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F.T.M. Nieuwstadt and C.A. Engeldal

Application of the recommended national air pollution model of the Netherlands to the NATO common data base for the Frankfurt area

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SUMMARY

The national air pollution model of the Netherlands, which is extensively described in this report, has been applied to the NATO/CCMS data base for the Frankfurt region. With this model the annual averaged concentration has been calculated. A distinction was made between the contributions due to area source emissions and those due to point source emissions. The results for the annual averaged concentration are presented in the form of isopleth maps and are also given for six specified receptor locations. The calculated concentrations are compared with preliminary results, which were presented at the meeting of the NATO/CCMS modeling panel in Quail Roost (September 1976).

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INTRODUCTION

As part of the Practical Demonstration of Urban Air Quality Simulation Models in the NATO/CCMS air pollution study, the proposed national air pollution model for the Netherlands (Nieuwstadt et al., 1976) has been applied to the standard data base for SO_2 of the Frankfurt region, as given in the NATO/CCMS document M.P. 2/1975, 2.4.

The yearly averaged concentration has been calculated. Programs to calculate the frequency distribution have not yet become available.

The following remarks should be made regarding the use of the data base. The area sources, which originally had been of the dimension 500 x 500 m, were transformed to area sources of 1 x 1 km. The corners of these area sources were chosen so as to coincide with the grid points of the calculation grid of 1 x 1 km, the dimensions of which are in the W-E direction $9\ \mathrm{km} < x < 48\ \mathrm{km}$ and in the N-S direction $17\ \mathrm{km} < y < 44\ \mathrm{km}$. The source height and the emission of an area source of 1 x 1 km were calculated from the data for the four original 500 x 500 m area sources. The area source emissions used in this calculation were obtained by multiplying the emissions given in the data base by a factor 1560/8760. This is the ratio of the number of yearly heating hours as given in the data base to the total number of hours in a year. For the height of the point sources the geometrical stack height of the data base was used, so that in the calculation no account was taken of the differences in terrain elevation. For the distribution function of wind speed, wind direction and stability classes the data based on the stability class definition by Klug ($h < 100$ m) were used, as given in the data base.

The calculations were performed with a total number of 540 area sources and 681 point sources on the B6700-computer of the Royal Netherlands Meteorological Institute. The total computer time for the calculation of the point sources was 39 min. and for the area sources 26 min.

DESCRIPTION OF THE MODEL

For the background on the choice of the national model and its parameters one is referred to Nieuwstadt et al. (1976) and to Kleine Commissie (1976).

1. The long-term Gaussian model

The concentration averaged over a long period (season, year) $\overline{C}$ [g/m^3] at ground level, as a result of a source at the location: (0,0,H), is described by

$$\overline{C}(x,y) = \sum_S \sum_N \left\{ \frac{2Q}{\sqrt{2\pi}\, u_N\, \sigma_{z_S}} \cdot f(\theta,S,N)\, \frac{n}{2\pi r} \cdot C_{L_S} \cdot \exp\left(- \frac{H^2_{S,N}}{2\sigma^2_{z_S}} \right) \right\}$$

In this equation r[m] is the horizontal distance from the source: $r = \sqrt{x^2 + y^2}$. The source has an emission Q[g/s].

The concentration is given in a sector $2\pi/n$ in width around the direction $\theta + 180^o$ (θ indicates the wind direction class, defined as a sector also $2\pi/n$ in width around θ).

The vertical dispersion coefficient σ_z [m] is classified according to stability classes (S).

The transport velocity of the plume u [m/s], calculated from the wind speed, is subdivided into wind speed classes (N). H [m] is the effective source height, which follows from the physical stack height h [m] and the plume rise Δh [m]. The function $f(\theta,S,N)$ gives the distribution over the wind speed, wind direction and stability classes. The coefficient C_{L_S} describes the influence exerted on the ground level concentration by the mixing height (8).

2. Stability classes (S)

To determine the stability class the KNMI-scheme, which is a modification of the Pasquill stability class definition, is chosen. The stability class is defined from the amount of clouds (in eights), the wind speed at a height of 10 m (in knots, 1 knot =

½ m/s), the time of the day and the season (Nieuwstadt et al., 1976).

The dispersion coefficients for high sources are classified after the stability class definition by Singer and Smith.
A tentative relation between the stability classes after the KNMI-definition and after the Singer and Smith definition is

KNMI		Singer and Smith
A	—	B_2
B	—	B_2
C	—	B_1
D ($u \leqslant 5.5$ m/s)	—	B_1
D ($u > 5.5$ m/s)	—	C
E	—	D
F	—	D

where u is the wind speed at a height of 10 m.

The results based on the stability class definition by Klug ($h < 100$ m) have been used in the calculations with the data base. The following relation between the Klug stability classes and the KNMI/Pasquill classes was chosen:

KNMI		Klug
A	—	V
B	—	IV
C	—	III_2
D	—	III_1
E	—	II
F	—	I

3. The distribution function of wind direction classes, stability classes and wind speed classes $f(\theta,S,N)$

The distribution function consists of a frequency distribution over 6 stability classes S (2), 3 wind speed classes N and 12 wind direction classes θ of the size of $2\pi/n = 30^\circ$ (345°-015°, 015°-045° etc.). This distribution function was calculated from the meteorological data given in the data base.

For the 3 wind speed classes the representative wind velocity at a height of 10 m is defined as

Wind speed class	Wind speed limits	Representative wind speed
1	1- 5 kts (0.5-2.5 m/s)	1.45 m/s
2	6-11 kts (3-5.5 m/s)	4.0 m/s
3	$\geqslant$ 12 kts ($\geqslant$ 6 m/s)	8.0 m/s

4. Dispersion coefficients (σ_z)

The dispersion coefficients are a function of the height above the earth's surface, because the turbulence on which the dispersion coefficients depend is a function of the height above the surface. The recommendation for the dispersion coefficients is therefore subdivided according to the effective source height H.

a) Low sources ($H \leqslant 10$ m) and area sources.

σ_z according to Pasquill

$\sigma_z = ar^b * C_{z_0}$ (σ_z and r in m)

Stability class	a	b
A	0.28	0.90
B	0.23	0.85
C	0.22	0.80
D	0.20	0.76
E	0.15	0.73
F	0.12	0.67

The coefficient C_{z_0} describes the effect of the surface roughness on the dispersion coefficient. The roughness of the area where the source is situated is characterized by the roughness length $z_0[m]$.

For $z_0 = 0.10$ m it follows that $C_{z_0} = 1$. For other values of z_0 the coefficient C_{z_0} becomes

$$C_{z_0} = (10\ z_0)^{0.53}\ r^{-0.22}$$

$z_0[m]$ is the roughness length and $r[m]$ the horizontal distance from the source (1).

Some representative values for z_0 are

flat country	(e.g. polder landscape with a few trees)	approx. 0.03 m
agricultural land	(e.g. airfield, arable land, polder with many trees)	approx. 0.10 m
cultivated land	(e.g. hothouse area, open area with much vegetation, scattered houses)	approx. 0.30 m
residential area	(e.g. area with many but low buildings, wooded area, industrial area with not too high obstacles)	approx. 1.00 m
urban area	(e.g. a big city with high buildings, industrial area with high obstacles)	approx. 3.00 m

For the calculations with the data base for the Frankfurt area the value of the roughness length is taken to be $z_0 = 3.00$ m.

b) High sources ($100 \leqslant H <$ circa 400 m).

σ_z according to Singer and Smith

$\sigma_z = ar^b$ (σ_z and r in m)

Stability class	a	b
B_2	0.411	0.907
B_1	0.326	0.859
C	0.223	0.776
D	0.062	0.709

c) Sources with an effective height $10\ \mathrm{m} < H < 100\ \mathrm{m}$.

The σ_z is determined for each value of r by means of a linear interpolation:

$$\sigma_z = \sigma_z(a)(100-H)/90 + \sigma_z(b)(H-10)/90$$

where $\sigma_z(a)$ is the σ_z calculated according to a) and $\sigma_z(b)$ is the σ_z calculated according to b).

d) Very high sources ($h \geqslant 150$ m and $H >$ approx. 400 m).

An effective height > 400 m was reached by three point sources in the data base. This occurred only for the lowest wind speed class. The calculation of the concentrations from these point sources has been done with the coefficients of Singer and Smith.

5. Plume rise (Δh)

The plume rise is calculated with formulas of Briggs.

$$\Delta h = 109\ Q_H^{3/4}/u \qquad Q_H < 6\ \mathrm{MW}$$

$$\Delta h = 143\ Q_H^{3/5}/u \qquad Q_H \geqslant 6\ \mathrm{MW}$$

The Q_H is the heat output of the sources in MW. The u is the wind velocity at the top of the stack (h) (calculated by means of the equation given in 7).

An upper limit to the plume rise is set by the equation

$$\Delta h = 115(Q_H/u)^{1/3}$$

This equation results from the plume rise formula of Briggs for stable conditions, with the temperature gradient parameter s equal to $1.4\ 10^{-4}$.

The Q_H is calculated with respect to an air temperature of 10° C.

6. Transport velocity (u)

The transport velocity of the plume must be representative of the entire layer in which the diffusion takes place. This velocity is calculated from the representative wind speed at a height of 10 m (u_{10}) for each wind speed class N (3). From the wind speed u_{10} the wind velocity u(z) at an arbitrary altitude z can be calculated by means of the equation given in 7.

In the calculation of the transport velocity a classification is applied after the effective source height, analogous to the classification of the dispersion coefficients (4).

a) Point sources ($H \leqslant 10$ m): the wind velocity at a height of 10 m: u_{10}.

Area sources: the wind velocity at the effective source height H (with a minimum of H = 10 m): u(H).

b) ($100 \text{ m} < H <$ approx. 400 m).

I. $H \leqslant \frac{1}{2}L$

$u = u(H)$ if $0.62\ \sigma_z \leqslant H$

$u = u(0.62\ \sigma_z)$ if $H \leqslant 0.62\ \sigma_z \leqslant \frac{1}{2}L$

$u = u(\frac{1}{2}L)$ if $0.62\ \sigma_z > \frac{1}{2}L$

II. $H > \frac{1}{2}L$

$u = u(H)$

in the case of $L \leqslant H \leqslant 3/2\ L$: $u = u(L)$

The σ_z is calculated according to 4b. The mixing height L is discussed in 8.

c) ($10 \leqslant H \leqslant 100$ m).

For all distances the transport velocity u is determined by a linear interpolation.

$$u = u(a)(100-H)/90 + u(b)(H-10)/90$$

where u(a) is the transport velocity calculated according to a) and u(b) is the transport velocity calculated according to b), with σ_z following from 4b and with H chosen equal to 100 m.

7. Wind profile according to a power law

The wind speed at an arbitrary height z [m] is calculated from the wind speed at a height of 10 m: u_{10} by means of the equation

$$u(z) = u_{10}\ (z/10)^p$$

The exponent p is a function of the stability class.

Stability class according to Pasquill	p
A	0.10
B	0.10
C	0.16
D	0.16
E	0.30
F	0.30

8. Mixing height

The mixing height sets a limit to the vertical dispersion. For each stability class one fixed mixing height is chosen.

Stability class according to Pasquill	L (in m)
A	1500
B	1500
C	1000
D	500
E	200
F	200

The influence of the mixing height on the ground level concentration is determined by the coefficient C_{L_S} (1).

	C_{L_S}
$0 < \sigma_z/L \leqslant 0.6\sqrt{1-H/L}$	1
$0.6\sqrt{1-H/L} < \sigma_z/L < 0.9$	$1+\left[\exp\left\{\frac{(2L-H)^2}{2\sigma_z^2}\right\}+\exp\left\{\frac{(2L+H)^2}{2\sigma_z^2}\right\}\right]\Big/\exp\left\{-H^2/2\sigma_z^2\right\}$
$\sigma_z/L > 0.9$	$\frac{1}{L}\,\frac{\sqrt{2\pi}\,\sigma_z}{2\exp(-H^2/2\sigma_z^2)}$

This last factor leads to the so-called uniform vertical distribution of the concentration in the mixing layer. In the evaluation of C_{L_S} the σ_z is calculated according to 4a, b or c.

When $h > L$ holds good, it is assumed that the plume is above the mixing layer and for that reason will not contribute to the concentration at ground level.
It is also assumed that for $H > 3/2\ L$ the plume will break through the inversion capping the mixing layer and will not contribute to the ground level concentration either. When $L \leqslant H \leqslant 3/2\ L$, the effective source height H is set equal to the height of the mixing layer L.

9. Area sources

An area source is for practical reasons subdivided into squares with a side of 1 km.
To calculate the dispersion from an area source the virtual point source equation is used. The virtual point source is situated in the middle of each square of the area source. The ground level concentration from each virtual point source is calculated with the equation

$$\bar{C} = \sum_{S}\sum_{N}\left\{\frac{Q\,f(\theta,N,S)}{u_N\left(\sqrt{\frac{\pi}{2}}\,\sigma_{z_S}\,\frac{2\pi r}{n}+\frac{A}{K}\right)}\quad C_{L_S}\exp\left(-\frac{H^2_{S,N}}{2\sigma^2_{z_S}}\right)\right\}$$

For an explanation of most of the parameters used in this equation see section 1.

The emission Q is the total emission [g/s] of the area source square. The initial vertical dispersion inside the area source is simulated by adding a virtual distance r_o [m] to the horizontal distance r [m] in the evaluation of σ_z: $\sigma_z(r + r_o)$.

The virtual distance r_o is determined from the equation $\sigma_z(r_o) = H$, where H is the effective source height of the area source and where the σ_z for each stability class is calculated according to 4a, b or c, the roughness correction included.

The initial horizontal mixing inside the area source is described by the term A/K in the denominator of the above equation. The A [m^2] is the area of the area source.
The factor K is a function of the size of the area source square. For a square of 1 x 1 km K can be chosen equal to 50.
The virtual point source model should not be used for calculating the ground level concentration inside the area source square.

RESULTS

In the figures 1, 2 and 3 isopleths of the annual averaged concentration are given for the concentrations respectively from the point sources, area sources and both groups combined.

In the receptor points the following concentrations have been calculated.

	Receptor points		Concentration in $\mu g/m^3$		
	x-coord.(km)	y-coord.(km)	point source	area source	total
1 :	22.29	26.53	21.0	57.5	78.5
2 :	28.25	28.15	17.0	48.1	65.1
3 :	24.76	28.98	20.8	67.5	88.3
4 :	16.00	27.00	28.8	41.3	70.1
5 :	19.00	32.00	15.3	29.5	44.8
6 :	34.00	27.00	11.7	29.7	41.4

No comparison with measured data could be made, because the measuring results will be available only at a later stage of the demonstration.

Some comparison with other calculations could be made, the preliminary results of which were given at the meeting of the modeling panel in Quail Roost, in September 1976.

Receptor points	1976 Tex. Air Contr. Brd			1976 Turner			1976 Irwin			this study		
	I	II	III	I	II	III	I	II	III	I	II	III
1	14	109	123	16	55	71	4	68	72	21	58	79
2	13	84	97	15	45	60	4	53	57	17	48	65
3	16	95	111	16	60	76	3	72	75	21	67	88
4	15	70	85	14	39	53	3	44	47	29	41	70
5	15	8	23	13	17	30	2	19	21	15	30	45
6	8	43	51	11	26	37	2	36	38	12	30	42

I	concentrations from the point sources in $\mu g/m^3$
II	concentrations from the area sources in $\mu g/m^3$
III	total concentration in $\mu g/m^3$

From Turner (1976) only the results for CDM-36 were compared. In the results of Irwin (1976) the comparison was made with the average over the five samples.

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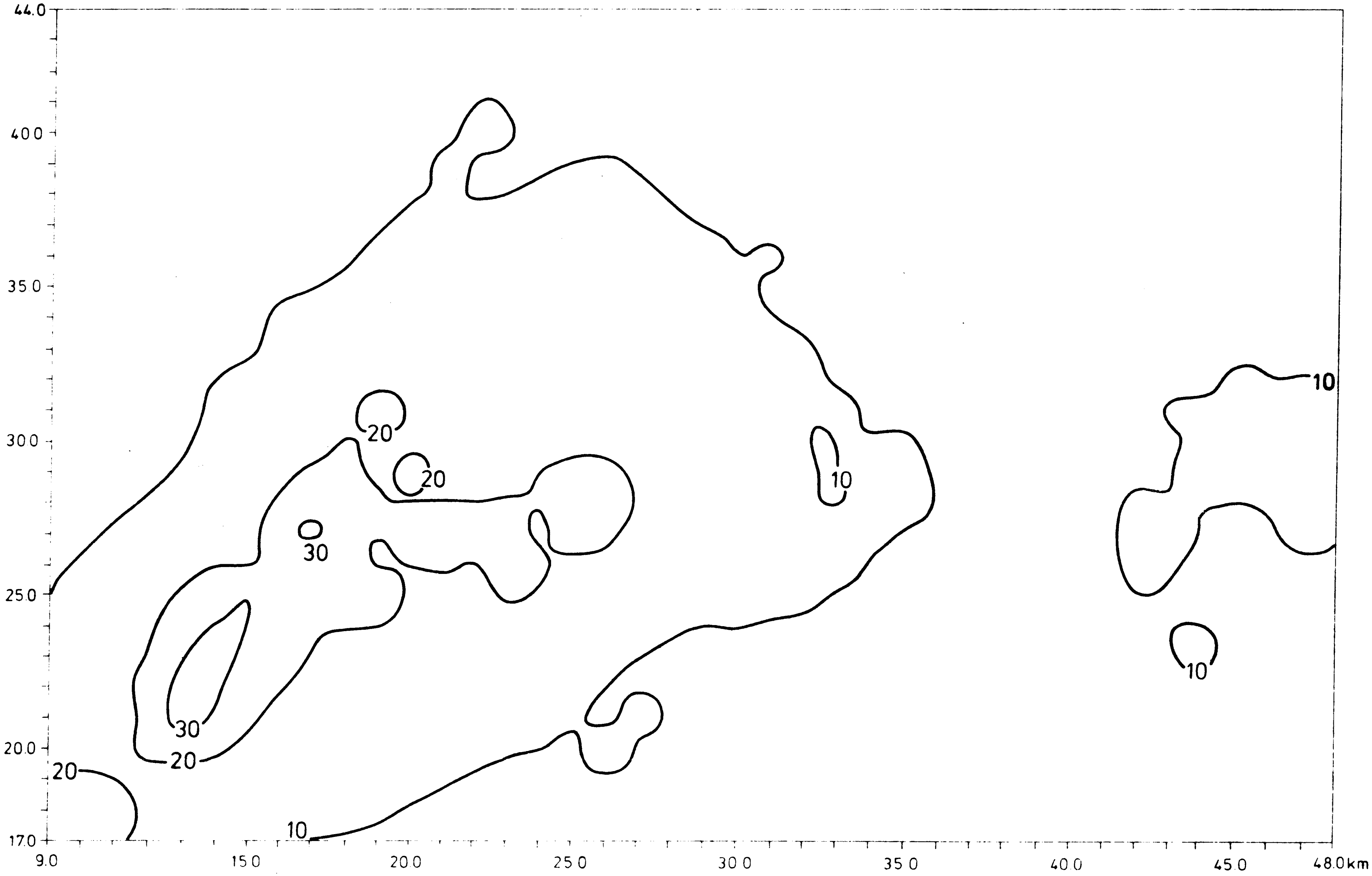

Fig. 1 Data base Frankfurt : annual averaged concentration in $\mu g/m^3$ due to emissions from point sources

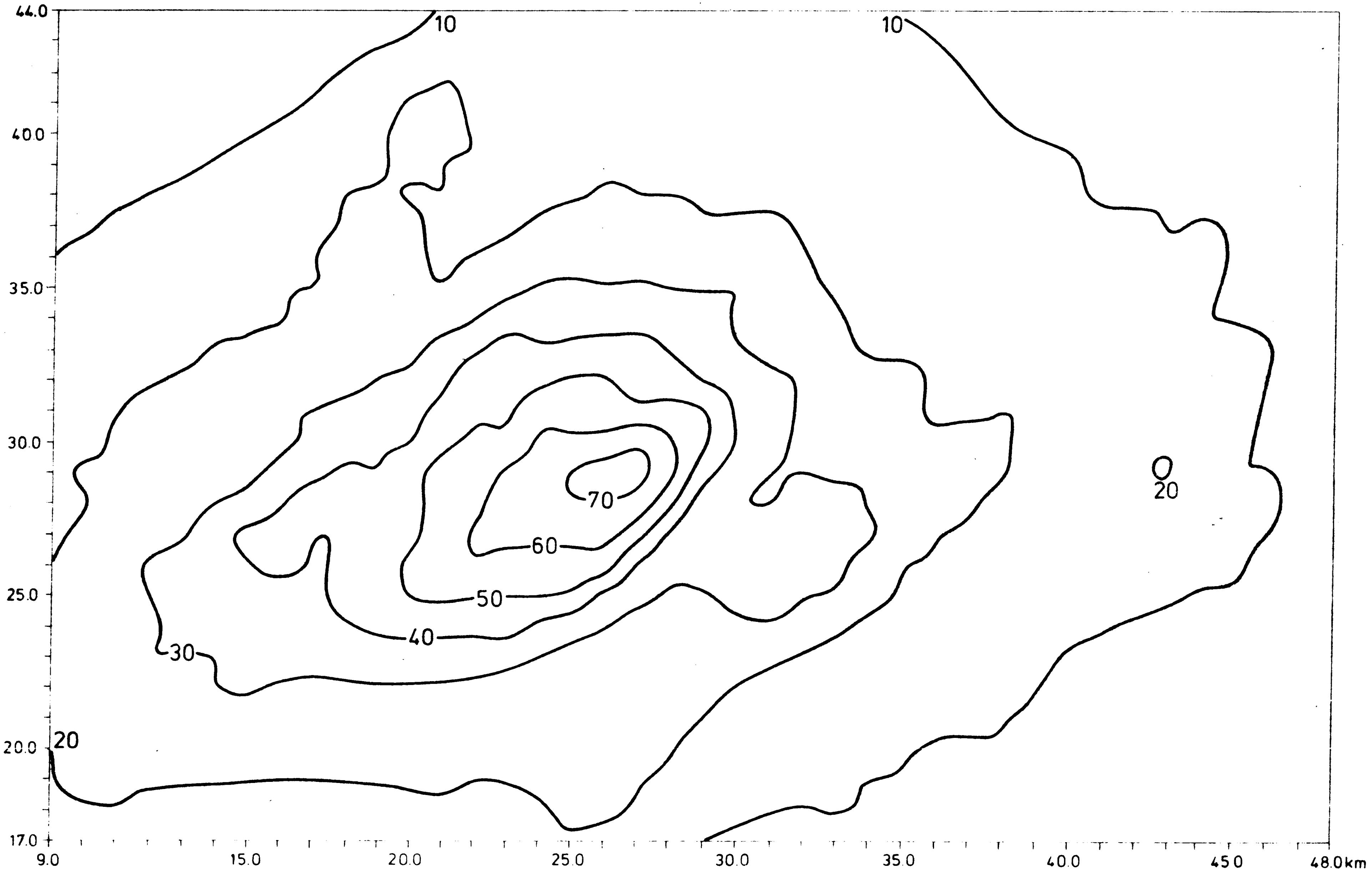

Fig. 2 Data base Frankfurt: annual averaged concentration in $\mu g/m^3$ due to emissions from area sources

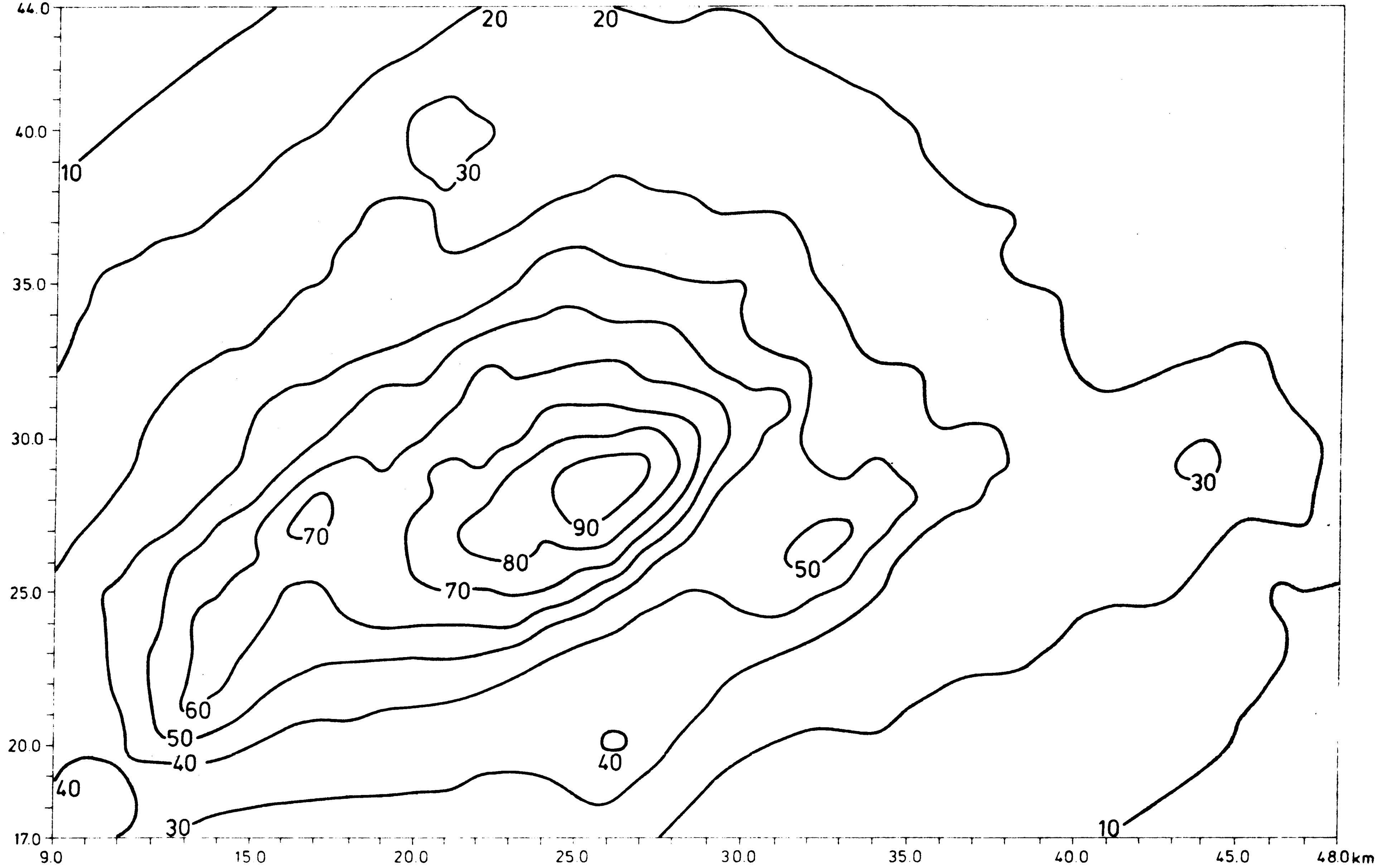

Fig 3 Data base Frankfurt· annual averaged concentration in $\mu g/m^3$ due to emissions from all sources