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A Model for Estimation of Airborne Pollution in long Time Intervals

C.F. Højerup

Risø National Laboratory, DK-4000 Roskilde, Denmark
September 1984

Risø-M-2444

A MODEL FOR ESTIMATION OF AIRBORNE POLLUTION IN LONG TIME INTERVALS

C.F. Højerup

Abstract. A model has been developed for calculation of concentrations in air and deposition rates on ground surface of pollutants emitted from chimneys.

The model can handle two pollutants simultaneously, one of which is generated from the other by chemical transformation during the transport.

A model for the lift of hot plumes is presented and incorporated in the dispersion model.

EDB descriptors: AIR POLLUTION; CHIMNEYS; DEPOSITION; DISPERSIONS; MATHEMATICAL MODELS; PLUMES; POLLUTANTS.

UDC 551.510.4 : 551.511

September 1984
Risø National Laboratory, DK 4000 Roskilde, Denmark

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The project is carried out at Risø National Laboratory, Department of Energy Technology.

The work is followed by a group of experts from government institutions and electric utilities:

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CONTENTS

	Page
Introduction	5
Qualitative description of the model	5
References	12
APPENDIX 1. Meteorological data	13
APPENDIX 2. Plume lift	16
APPENDIX 3. Dispersion model for one pollutant	24
APEPNDIX 4. Dispersion model for one pollutant	30

Dansk resumé. Der er udviklet en model til beregning af koncentrationerne i luft og depositionshastighederne på jordoverfladen af forurenende stoffer, der udsendes fra skorstene.

Modellen kan behandle to samtidige stoffer, af hvilke det ene dannes fra det andet ved kemiske processer under transporten.

En model for opstigning af en varm røgfane præsenteres og er indbygget i spredningsmodellen.

Introduction

For use in the project "Environmental consequences of energy production" (1), a model has been developed to calculate the concentrations in air and the deposition on ground surface of pollutants emitted from chimneys.

The model is restricted to distances not over ~ 100 km and to time intervals not shorter than ~ 1 month.

Qualitative description of the model

The model assumes a homogeneous distribution of the smoke across the vane. This can be compared to the Gaussian dispersion model, which considers Gaussian distributions of the smoke in the cross wind directions.

Averaging over long time intervals makes the concentration in a given horizontal sector homogeneous over the sector and proportional to the probability that the wind is blowing in a direction from the chimney that lies within the sector. Almost the same result is obtained when the Gaussian cross-wind (y) distribution is averaged over a sector.

In the vertical (z) direction the two distribution functions are a little more different. The present model assumes a vertical extension of the vane which is $4 \cdot \sigma_z(x)$, where $\sigma_z(x)$ is the vertical dispersion parameter of the Gaussian model. When the vane has broadened suffficiently it will reach either the ground or the inversion layer, which will then limit the vertical expansion.

Fig. 1 shows how the vertical plume extension is assumed to be in this model.

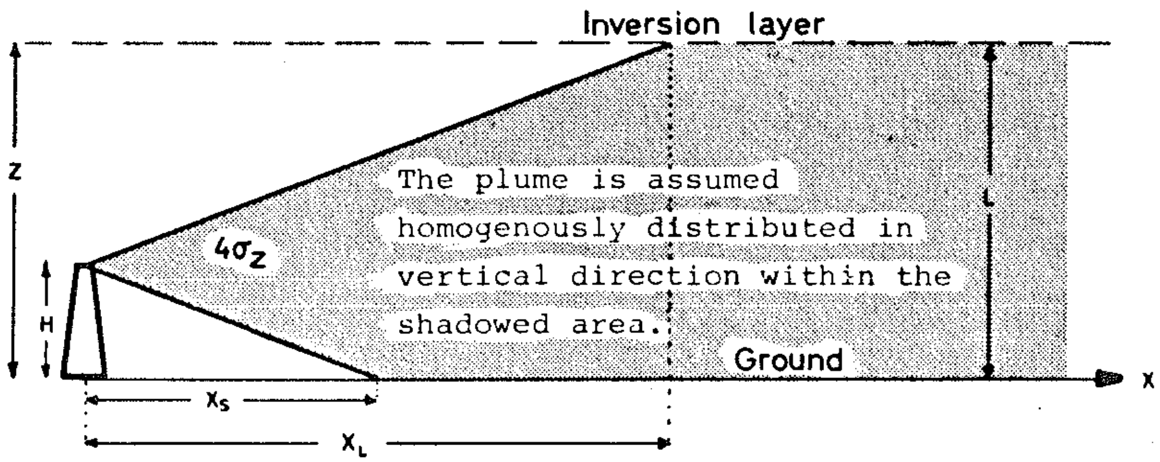

Fig. 1. Sketch of the plume.

The concentration profile of this model is compared to the corresponding Gaussian variation in Fig. 2.

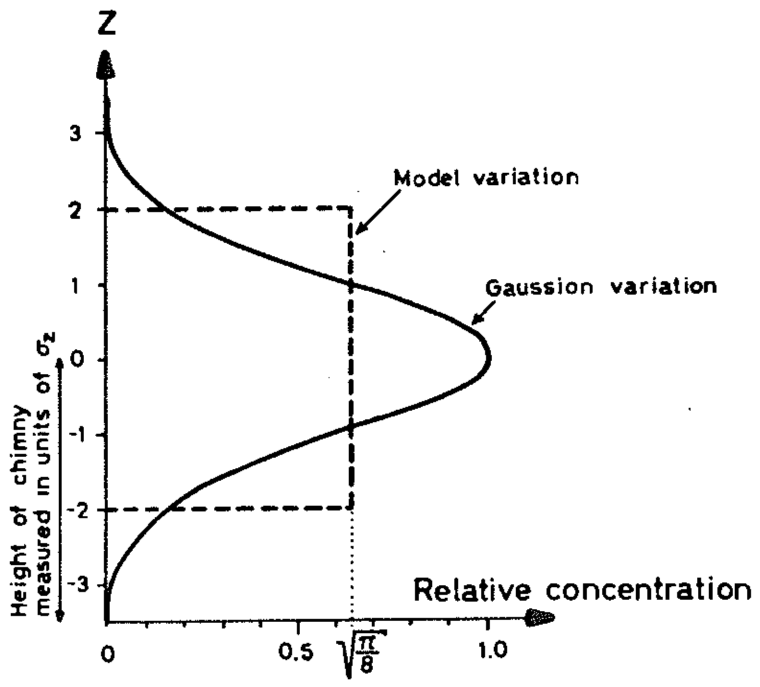

Fig. 2. Vertical concentration profiles in the Gaussian model and in this model.

The concentrations along ground surface according to the two models are qualitatively pictured in Fig. 3. The main difference between the two models is seen to be the (small) contribution to the ground level concentration at short distances from the chimney in the Gauss-model, where the present model assumes zero concentration until the distance x_S. At this point the model jumps to about twice the Gauss-model value.

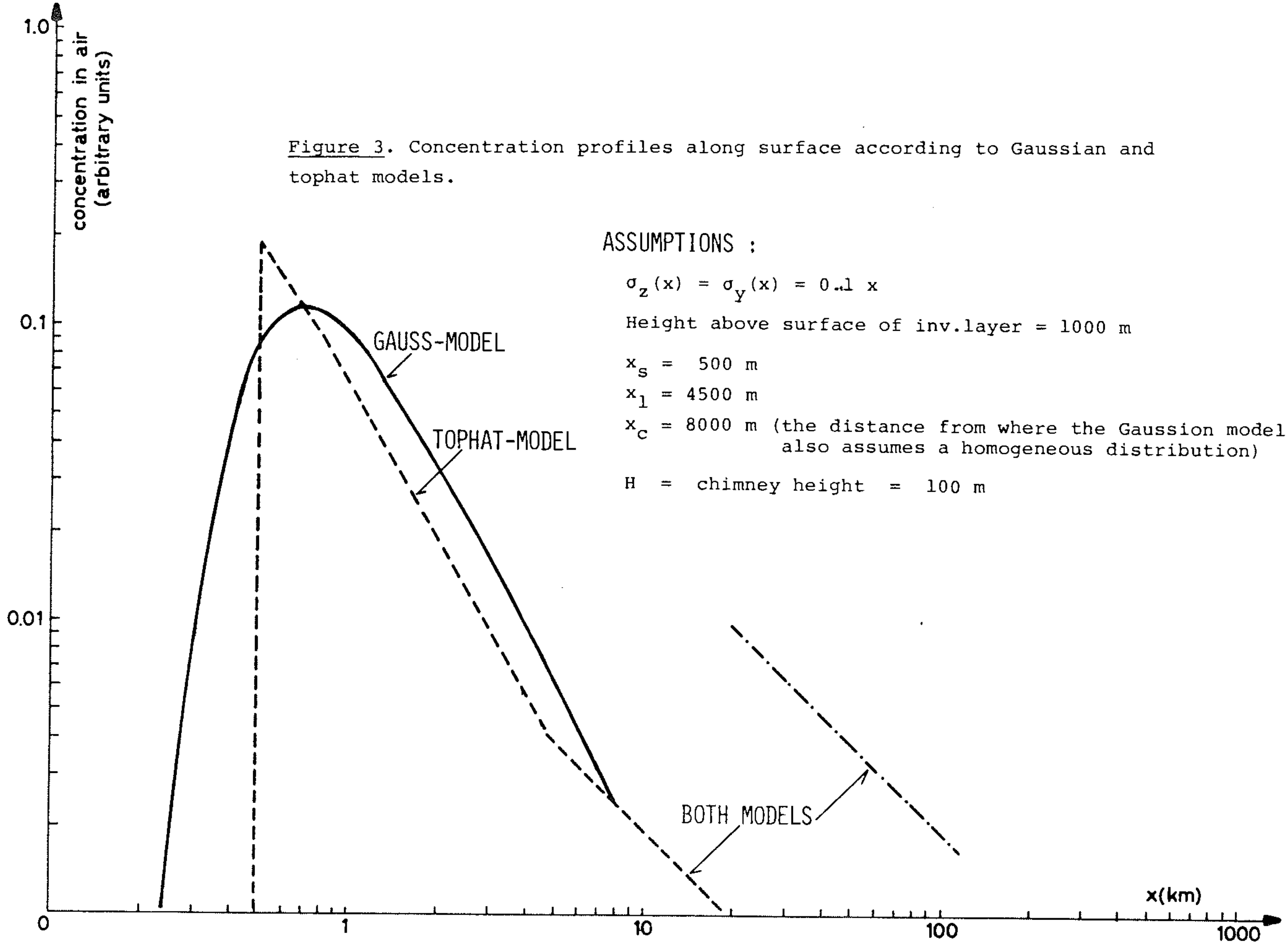

Figure 3. Concentration profiles along surface according to Gaussian and tophat models.

ASSUMPTIONS :

$\sigma_z(x) = \sigma_y(x) = 0.1\ x$

Height above surface of inv.layer = 1000 m

x_s = 500 m

x_1 = 4500 m

x_c = 8000 m (the distance from where the Gaussion model also assumes a homogeneous distribution)

H = chimney height = 100 m

The meteorological data are long-time averages of frequencies of stability categories, wind speeds, wind directions, and precipitations. The data are drawn from an input file and may, therefore, readily be exchanged with other ones. This would be necessary to do, for instance, if the number of subperiods in a year is changed from the present 2, or whenever the Risoe data are deemed non-appropriate for the actual problem. The structure of the meteorological file is described in more detail in appendix 1.

When the plume leaves the chimney, it will usually have a vertical velocity and, also, a temperature much higher than the surrounding air. The centerline of the vane will therefore rise during some time. The problems about the plumerise are treated in appendix 2, where a model is described, which is largely consistent with the present "top-hat" model, and which delivers as output an effective "chimney-height", and the distances x_S and x_L where the vane strikes the ground and the inversion layer, respectively.

The mathematical formulation of the simple dispersion model treating only one pollutant is given in appendix 3, and in appendix 4 the model is further extended to enable the calculation of two pollutants simultaneously, one of which is formed from the other during the transport. Only transformations of the kind where the formation rate of the secondary pollutant is proportional to the concentration of the primary pollutant can be treated.

In the appendices formulae are derived for the concentrations c_1 and c_2, and the deposition rates d_1 and d_2 of such two substances.

It is found that

$$c_1(x) = P_i \sum_{j=1}^{7} \sum_{k=1}^{5} (f_j \cdot c_{1,jk}{}^{R}(x) + (1-f_j) \cdot c_{1,j,k}{}^{NR}(x))$$

where

- i is the sector under consideration
- j sums over stability categories and
- k sums over wind velocity group
- f_j is the probability of rain

and

$$c_{1,j,k}^{R}(x) \text{ and } c_{1,j,k}^{NR}(x)$$

are the contributions from stability category no. j and velocity group no. k under "rain" and "no-rain" conditions.

The expressions for c^R and c^{NR} are identical, when the wet-deposition parameter c_{w1} is put equal to zero in the NR-case:

$$c_{1,j,k}^{R}(x) = P_j^{\,i} P_{j,k}^{\,i} \cdot \frac{Q_1}{u_{j,k}^{\,i} \cdot \Delta y(x) \cdot \Delta z_{j,k}(x)} \cdot$$

$$\cdot \; e^{-\frac{1}{u_{j,k}^{\,i}} \cdot ((\lambda_1 + C_{w1}) \cdot x + c_{d1} \cdot INT_{j,k})}$$

$$c_{1,jk}^{NR}(x) = c_{1,j,k}^{R}(x) \text{ with } c_{w1} = 0$$

$$INT_{j,k} = \int_{x_S^{j,k}}^{x} \frac{dx'}{\Delta z_{j,k}(x')}$$

and for the second pollutant

$$c_2(x) = P_i \sum_j \sum_k (f_j(c_{2,j,k}{}^R(x) + \frac{\lambda_1 \cdot Q_1}{u_{j,k}{}^i} \cdot \text{Integral}_{j,k}{}^R) +$$

$$(1 - f_j)(c_{2,j,k}{}^{NR}(x) + \frac{\lambda_1 \; Q_1}{u_{j,k}{}^i} \cdot \text{Integral}_{j,k}{}^{NR}))$$

where $c_2{}^R$ and $c_2{}^{NR}$ are the equivalents of $c_1{}^R$ and $c_1{}^{NR}$, only that all 1's are exchanged by 2's.

The $\text{Integral}_{j,k}{}^R$ and $\text{Integral}_{j,k}{}^{NR}$ are given by similar expressions (in the NR-case, c_{w1}, and c_{w2} are zero):

$$\text{Integral}_{j,k}{}^R = \int_o^x e^{-\frac{1}{u_{j,k}{}^i} \cdot ((\lambda_1 - \lambda_2 + c_{w1} - c_{w2}) \cdot x' + (c_{d1} - c_{d2}) \int_{x_S}^{x'} \frac{dx''}{\Delta z(x'')})} dx'$$

This integral is espressed by means of either the error-function or the Dawson-integral.

The deposition rates d_1 and d_2 are easily calculated when the concentrations are known, as the wet deposition contribution is given by

$$c_w \cdot f_j \cdot c_{j,k}{}^R(x) \cdot \Delta z_{j,k}(x) \qquad \text{per unit area}$$

and the dry deposition contribution is zero for $x < x_S{}^{j,k}$,

and for $x > x_S{}^{j,k}$ is given by

$$c_d \cdot (f_j \cdot c_{j,k}{}^R(x) + (1 - f_j) \cdot c_{j,k}{}^{NR}(x))$$

References

1. Environmental Impacts from Energy Production. EFP-82 research project.

The present work is based on previous works by many authors. The papers most heavily leaned upon are:

2. JENSEN, N.O. (1973). Occurrences of stability classes, wind speeds, and wind directions as observed at Risø. Risø-M-1666.

3. HEDEMANN JENSEN, P. (1975). POPDOS, a computer model for calculating individual and population doses within a radius of 1000 km. Internal Health Physics Report, 1612-940.111, A 1009.

4. THYKIER-NIELSEN, S. and LARSEN, S.E. (1982). The importance of depositon for individual and collective doses in connection with routine releases from nuclear power plants. Risø-M-2205.

5. THYKIER-NIELSEN, S. (1979). Risø model til beregning af konsekvenser af frigørelse af radioaktivt materiale til atmosfæren. Risø-M-2149.

6. HANNA, S.R., BRIGGS, G.A., HOSKER, R.P. (1982). Handbook on Atmospheric Diffusion. DOG/TIC-11223.

APPENDIX 1

Meteorological data

Meteorological data are assumed present on a file METDATA. It contains statistical data (of course appropriate for the geographical area under consideration) for 12 wind directions (30^{o} sectors), 7 stability categories (the Pasquill categories A,B,C,D,E,F, and G) and 5 wind velocity groups.

The format is free-field.

The first record contains one number, NPY, which is the number of subperiods in a year.

The 2. record contains 7 numbers, DTDZ[1:7], which are the vertical temperature gradients for the 7 stability categories.

The 3. record also holds 7 numbers, ML[1:7], which are the inversion layer heights (m) for the 7 stabilities.

The 4. record contains the 7 rain frequencies, RP[1:7].

The following 7 records each hold 3 numbers, H0, H1, H2, which, for a particular stability category, defines the vertical dispersion parameter of the Gaussian dispersion model, $\sigma_z(x)$, in meters according to the formula

$$\log(\sigma_z(x)) = H0 + H1 \cdot \log(x) + H2 \cdot (\log(x))^2$$

with x in km. (The extension of the vane in this model is $4 \cdot \sigma_z(x)$).

Then follows the winddata ordered by sector. There are 12 sectors of 30^{o} each. In sector no. 1 the wind is blowing from north ($\pm 15^{o}$), in sector no. 4 the wind is blowing from east ($\pm 15^{o}$).

For each and one sector then comes:

1. record: Frequency in % for the wind to be in this sector (1 number).

For each and one stability category comes:

1. record: Frequency in % for this stability category to occur, when the wind is in this sector, (1 number). Then 5 numbers indicating the frequencies in % for the wind velocity to lie in the 5 groups:

Group	1	2	3	4	5
m/sec	0-1	1-3	3-6	6-10	> 10

2. record: The first number giving the average wind velocity in this sector and stability category. The next 5 numbers giving the actual average velocities of the 5 groups.

When last sector and last category are finished the whole thing is repeated as many times as indicated by NPY, the number of subperiods per year. The first few records of a METDATA file is shown below.

Structure of a METDATA file:


```
                                          Comments:
2                                         No. of subperiods per year
 -.020,-.018,-.016,-.010,.010,.0275,.050  Temperature gradients
1600,1400,1000,500,300,180,180            Inversion layer heights
.005,.015,.025,.095,.045,.025,.025        Weighted rain probability
2.61162, 2.02163, 0.548155                Coeff. for SIGMA-Z in cat. A
2.04447, 1.05700, 0.030341                Do. for category B
1.78625, 0.91882,-0.003980                Do. for C
1.48448, 0.73303,-0.074596                Do. for D
1.32948, 0.68087,-0.105925                Do. for E
1.13766, 0.65502,-0.121964                Do. for F
1.13766, 0.65502,-0.121964                Do. for G
6.2                                       Prob. of wind in sector 1
 0.5, 0.0, 5.0,30.0,45.0,20.0             Prob. of A, Prob. of group 1-5
7.0, 0.1, 2.5, 4.4, 7.3,11.2              Mean vel. in A and in gr. 1-5
 1.8, 1.4,11.1,31.9,34.7,20.8             Prob. of B, Prob. of group 1-5
6.8, 0.5, 1.8, 4.4, 7.5,12.5              Mean vel. in B and in gr. 1-5
 3.4, 1.4, 4.3,24.5,49.6,20.1             C
7.5, 0.6, 2.4, 4.5, 7.6,12.2              C
63.2, 0.7, 9.8,30.2,40.6,18.6             D
7.0, 0.5, 2.1, 4.4, 7.6,12.7              D
26.3, 3.7,15.9,34.2,37.8, 8.3             E
5.6, 0.4, 1.9, 4.3, 7.4,12.3              E
 4.0,11.0,34.1,29.9,21.3, 3.7             F
3.8, 0.3, 1.9, 4.1, 7.3,11.0              F
 0.7, 7.1,64.3,21.4, 7.1, 0.0             G
2.4, 0.5, 1.6, 4.2, 6.5,10.0              G


5.1                                       Prob. of wind in sector 2
 0.2, 0.0,14.3,14.3,57.1,14.3             Etc. for sector 2
6.4, 0.1, 1.9, 4.5, 7.1,10.0
 0.4, 0.0,21.4,35.7,28.6,14.3
6.1, 0.1, 2.5, 4.8, 7.4,12.4
 1.1, 0.0, 7.9,42.1,26.3,23.7
6.8, 0.1, 2.0, 4.2, 8.0,11.9
65.0, 1.2, 9.7,32.3,44.0,12.8
6.4, 0.6, 2.0, 4.4, 7.5,11.9
26.4, 3.2,15.7,38.8,39.2, 3.1
5.2, 0.4, 1.9, 4.4, 7.3,10.8
 5.8, 7.9,25.1,42.9,22.5, 1.6
4.2, 0.3, 2.2, 4.4, 7.0,10.6
 1.1, 8.3,27.8,55.6, 8.3, 0.0
3.4, 0.5, 1.8, 4.1, 7.5,10.0
4.1
 0.5, 8.3,25.0,41.7,25.0, 0.0
4.1, 0.5, 2.4, 3.9, 7.2,10.0
 0.5, 0.0, 8.3,75.0,16.7, 0.0
4.7, 0.1, 2.8, 4.3, 7.6,10.0
 1.6, 0.0,11.6,53.5,34.9, 0.0
4.9, 0.1, 2.3, 4.2, 6.9,10.0
57.7, 1.5,15.9,42.3,35.7, 4.6
5.3, 0.6, 2.0, 4.4, 7.4,11.1
```

APPENDIX 2

Plume Lift

The model

The plume release is viewed as a series of spheres with initial radii equal to the chimney radius, RO. The spheres are moving with an initial vertical velocity WO and with a constant horizontal velocity which equals the wind velocity, U. The spheres are supposed to expand (by mixing with the surrounding air) in such a way that the radius at time t after release is given by

$$R(t) = RO + \Delta Z(t)$$

where $\Delta Z(t)$ is the (half) vertical extension of the vane at time t, i.e. at the distance $x = U \cdot t$.

A sphere is worked upon by to forces, the buoyancy, KB, and the friction, KF.

The buoyancy, KB, is given by

$$KB = g \cdot (\rho_e - \rho_p) \cdot V$$

where g is the acceleration of gravity (9.81 m/sec^2), V is the volume of the sphere and ρ_e and ρ_p are the densities of the environmental air and the plume, respectively. For the present purpose the densities may be assumed to be dependent on temperature only, viz.

$$\rho = 1.29 \cdot \frac{273}{T} \simeq \frac{352}{T} (\mathrm{kg/m^3})$$

The frictional force, KF, is directed opposite to the vertical velocity, W, and the size is given by

$$KF = 1/2\ \rho W^2 \cdot \pi R^2 \cdot c$$

where the parameter c for large Reynolds numbers (which we are dealing with here) is nearly constant, $c \simeq 0.5$. Thus we get

$$KF = 1.0 \cdot W^2 R^2 \qquad (N)$$

when W is in m/sec, and R in m. KF is taken to be positive when directed downwards.

The combined force on the sphere is then

$$K = KB - KF$$

which will accelerate the sphere with

$$\frac{dW}{dt} = \frac{K}{M} = \frac{K}{V \cdot \rho_p}$$

In a time increment, Δt, the velocity W will change to

$$W' = W + \frac{dW}{dt} \Delta t$$

The temperature distribution in the surrounding air, TE(z), is a function of height above surface, z

$$TE(z) = TEO + \frac{dT}{dz} \cdot z$$

where the atmosphere temperature gradient, $\frac{dT}{dz}$,

may have values from -0.02 K/m (very unstable conditions) to + 0.05 K/m (very stable conditions).

The temperature of the sphere is more intrigate to assess. We shall use the following recipe:

The initial temperature at the chimney outlet is TPO. Whenever a parcel of air is moved adiabatically from one height, z1, to another height z2, the temperature of the parcel will change according to the equation

$$c_p \cdot dT = \frac{1}{\rho} dp$$

where c_p is the specific heat of air at constant pressure, and p stands for the pressure. As the pressure gradient with height is

$$\frac{dp}{dz} = - \rho \cdot g$$

we get

$$\left(\frac{dT}{dz}\right)_{adiab.} = \frac{dT}{dp} \cdot \frac{dp}{dz} = - \frac{g}{cp} \simeq -0.01 \text{ K/m}$$

Thus, the temperature will fall with 1K for every 100 m, the parcel is lifted when no heat is exchanged with the surroundings.

If the sphere volume is increased from a value, V1, to another value V2 > V1, by introduction of ambient air into the sphere, a mixing temperature, TP2, will arise, given by

$$TP2 = \frac{M1 \cdot TP1 + (M2-M1) \cdot TE}{M2}$$

As $M = \rho_o \frac{T_o}{T} V$

$$TP2 = \frac{V2}{\frac{V1}{TP1} + \frac{V2 \cdot V1}{Te}}$$

We shall assume that if a gas sphere simultaneously expands from V1 to V2 and rises from z1 to z2, then the temperature will be

$$TP(V2,z2) = \frac{V2}{\frac{V1}{TP(V1,z1)} + \frac{V2 -V1}{TE(zM)}} -0.01 \cdot (z2-z1)$$

where zM is some height between z1 and z2, e.g. (z1+z2)/2.

By calculating the above quantities in successive time steps we can get the correlation between the sphere centre's height and distance from the chimney.

It turns out that with atmospheric temperature gradients,

$$\frac{dT}{dz} < -0.01 \text{ K/m}$$

(unstable conditions), the plume will continue to rise, if its initial temperature is larger than that of the ambient air.

The upper surface of the sphere will eventually reach the inversion layer assumed to be located at a height ML, (which depends on the temperature gradient). When this happens we shall assume no further rise of the plume centre. In some cases the rate of rise will become very slow, and it may happen that the expansion of the sphere will make its lower surface touch the ground. For simplicity we shall assume that the rise of the centre ceases, when this happens.

With the three criteria for cease of rise, buoyancy = 0, striking of inversion layer or striking of ground, the plume will always reach a final height.

One case, though, is not covered. If the chimney outlet is higher than the inversion layer, the above model will not work.

As the lowest inversion height is assumed to be 180 m (for stability categories F and G, which occur for less than 7% of the time), only for very tall chimneys there will be a small error by limiting the final plume height to the inversion layer height.

An algorithm has been written which performs the above calculations and some results are reproduced in table 1 and figures 2-1, 2-2 and 2-3.

Table 1. Final centre heights for plumes under varying conditions. Heights are in meters above terrain.

Ch.height=100 m. Plume init. vel.=10 m/s. Plume init. temp.=393 K							
Stab.cat.		A	B	C	D	E	F
Temp.grad.(K/m)		-0.020	-0.018	-0.016	-0.010	+0.001	+0.0275
Inv.height(m)		1600	1400	1000	500	300	180
Wind	1	1417[1]	1290[1]	942[1]	485[1]	294[1]	175[1]
Velocity	6	136[2]	165[2]	248[2]	287[3]	261[3]	173[1]
(m/s)	12	119[2]	130[2]	148[2]	182[3]	190[3]	170[1]
Ch.height=100 m. Plume init. vel.=20 m/s. Plume init. temp.=393 K							
Wind	1	1418[1]	1291[1]	943[1]	485[1]	294[1]	175[1]
Velocity	6	148[2]	179[2]	598[2]	297[3]	270[3]	174[1]
(m/s)	12	128[2]	141[2]	161[2]	195[3]	200[3]	171[1]
Ch.height=100 m. Plume init. vel.=20 m/s. Plume init. temp.=493 K							
Wind	1	1427[1]	1299[1]	952[1]	488[1]	294[1]	175[1]
Velocity	6	151[2]	192[2]	617[2]	364[1]	281[1]	174[1]
(m/s)	12	127[2]	143[2]	167[2]	220[3]	224[3]	172[1]
Ch.height=200 m. Plume init. vel.=20 m/s. Plume init. temp.=493 K							
Wind	1	1432[1]	1304[1]	959[1]	491[1]	295[1]	180[4]
Velocity	6	255[2]	307[2]	636[2]	413[1]	291[1]	180[4]
(m/s)	12	229[2]	246[2]	276[2]	321[3]	283[1]	180[4]

Plume lift stopped by

1) vane hitting inversion layer
2) vane hitting ground
3) zero buoyancy
4) chimney higher than inversion layer.

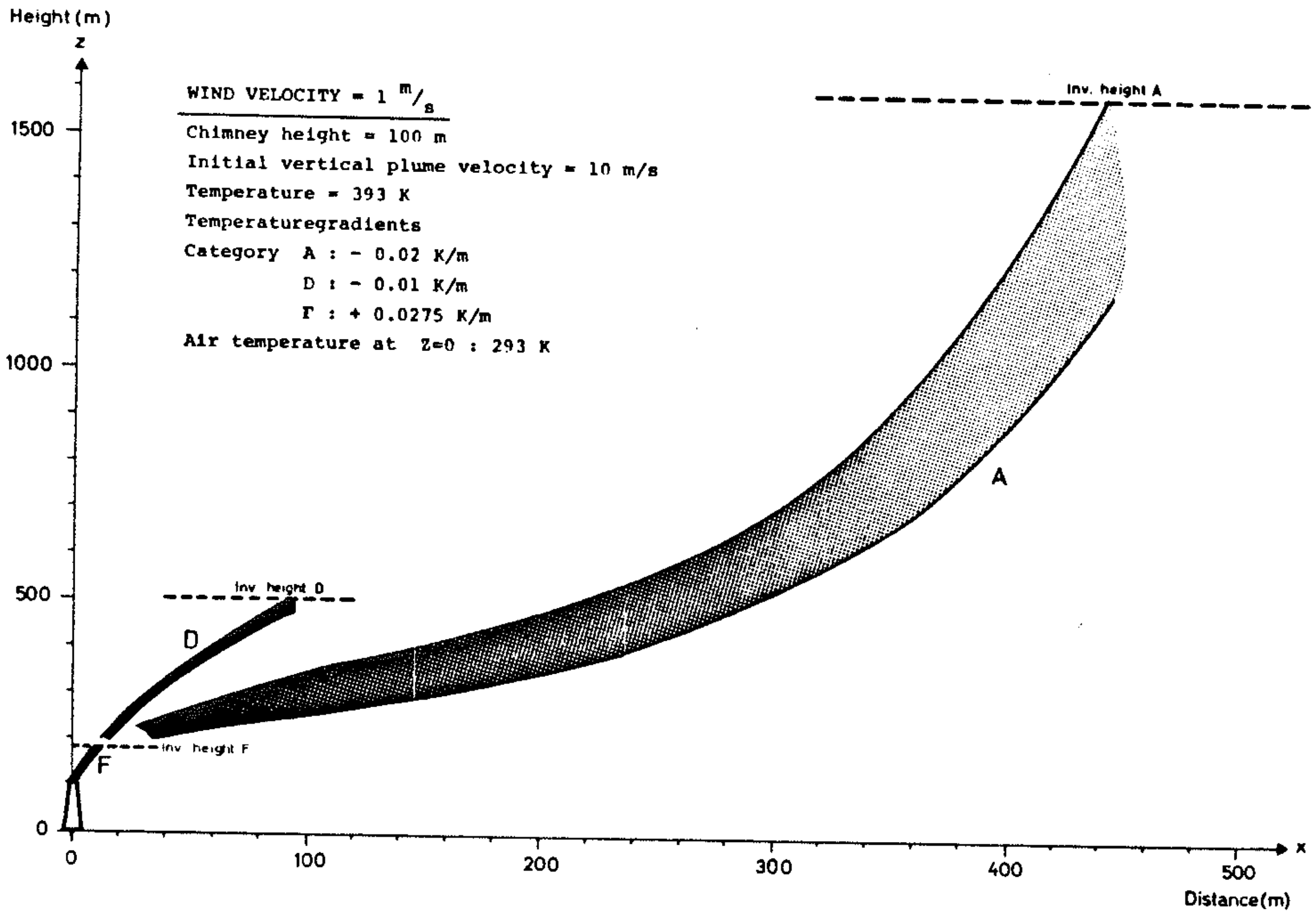
Height (m)
z
1500
1000
500
0
WIND VELOCITY = 1 m/s
Chimney height = 100 m
Initial vertical plume velocity = 10 m/s
Temperature = 393 K
Temperaturegradients
Category A : - 0.02 K/m
D : - 0.01 K/m
F : + 0.0275 K/m
Air temperature at Z=0 : 293 K
Inv. height A
A
Inv. height D
D
Inv. height F
F
0
100
200
300
400
500
x
Distance(m)

Figure 2-1.

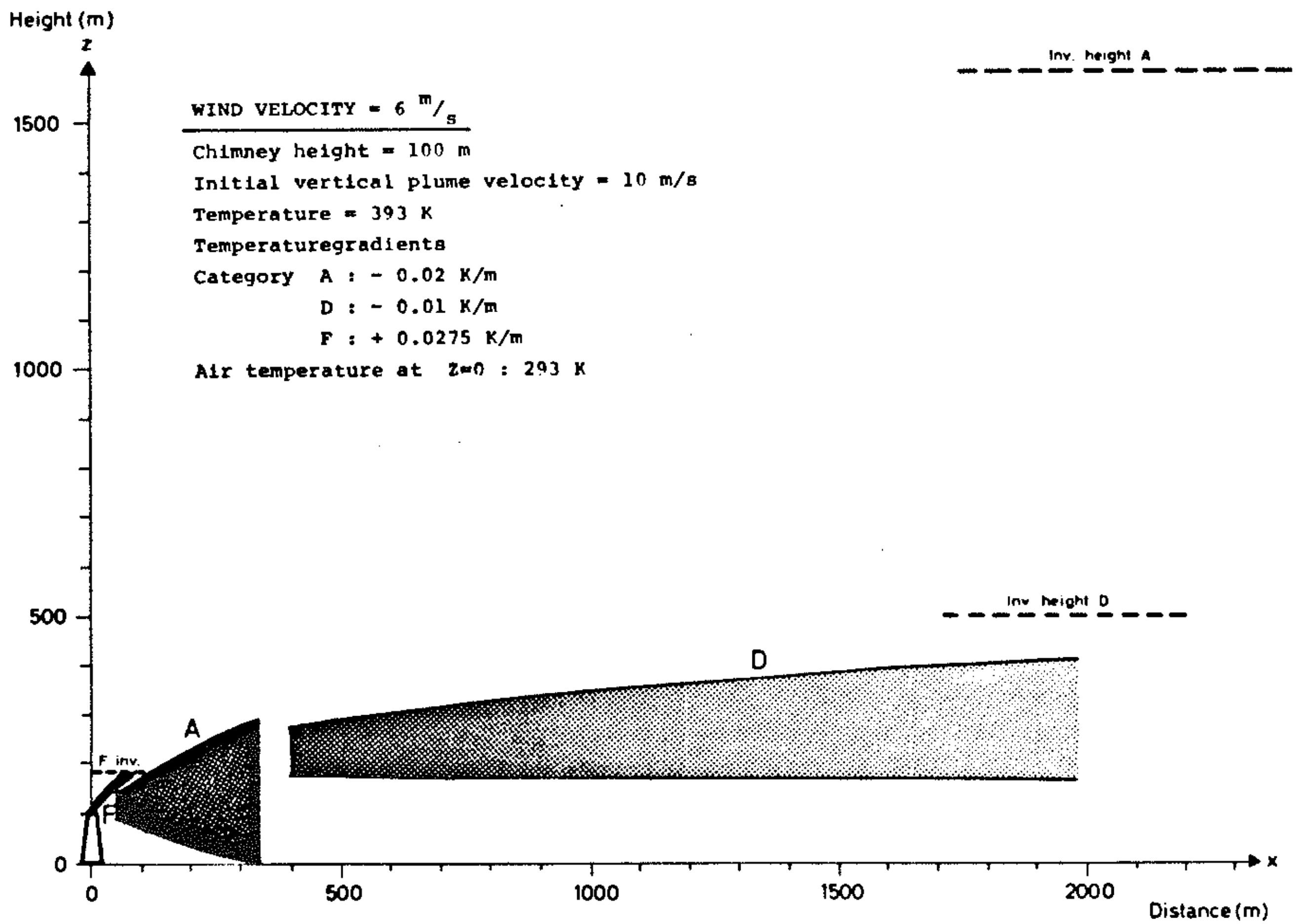
Height (m)
z
1500
1000
500
0
0
500
1000
1500
2000
x
Distance (m)
WIND VELOCITY = 6 m/s
Chimney height = 100 m
Initial vertical plume velocity = 10 m/s
Temperature = 393 K
Temperaturegradients
Category A : - 0.02 K/m
D : - 0.01 K/m
F : + 0.0275 K/m
Air temperature at Z=0 : 293 K
Inv. height A
Inv. height D
F inv.
A
D
F

Figure 2-2.

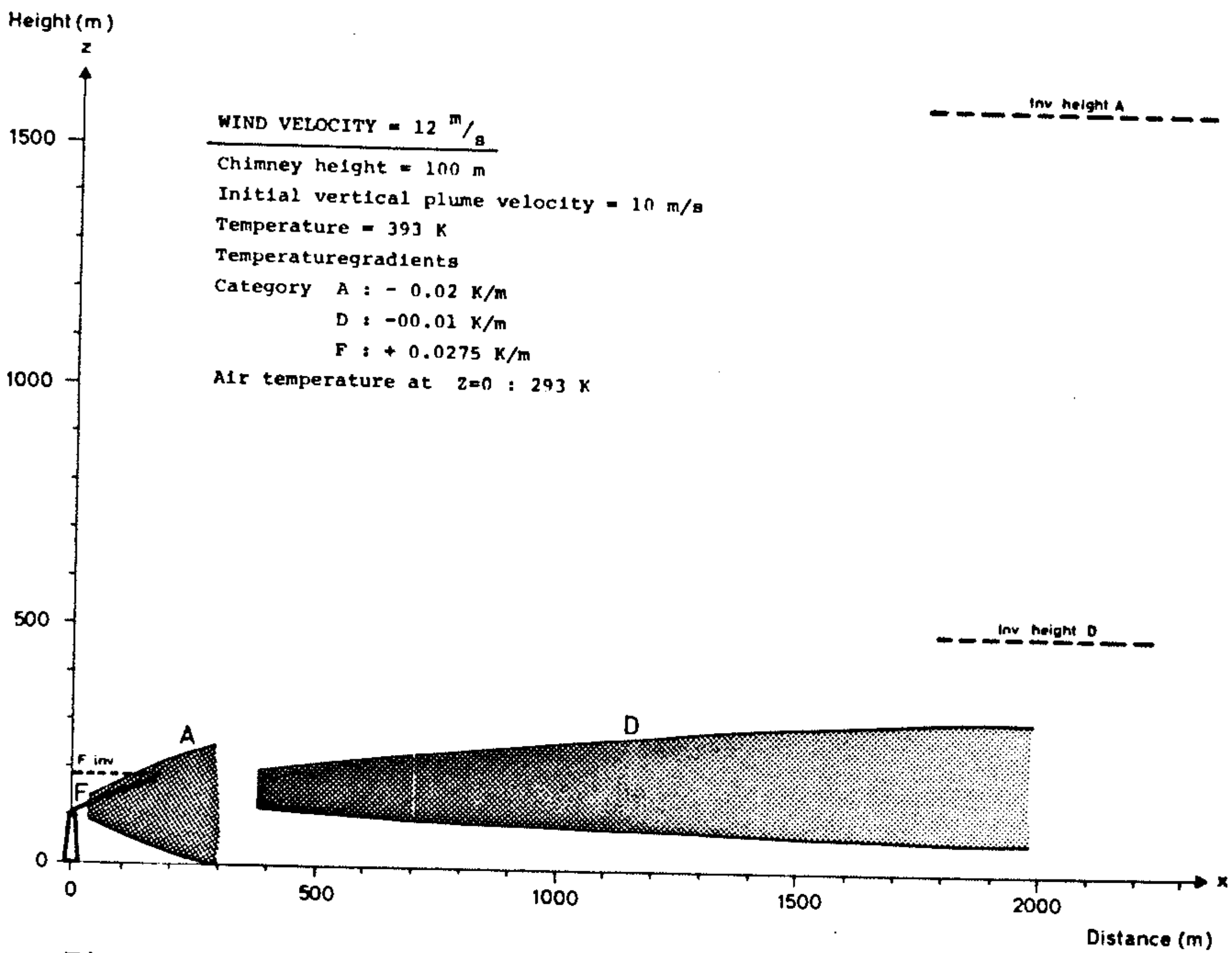
Height (m)
z
1500
1000
500
0
WIND VELOCITY = 12 m/s
Chimney height = 100 m
Initial vertical plume velocity = 10 m/s
Temperature = 393 K
Temperaturegradients
Category A : - 0.02 K/m
D : -00.01 K/m
F : + 0.0275 K/m
Air temperature at Z=0 : 293 K
Inv height A
Inv height D
F inv
F
A
D
0
500
1000
1500
2000
x
Distance (m)

Figure 2-3.

APPENDIX 3

A model for calculating air concentration and deposition rate of a pollutant, emitted from a chimney and not generated during the transport away from the chimney.

The compass rose is divided into 12 sectors of 30^o. The midline of sector no. 1 points towards north, and the midline of sector no. 4 points to the east, see Fig. 3-1. When the wind is in sector no. 1 it means that the wind is blowing from north towards south. If the direction from a point to a chimney lies in sector no. i, we shall assume that only for wind directions in the same sector the air concentration of the pollutant will be greater than zero at the point. Another way to put it: Whenever the wind direction lies in a certain sector, we shall assume that its direction is exactly in the midline of that sector and that the smoke spreads homogeneously out in the sector.

As to the vertical distribution we assume that the vane expands symmetrically upwards and downwards in such a way that the vetical extension of the vane at a distance x from the chimney is $4 \cdot \sigma_z(x)$, where $\sigma_z(x)$ is the dispersion parameter of the Gaussian dispersion model.

The distribution within the vane is assumed to be homogeneous, and outside the vane to be zero. As illustrated in Fig. 3-2 the upper and lower vane fronts will sooner or later reach the inversion layer and the ground surface, respectively. If the distances, where this occur, are denoted x_L and X_S, we can see that the vertical vane extension, $\Delta z(x)$, is given by

$$\Delta z(x) = \begin{cases} 4 \cdot \sigma_z(x) & \text{if } x < x_{min} \\ L - H + 2 \cdot \sigma_z(x) & \text{if } x < x_S \text{ and } x_L < x_S \\ H \quad + 2 \cdot \sigma_z(x) & \text{if } x < x_L \text{ and } x_L > x_S \\ L & \text{if } x > x_{max} \end{cases}$$

where x_{min} stands for the smaller of x_L and x_S and x_{max} for the greater of x_L and x_S.

For the horizontal cross-wind extension we had

$$\Delta y(x) = \frac{2\pi}{12} \cdot x$$

If the wind velocity is u m/sec and the chimney expels Q gram per second of some pollutant in the sector under consideration, a simple mass balance gives the following expression for the concentration c(x) of the pollutant:

$$Q = c(x) \cdot u \cdot \Delta y(x) \cdot \Delta z(x)$$

or

$$c(x) = \frac{Q}{u \cdot \Delta y(x) \cdot \Delta z(x)}$$

This holds if there is no removal of matter from the smoke on the distance from the chimney to the point x.

However, there are mechanisms which act to remove matter from the smoke:

1) Precipitation or wash-out occurs when it is raining. It is assumed that the raindrops starts above the vane and therefore remove matter at a rate proportional to the concentration and to the vertical extension of the vane. At some distance, x, the quantity, $\Delta M_w(x)$(gr/sec/m^2) will be deposited by precipitation:

$$\Delta M_w(x) = c_w \cdot c(x) \cdot \Delta z(x)$$

where c_w is the wash-out coefficient (sec^{-1}) and c(x) now means the concentration at the distance x corrected for wash-out.

c_W is dependent on rain-intensity, drop-sizes, particle-sizes or whether the pollutant considered is a gas. Here we shall assume c_W an input constant, characteristic for the pollutant, properly averaged for the weather conditions in the area.

2) Dry deposition takes place when the smoke touches the ground or obstacles on the ground.

For this model dry deposition is only active for distances $x > x_S$, Fig. 3-2. It is assumed that per second and m^2 a quantity, $\Delta M_D(x)$, is deposited:

$$\Delta M_D(x) = c_D \cdot c(x)$$

where the dry deposition coefficients c_D (m/sec) will be dependent on surface roughness, wind velocity, pollutant etc. We shall assume c_D an input constant connected to the pollutant, properly averaged for landscape, velocities etc.

Expressing the mass balance for the area of a sector between the radii x and x+dx that the flow through the inner surface, $\Delta y(x) \cdot \Delta z(x)$, must equal the flow through the outer surface, $\Delta y(x+dx) \cdot \Delta z(x+dx)$, plus the amount deposited between x and x+dx, yields a differential equation for the concentration, c(x):

$$\frac{dc(x)}{c(x)} = - dx\left(\frac{1}{x} + \frac{\Delta z'(x)}{\Delta z(x)} + \frac{1}{u} c_W + \frac{1}{u} c_D \cdot \frac{1}{\Delta z(x)} \right)$$

which is integrated to

$$c(x) = \frac{Q}{u \cdot \Delta y(x) \cdot \Delta z(x)} \cdot e^{-\left(\frac{1}{u}\left(c_W \cdot x + c_D \cdot \int_{x_S}^{x} \frac{dx'}{\Delta z(x')}\right)\right)}$$

For the time-averaged concentration in sector no i at the distance x from a chimney, releasing Q per second, we get:

$$c(x) = P^i \sum_{j=1}^{7} \sum_{k=1}^{5} (f_j \cdot c_{jk}^R(x) + (1-f_j) \cdot c_{jk}^{NR}(x))$$

where

$$c_{jk}^{R}(x) = \frac{Q \cdot P_j{}^{i} \cdot P_{kj}{}^{i}}{u_{kj}{}^{i} \cdot \Delta y_j(x) \cdot \Delta z_j(x)} \cdot e^{-\frac{1}{u_{jk}{}^{i}}\left(c_w \cdot x + c_D \cdot \int_{x_S{}^{j}}^{x} \frac{dx'}{\Delta z(x')}\right))}$$

is the contribution from periods <u>with</u> rain and

$$c_{jk}^{NR}(x) = \frac{Q \cdot P_j{}^{i} \cdot P_{kj}{}^{i}}{u_{kj}{}^{i} \cdot \Delta y_j(x) \cdot \Delta z_j(x)} \cdot e^{-\frac{1}{u_{jk}{}^{i}}\left(c_D \cdot \int_{x_s{}^{j}}^{x} \frac{dx'}{\Delta z_j(x')}\right))}$$

is the contribution from periods <u>without</u> rain.

P^i = the probability that the wind is in sector no. i.

$P_j{}^i$ = the probability for stability category j when the wind is in sector i.

$P_{kj}{}^i$ = the probability for the wind velocity to be i group k, when stability j and sector i.

$u_{kj}{}^i$ = the wind velocity corresponding to $P_{kj}{}^i$.

f_j = the probability for rain, when stability j.

c_W and c_D = wet and dry deposition factors, respectively.

The deposition rate, D(x), is obtained in a similar manner by summation over stabilitites and wind velocities:

$$D(x) = Q \cdot P^i \sum_{j=1}^{7} \sum_{k=1}^{5} (c_w \cdot c_{jk}{}^{R}(x) \cdot \Delta z_j(x) \cdot f_j +$$

$$\delta(x > x_S{}^{j,k}) \cdot c_D \cdot (c_{jk}{}^{R}(x) \cdot f_j + c_{jk}{}^{NR}(x) \cdot (1-f_j))$$

where

$\delta(x>x_S{}^{j,k})$ is 1 when $x \geq x_S{}^{j,k}$ and otherwise 0.

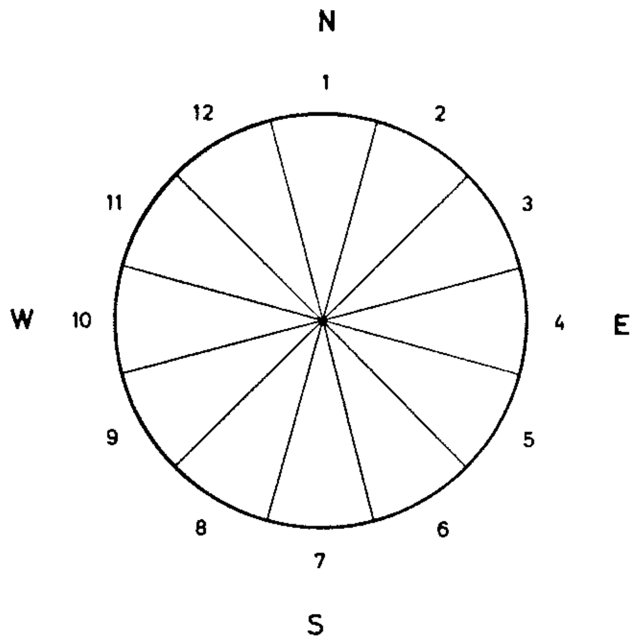

Figure 3-1. Windsectors.

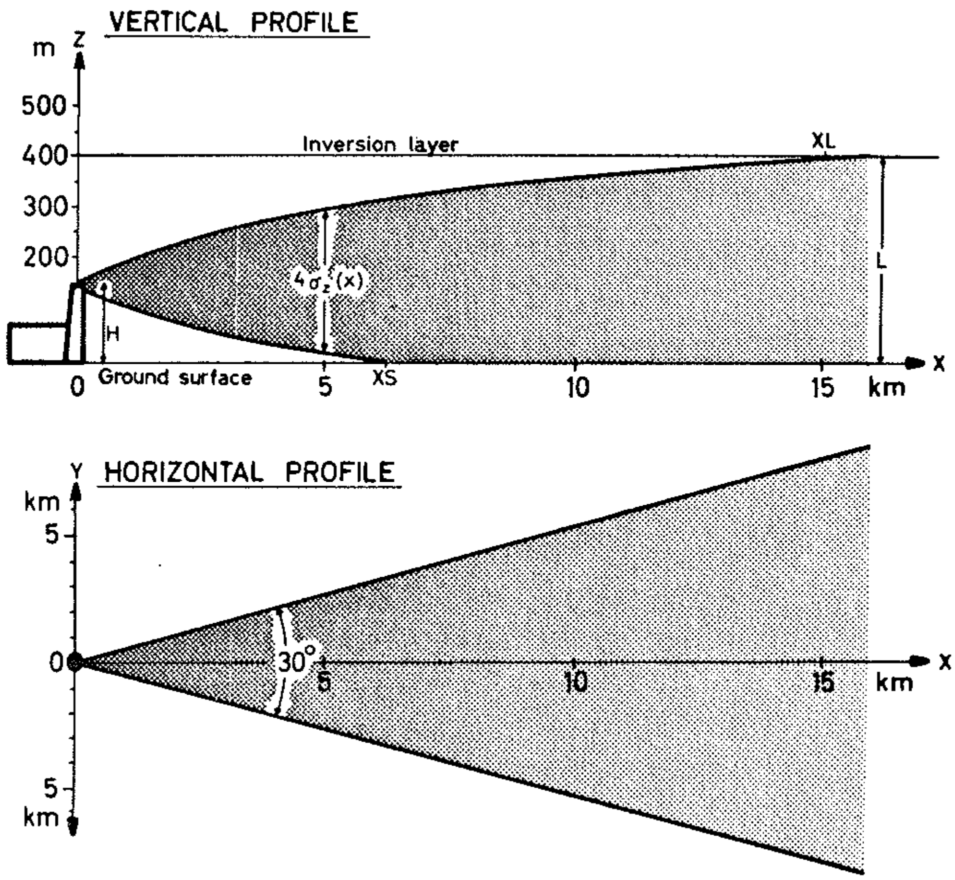

Figure 3-2. Illustration of the assumed plume profiles with indication of the distances x_S and x_L.

APPENDIX 4

A model for calculating air concentrations and deposition rates for two pollutants emitted from a chimney. Pollutant no. 1 is transformed into pollutant no. 2 at a certain rate during the transport.

Some materials emitted in smokes from chimneys will be transformed into other materials during the flight. Examples are SO_2 which is oxidized to SO_4 and NO, which is oxidized to NO_2.

Insofar the kinetics of the transformation are so that the rate of formation of the secondary product is proportional to the concentration of the primary product, a model can be made for the calculation of the two concentrations and the two deposition rates.

The model is quite similar to the model described in app. 3. For the primary product the expressions are excactly the same as deduced in app. 3, except that an extra removal term enters the formulae in complete parallel to the precipitation term:

$$c_1(x) = \frac{Q_1}{u\cdot\Delta y\cdot\Delta z} \; e^{-\frac{1}{u}\left((\lambda_1+c_{w1})\cdot x+c_{D1}\cdot\int_{x_s}^{x}\frac{dx'}{\Delta z(x')}\right)}$$

where the subscript 1 stands for the primary product and λ_1 is the "decay-constant" for transformation into the secondary product.

If the same procedure is followed as in app. 3 for the differential equation for the secondary product, an inhomogeneous differential equation for $c_2(x)$ is obtained:

$$\frac{dc_2(x)}{dx} + \left(\frac{\Delta y'}{\Delta y} + \frac{\Delta z'}{\Delta z} + \frac{1}{u}\,c_{w2} + \frac{1}{u}\,c_{D2}\cdot\frac{1}{\Delta z}\right)\cdot c_2(x) = \frac{\lambda_1\cdot c_1(x)}{u}$$

It has the solution

$$c_2(x) = \frac{1}{u \cdot \Delta y \cdot \Delta z} \qquad e^{-\frac{1}{u}\left((\lambda_2+c_{w2})\cdot x + c_{D2}\int_{x_S}^{x}\frac{dx'}{\Delta z(x')}\right)}$$

$$\cdot\left(Q_2 + \frac{\lambda_1 Q_1}{u}\int_{o}^{x} e^{-\frac{1}{u}\left((\lambda_1-\lambda_2+c_{w1}-c_{w2})\cdot x' + (c_{D1}-c_{D2})\int_{x_S}^{x}\frac{dx''}{\Delta z(x'')}\right)} dx'\right.$$

In order to evaluate the integral ($\int_o^x$) we shall approximate the second integral

$$I(x') = \int_{x_S}^{x'} \frac{dx''}{\Delta z(x'')}$$

with a polynomial of not more than second degree:

$$I(x') = a + bx' + cx'^2$$

Remembering that

$$\Delta z(x) = \begin{cases} 4\sigma_z(x) & \text{for } x \leq \min(x_S, x_L) \\ H + 2\sigma_z(x) & \text{for } x > x_S,\ x_S < x_L \\ L - H + 2\sigma_z(x) & \text{for } x > x_L,\ x_S > x_L \\ L & \text{for } x \geq \max(x_S, x_L) \end{cases}$$

we have that

for $x' < x_S$: $\qquad I(x') = 0$

$$x' > x_M = \max(x_S, X_L):\ I(x') = I(x_M) + \frac{1}{L}(x' - x_M)$$

In between x_S and x_L it turns out that a second order polynomial in x approximates I(x) nicely. We can now evaluate the original integral. Depending on wether c is zero or not, we get two different types of integral:

1) $c = 0$:

$$I(x) = \int_o^x e^{\frac{1}{u}((\lambda_2 - \lambda_1 + c_{w2} - c_{w1})\cdot x' + (c_{D2} - c_{D1})(a + bx'))} dx'$$

$$\underline{=} \int_o^x e^{k_o} \cdot e^{k_1 \cdot x'} dx' = e^{k_o} \cdot \begin{cases} x \text{ for } k_1 = 0 \\ \frac{1}{k_1}(e^{k_1 \cdot x} - 1) \text{ for } k_1 \neq 0 \end{cases}$$

where

$$k_o = \frac{1}{u}(c_{D2} - c_{D1}) \cdot a$$

$$k_1 = \frac{1}{u}(\lambda_2 - \lambda_1 + c_{w2} - c_{w1} + b\cdot(c_{D2} - c_{D1}))$$

2) $c \neq 0$:

$$I(x) = \int_o^x e^{\frac{1}{u}((\lambda_2 - \lambda_1 + c_{w2} - c_{w1})\cdot x' + (c_{D2} - c_{D1})(a + bx' + cx'^2))} dx'$$

$$\underline{=} \int_o^x e^{k_o} \cdot e^{k_2 \cdot x'^2 + k_1 x'} dx'$$

where

$$k_2 = \frac{1}{u}(c_{D2} - c_{D1})\ c,$$

and k_1 and k_o as above.

If $k_2>0$ the integral can be expressed by means of the Dawson-integral:

$$\mathrm{DAWSON}(x) = e^{-x^2} \int_0^x e^{t^2}\, dt$$

for which a standard algorithm, DAW(x), is available

We get

$$I(x) = e^{k_0 - \frac{k_1^2}{4k_2}} \cdot \frac{1}{\sqrt{k_2}} \left(e^{k_2 (x+\frac{k_1}{2k_2})^2} \cdot \mathrm{DAW}\left(\sqrt{k_2}\left(x + \frac{k_1}{2k_2}\right)\right) - e^{\frac{k_1^2}{4k_2}} \cdot \mathrm{DAW}\left(\sqrt{k_2} \cdot \frac{k_1}{2k_2}\right)\right)$$

In the case that $k_2<0$ the error function plays the role of the Dawson-integral. The error function, erf(x), is given by

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

and is a standard function on most computer installations.

We get

$$I(x) = e^{k_0 - \frac{k_1^2}{4k_2}} \frac{\sqrt{\pi}}{2\sqrt{-k_2}} \left(\mathrm{erf}\left(\sqrt{-k_2}\left(x + \frac{k_1}{2k_2}\right)\right) - \mathrm{erf}\left(\sqrt{-k_2} \cdot \frac{k_1}{2k_2}\right)\right)$$

The final expressions for the time-averaged concentrations in sector no i, at the distance x from a chimney releasing Q_1 and Q_2 per second are then:

$$c_1(x) = P^i \sum_{j=1}^{7} \sum_{k=1}^{5} (f_j \cdot c_{1,j,k}^{R}(x) + (1-f_j) \cdot c_{1,j,k}^{NR}(x))$$

where

$c_{1,j,k}^{R}(x)$ and $c_{1,j,k}^{NR}(x)$ are the "rain" and "no-rain" contributions as in app. 3.

For $c_2(x)$ we get a much more complicated expression consisting of two terms. The first term is analogous to the expression for $c_1(x)$ and takes care of the amount Q_2 which is directly emitted from the chimney. The other term, then, adds the contribution transformed from $c_1(x)$:

$$c_2(x) = P^i \sum_{j=1}^{7} \sum_{k=1}^{5} (f_j \cdot c_{2,j,k}^{R}(x) + (1-f_j) \cdot c_{2,j,k}^{NR}(x))$$

$$+ \lambda_1 \cdot Q_1 \cdot \mathrm{Int}_{jk}^{R} \cdot f_j + (1-f_j) \cdot \mathrm{Int}_{j,k}^{NR})$$

the "rain" and "no-rain" integrals $\mathrm{Int}_{j,k}^{R}$ and Int_{jk}^{NR} are given by:

$$\mathrm{Int}_{j,k}^{R} = \frac{P_j^{\,i} \cdot P_{jk}^{\,i}}{u_{jk}^{\,i}\ \Delta y_j(x) \cdot \Delta z_j(x)}\ e^{-\frac{1}{u_{jk}^{\,i}}((\lambda_2 + c_{w,2}) \cdot x + c_{D,2} \int_{x_s}^{x}{}^{j} \frac{dx'}{\Delta z_j(x')})}$$

$$\cdot \frac{1}{u_{j,k}^{\,i}} \int_{o}^{x} e^{-\frac{1}{u_{jk}^{\,i}}((\lambda_1 - \lambda_2 + c_{w1} - c_{w2})x' + (c_{D1} - c_{D2} \int_{x_s}^{x}{}^{j} \frac{dx''}{\Delta z_j(x'')})}\ dx'$$

and an analogous expression for $Int_{j,k}{}^{NR}$, where c_{w1} and c_{w2} are zero.

The formulae for deposition rates $D_1(x)$ and $D_2(x)$ are unchanged from app. 3, as they utilize the air concentrations already calculated.

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Abstract

A model has been developed for calculation of concentrations in air and deposition rates on ground surface of pollutants emitted from chimneys.

The model can handle two pollutants simultaneously, one of which is generated from the other by chemical transformation during the transport.

A model for the lift of hot plumes is presented and incorporated in the dispersion model.

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