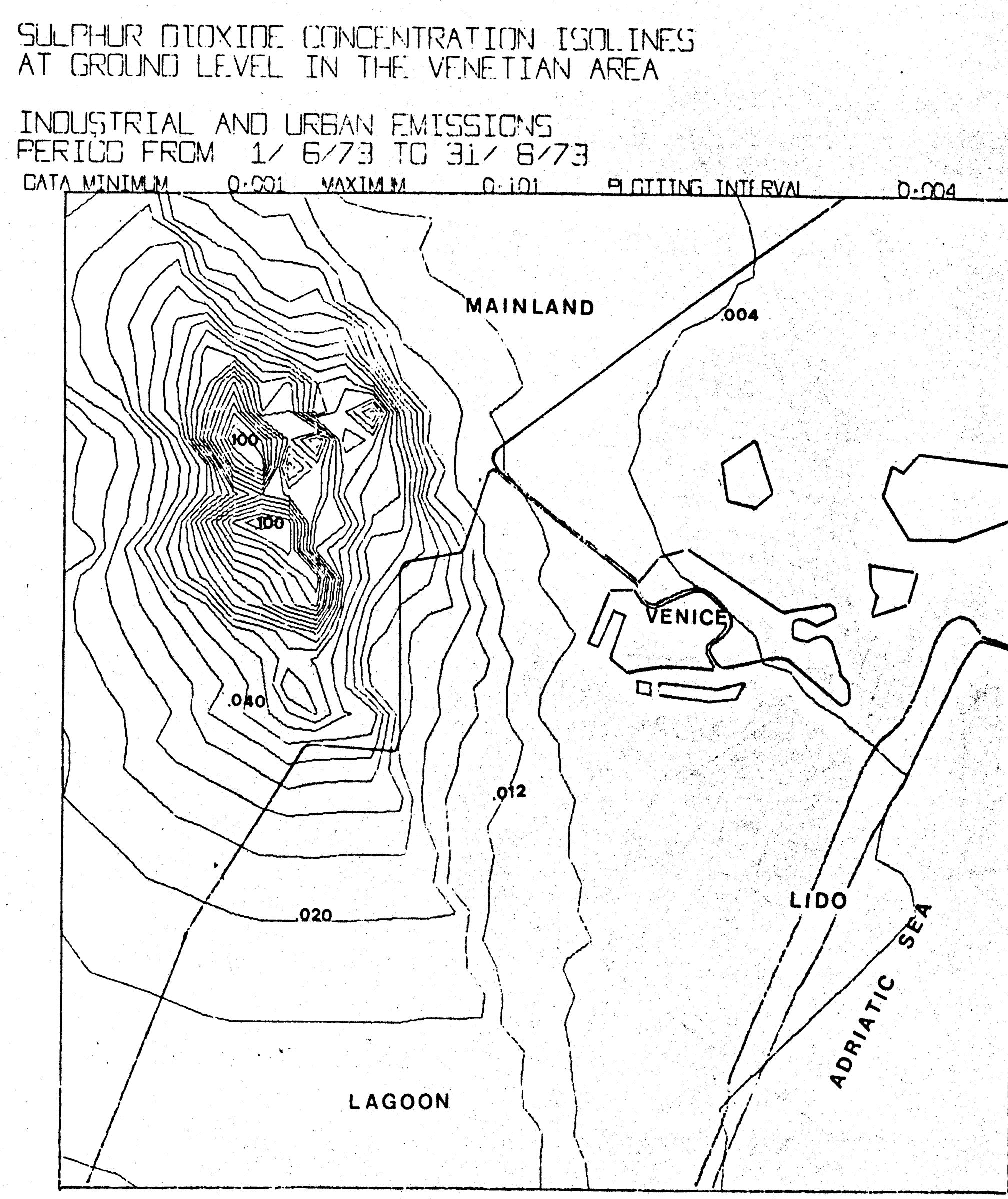



Fig. 10 Concentration values are in ppm.

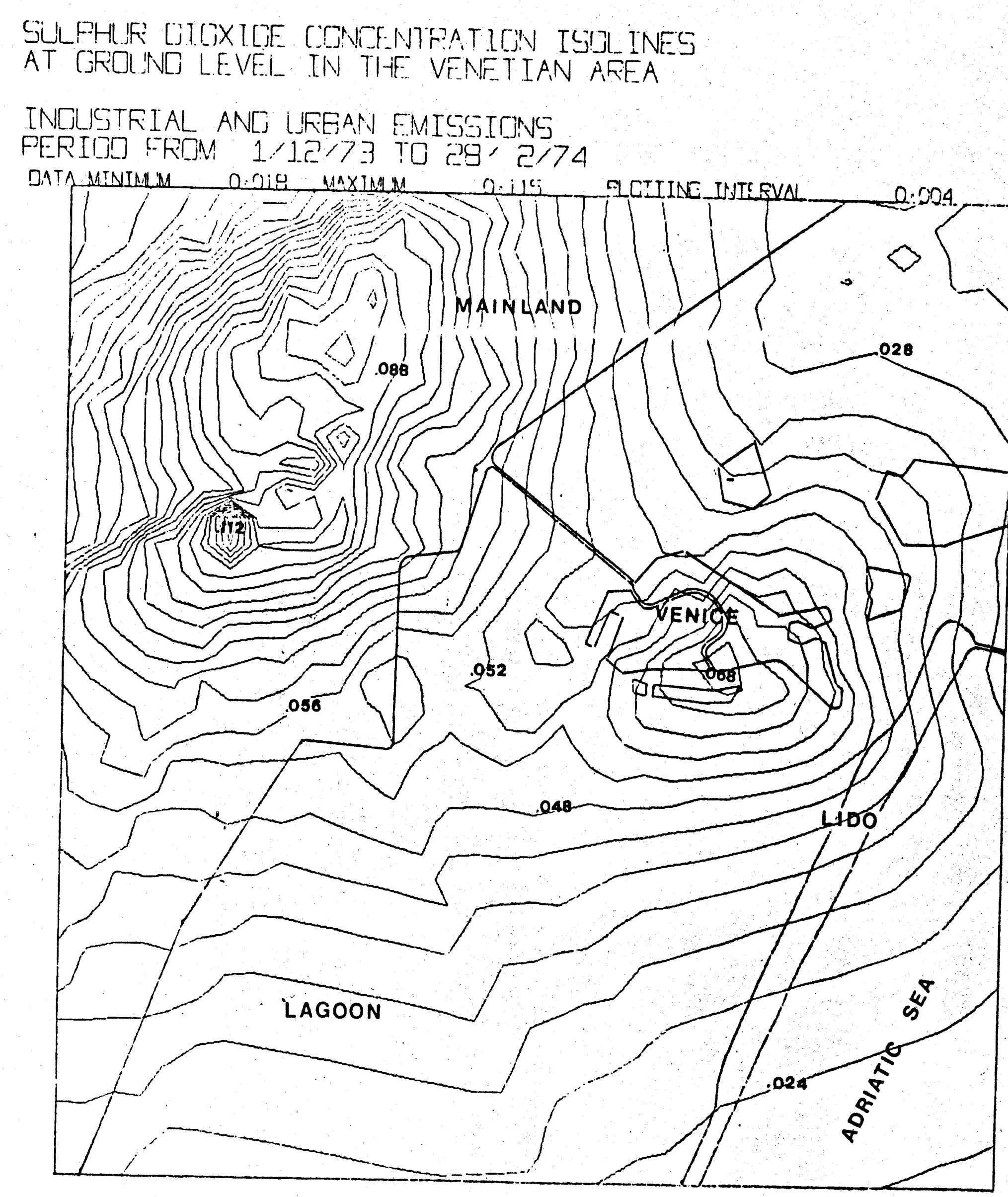
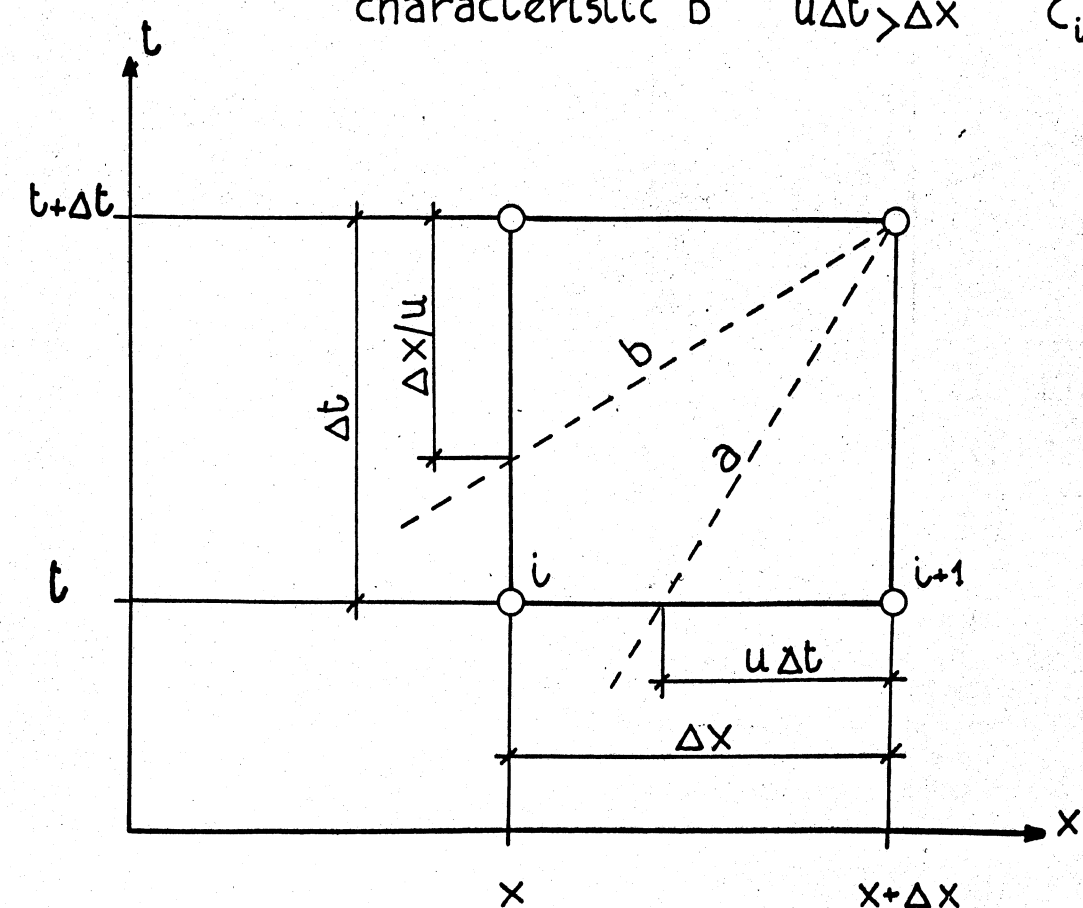



Fig. 11 Concentration values are in ppm.

FIG. 12 - CARLSON'S scheme applied to convection along x-axis

characteristic a $\quad u\Delta t < \Delta x \quad C_i^{t+\Delta t} = \dfrac{C_i^t \cdot (\Delta x - u\Delta t) + C_{i-1}^t u \Delta t}{\Delta x}$

characteristic b $\quad u\Delta t > \Delta x \quad C_i^{t+\Delta t} = \dfrac{C_{i-1}^t \Delta x/u + C_{i-1}^{t+\Delta t} \cdot (\Delta t - \Delta x/u)}{\Delta t}$



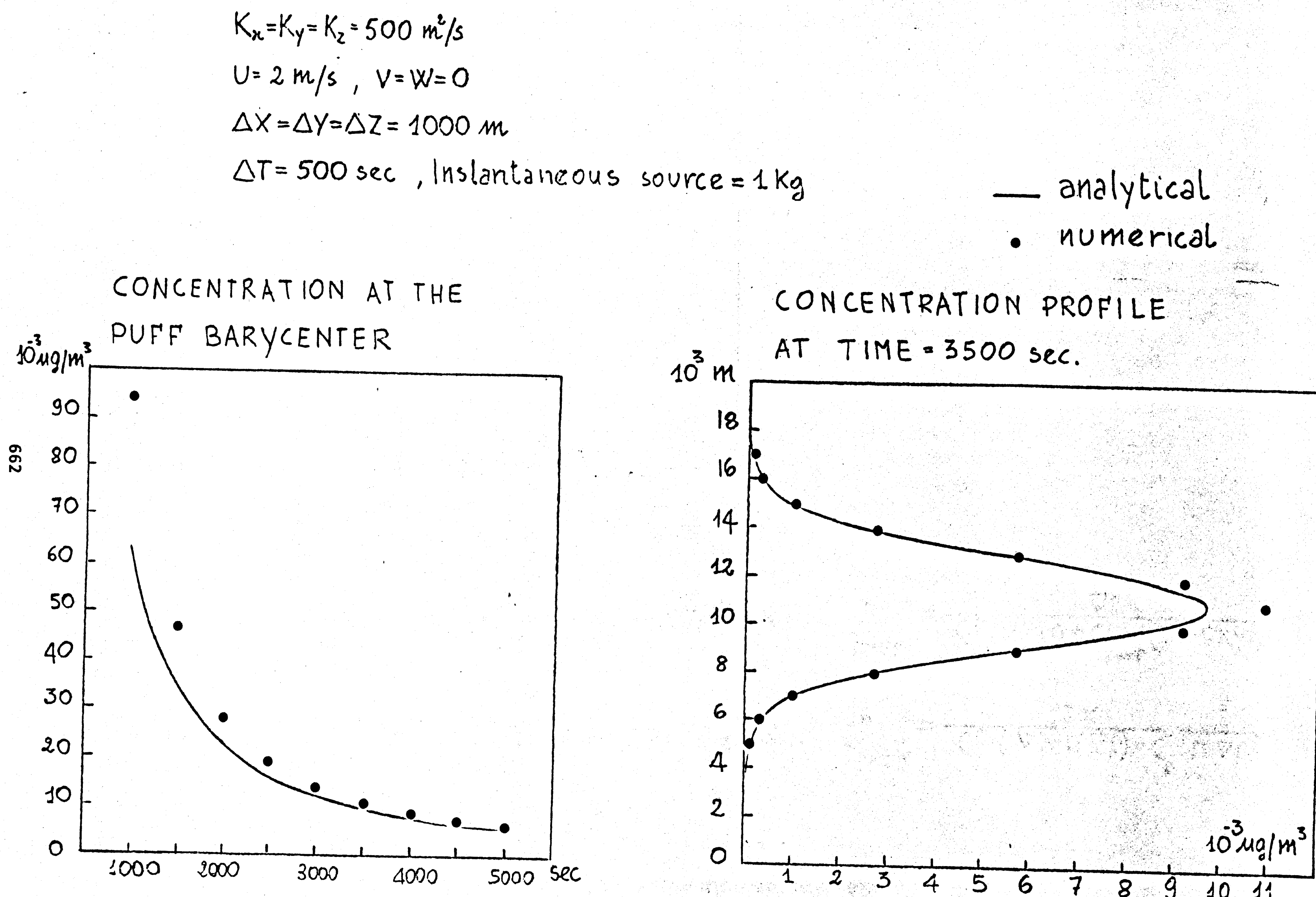



FIG. 13 Comparison of analytical with numerical solution