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An Operational atmospheric transport model for Priority Substances; specification and instructions for use

J.A. van Jaarsveld

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Translation: H.B.J.M. Volman

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Summary

This report is made to support the use of the OPS long term model for the calculation of dispersion and deposition of primary released material in the atmosphere. Next to a short description of the model, this report contains also a specification of the model and an explanation to the user-definable input parameters. The spatial scale of the model ranges from local (100 m from the source) to national (the Netherlands) and the time scale from a specific month to long term (10 years). Influences of sources in all European countries can be accounted for, which makes it possible to calculate local contributions as well as background values in the Netherlands.

The structure of the model system is chosen in such a way that dispersion and transport parameters are defined internally and the pollutant-specific parameters externally. This approach offers the possibility of using the model for a wide range of pollutants.

Default values for parameters are included in the model for a number of polluting substances to enhance the ease of use of the model and perhaps also to stimulate standardization.

Atmospheric processes which are included in the model are dispersion, dry deposition, wet scavenging and chemical transformation. Modelling of these processes is based on meteorological observations of relevant parameters in the National Air Quality Monitoring Network (LML) and from the Royal Netherlands Meteorological Institute (KNMI) over the period of interest. The relevant data is stored in a climatological database which is part of the modelling system. Next to modelling gaseous components, this model handles also aerosols in which case the deposition properties are coupled to the size distribution of the particles.

Validation of the model on a regional scale is carried out using observations of the LML and the Netherlands National Precipitation Chemistry Network (LMR). From this comparison it can be concluded that this model describes the monthly variations in The Netherlands very well. The uncertainty in calculated values caused by the model or implicit parameters in the model on a regional or mesoscale is quantified as:

concentration in air:	10%	deposition (dry+wet):	15%	(long term)
	15%		20%	(specific year)
	20%		30%	(specific halfyear)
	30%		40%	(specific month)

Validation of model results close to single sources has not (yet) been possible. However a comparison on this aspect with a model used in The Netherlands for regulatory purposes (Nationale Model) shows differences less than 35% in all cases.

Samenvatting.

Onderliggend rapport is bedoeld als ondersteuning bij het gebruik van het OPS lange termijn model voor de berekening van verspreiding en depositie van stoffen in de atmosfeer.

Naast een beknopte beschrijving van het OPS-model, bevat dit rapport specifikatie en validatie van het model en een toelichting bij de invoerparameters. De ruimtelijke schaal van het model loopt van lokaal (100 m afstand van een bron) tot Nederland plus direkte omgeving en de tijdschaal van een specifieke maand tot lange termijn (10 jaar). Bijdragen van gebieden ver buiten Nederland kunnen worden meegenomen, zodat het mogelijk is zowel de lokale situatie te beschrijven alsook de achtergrondkonditie.

De opzet van het model is zodanig dat verspreidingsparameters zoveel mogelijk impliciet zijn en stofspecifieke parameters zoveel mogelijk extern worden gespecificeerd, waardoor het model voor een breed scala van stoffen kan worden toegepast. Van een aantal stoffen zijn advieswaarden voor de genoemde parameters opgenomen, met als doel het gebruiksgemak en wellicht ook de standaardisatie te bevorderen.

De atmosferische processen die in het model zijn opgenomen zijn: dispersie, droge depositie, natte depositie en omzetting. Beschrijving van deze processen is zoveel mogelijk gebaseerd op waarnemingen van relevante meteorologische parameters in het Landelijk Meetnet Luchtkwaliteit (LML) en van het KNMI voor de periode waarover gemiddeld wordt. De hiervoor benodigde gegevens zijn ondergebracht in een bestand van klimatologieën welke onderdeel is van het modelsysteem. Naast gasvormige stoffen kunnen met dit model ook deeltjesvormige stoffen worden gemodelleerd. Voor deze laatste kategorie zijn de depositie-eigenschappen volledig gekoppeld aan de deeltjesgrootte-verdelingen van die stoffen.

Validatie van het model voor regionale en landelijke schaal is geschied aan de hand van waarnemingen van het LML en het Landelijk Meetnet Regenwatersamenstelling (LMR). Uit het resultaat hiervan kan gekonkludeerd worden dat dit model de maandelijkse variaties zoals die in Nederland optreden, uitstekend kan beschrijven. De onzekerheid in berekende grootheden op regionale en landelijke schaal, veroorzaakt door het model of impliciete modelparameters is gekwantificeerd als:

koncentratie in lucht:	10%	depositie:	15%	(lange termijn)
	15%		20%	(specifiek jaar)
	20%		30%	(specifiek half jaar)
	30%		40%	(specifieke maand)

Validatie van uitspraken over individuele bronnen is (nog) niet mogelijk gebleken; vergelijking van dit aspekt met het Nationale Model levert echter verschillen op die kleiner zijn dan 35%.

1. Introduction

To calculate the dispersion of air pollution, the so-called "National Model" can be used in the Netherlands (Subcommittee on Models, 1976; Working Group on Dispersion of Air Pollution, 1984). Over the years, this long-term model has acquired the status of a concensus model, and is generally used as such. For a number of applications, however, the model is not, or not totally, suitable, such as for the calculation of dispersion over distances greater than about 20 kilometres and for the calculation of deposition. The above-mentioned limitations were reason for developing a dispersion model which - while retaining the advantages of the statistical approach - can calculate both the concentration and deposition of a substance close to a source, as well as the background concentration and background deposition at that location caused by other sources in Europe. This model, called TREND model (van Jaarsveld and Onderdelinden, 1989), is used to calculate the dispersion and deposition of substances such as SO_x, NO_x and heavy metals in the Netherlands. Besides dispersion of the primary components, the dispersion and deposition of their daughter products (SO_4^{2-}, NO_3^-) are here also included. Relatively much attention has also been paid to a stability- and particle size-dependent description of deposition, and to dispersion and deposition within and outside surface sources.

To arrive at a model that could be used more universally for substances with divergent properties, an approach has been chosen whereby general characteristics of dispersion have as far as possible been incorporated in the model system, and substance-specific properties are as far as possible determined using external - to be indicated by the user - parameters. This development has led to the "Operational Priority Substances model" (OPS model).

The availability of measurements of both gaseous components and aerosols in the Netherlands (National Air Quality Monitoring Network, and National Rainwater Composition Monitoring Network) make it possible to validate models for various aspects (concentration, deposition, variations in time and space) and to quantify subsequently the uncertainty involved. Since the OPS model calculates concentrations and depositions in exactly the same manner as the TREND model, it can be stated that comparisons with measurements performed for that model are also applicable to the OPS model.

Note that it here concerns validation for larger source areas. The general design of the OPS model is such that the user inputs interactively the data required for the calculation, whereby recommended values or self-selected values can be chosen for substance-specific parameters. Files can be made from the source and/or receptor data entered, which can be used in subsequent calculations, so that fewer operations are then required.
Apart from a model specification, this report also aims to be a reference book for the user seeking background information relating to the input parameters, as well as a manual in general. The subjects considered are successively: a brief description of the physical basis of the model and the processes incorporated therein (chapter 2), model validation with an assessment of its reliability (chapter 3), a specification of the application range (chapter 4), technical aspects of the model and its implementation (chapter 5), a manual on the parameters to be entered (chapter 6), and, finally, a few appendices containing, among other things, three examples of application of the model.

2. **Brief model description**

This chapter will present only an overall picture of the model. More detailed information can be found in the description of the TREND model (van Jaarsveld and Onderdelinden, to be published in 1989).
The model used here is of the same type as the so-called "National Model" (Subcommittee on Models, 1976).
This implies that the dispersion of material from a source is considered to take place at the prevailing wind speed and wind direction, and to be spatially bounded by:

- in the horizontal: a sector with an angle of 30 degrees
- in the vertical: the ground and the possible presence of an inversion layer (in the case of high sources, possibly also an inversion layer as a lower boundary)

Here, the spread from the source is taken to develop into a Gaussian form, at a rate depending on the atmospheric conditions.
To enable calculation of an average concentration at a particular point on the basis of these assumptions, the possible meteorological situations are divided into a number of classes. Next, a representative concentration is calculated for each meteoclass, and after summation of these concentrations, weighted by the frequency of occurrence of the classes, the period-averaged concentration is obtained.

The model described here was initially designed to explain concentration variations in time and space observed in the Netherlands in terms of emission, dispersion and deposition processes.
In view of the availability of meteorological data from the National Air Quality Monitoring Network (LML) such as wind direction, wind speed and solar radiation, it was obviously to utilize these data as far as possible for the characterization of the above-mentioned processes.
The selection of the meteoclassification and the associated parameters to be incorporated into the model is partly based on an analysis of concentration levels observed in the above-mentioned monitoring network.
The most clear-cut conclusion from this was that the concentration levels occurring in the Netherlands (especially SO_2 and its secondary products) can only be explained if influences of sources in a large area are included

together with large-scale climatological phenomena such as, for example, snow cover. This has led to the TREND model (van Jaarsveld and Onderdelinden, 1989), of which the OPS model described here is a direct derivative.

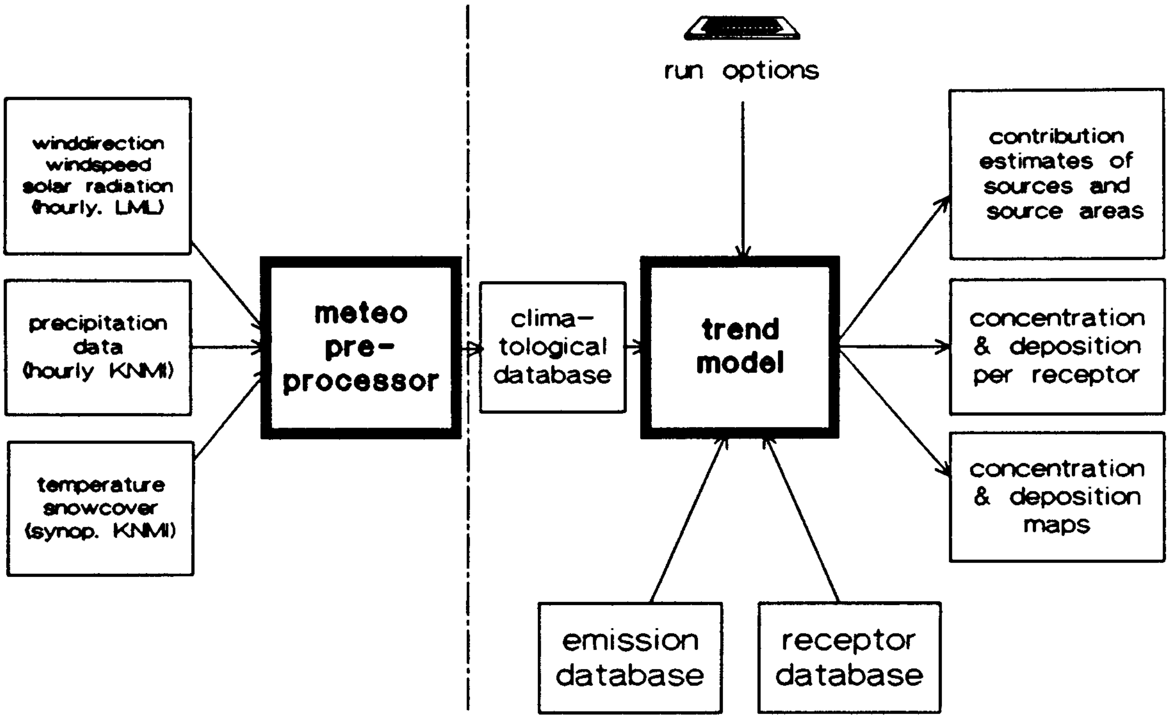


Figure 1: Schematic representation of the TREND/OPS model system. The meteo-preprocessor is in principle used only once.

The structure of the model system is presented schematically in figure 1. The collection of meteorological data from various files and the calculation of derived parameters take place in the meteo-preprocessor. This program produces meteostatistics for each period (summer, winter, year) and for each area of interest, which are stored in a climatological database. In performing calculations, the model chooses its meteo-input from the climatological database, so that the preprocessor is no longer required for this operation and for this reason has also not been incorporated as a part of the OPS model. The remaining model input consists of emission data, data on the locations for which calculations have to be performed, and data on specific properties of the substance to be modelled.

The model produces the calculated concentration and/or deposition fields, as specified by the user. In addition to printed output, files can also be made which serve as input for presentation software.
The similarities between the OPS model and the afore-mentioned "National Model" include:

- dispersion coefficients
- wind-direction sector division (12 sectors of 30°)
- treatment of wind speed
- effects of terrain roughness
- treatment of plume rise

The main differences are:

- meteoclass division
- mixing layer penetration
- height-dependent wind direction (wind shear)
- actual (measured) wind speed per meteoclass
- actual (calculated) mixing height per meteoclass
- calm hours have been included in the meteostatistics
- dispersion from surface sources with variable dimensions
- addition of calculation of (non-linear) transport over a large distance
- addition of calculation of dry deposition
- addition of calculation of wet deposition
- addition of calculation of (heavy) particles

2.1 **Meteostatistics**

The meteorological situations have been divided into:

- 12 wind direction classes (sectors of 30°)
- 6 stability/mixing height classes

The stability/mixing height classification is as follows:

ABC - the stability classes A, B and C (classification according to Pasquill, see Subcommittee on Models,(1976)) corresponding to an unstable atmospheric structure have been grouped together because of their low frequency of occurrence in the Netherlands.
Dl - this class represents the neutral stability class D for mixing heights of less than 250 m.
Dm - as above, for mixing heights of between 250 and 600 m.
Dh - as above, for mixing heights of more than 600 m.
E - the class for lightly stable atmosphere.
F - for stable atmospheric situations.

The (most common) situation with neutral atmospheric structure is here subdivided according to mixing height instead of the customary wind speed, making it possible to describe the spread from high sources more satisfactorily. Tall sources can emit above the mixing layer during periods with low mixing height and do not then contribute to concentrations at ground level.

The statistics of wind direction, wind speed, stability and other relevant parameters, which the model requires as input, are obtained from measurements made at a selected number of stations of the LML during the period 1977 to 1988, supplemented with KNMI data on the probability and intensity of precipitation (1981 to 1988). The selection of the stations can be geared to the chosen part of the Netherlands.

The friction velocity u_* and the Monin-Obukhov length L are calculated from above measurement data by means of a parameterization of the sensible heat flux. On the basis of this, the Pasquill stability class is determined using a relationship given by Golder (1972), assuming an average roughness length of 0.15 m in the Netherlands. A mixing layer height is hourly calculated from the same data, by a similar procedure as used by van Dop *et al.* (1982). The aerodynamic resistance r_a and the boundary layer resistance r_b are also calculated every hour. These parameters are included in the statistics for describing the dry deposition process.

2.2 Long-range transport

For the transport of pollutants over greater distances, wind fields are generated from the time behaviour of the wind direction and wind speed averaged over the Netherlands, obtained from measurements at five television masts with heights varying between 135 and 320 m. Estimates of the atmospheric stability and the magnitude of the mixing height at the time of emission and during transport are likewise obtained from the simultaneous values averaged over the Netherlands.
To make it possible to incorporate the data on transport over greater distances, three separate statistics have been chosen:

1. for a source-receptor distance of 0 km (local situations).
2. for a source-receptor distance of 100 km (transport over intermediate range).
3. for a source-receptor distance of 600 km (long-range transport).

When applying the model, the model automatically interpolates linearly between the data of the three statistics, depending on the actual source-receptor distance. The differences between these three statistics arise chiefly from the wind direction distribution and the magnitudes of the mixing heights. Table 1 gives, per stability class, the frequency, the wind speed and the (calculated) mixing height for each of the statistics. In relation to transport over a large distance, the following can be noted about the parameters in this table:

- the stability class is that which occurs at the time of emission,
- the wind speed is an average over the transport distance normalized to a height of 10 m,
- the mixing height is the maximum mixing height which occurs during the transport,
- the wind speed and the mixing height follow from a harmonic averaging of their respective hourly values.

Table 1. A few figures from the meteostatistics based on observations throughout the Netherlands during the period 1979-1989. Assumed average roughness length: 0.15 m.

class	1 (distance= 0 km) freq. (%)	wind speed (m/s)	mixing height (m)	2 (distance=100 km) freq. (%)	wind speed (m/s)	mixing height (m)	3 (distance=600 km) freq. (%)	wind speed (m/s)	mixing height (m)
ABC	10	2.9	610	10	2.9	980	9	3.2	1100
D1	24	2.1	130	12	2.8	180	<1	2.4	240
Dm	33	4.6	375	36	4.5	380	18	4.2	460
Dh	19	5.6	820	30	3.8	850	65	4.1	930
E	6	2.8	140	7	2.3	210	5	2.1	690
F	8	1.4	80	5	1.2	220	3	1.5	830

2.3 **Dry deposition**

The OPS model describes dry deposition of material from the lower layer of the atmosphere assuming a height-independent deposition rate (Onderdelinden *et al.*, 1984):

$$F = V_d(z).C(z) \tag{1}$$

where $V_d(z)$ is the deposition velocity and $C(z)$ is the concentration at height z. $V_d(z)$ is defined as the reciprocal of three resistances in series (Wesely and Hicks, 1977):

$$V_d(z) = (r_a(z) + r_b + r_c)^{-1} \tag{2}$$

where $r_a(z)$ is the aerodynamic resistance between a height of 0 and z (m), r_b is the resistance over the laminar boundary layer, and r_c is the surface resistance, all in s/m.

Concerning these three parameters, the model assumes the following:

- The magnitude of r_a and r_b is entirely determined by the stability of the atmosphere in combination with the surface roughness, and is independent of the substance to be modelled.
- The magnitude of r_c depends solely on the properties of the substance and the ground.

This implies that r_a and r_b can be included in the (universal) meteostatistics, and that with the parameter r_c the dry deposition properties of a particular substance are incorporated. The development of a vertical concentration gradient as a result of loss of material to the ground has been incorporated in the model as (van Egmond and Kesseboom, 1983):

$$C(4) = C(50).\phi \tag{3}$$

where $$\phi = \frac{(r_a(50) + r_b + r_c)}{(r_a(\ 4) + r_b + r_c)} \tag{4}$$

assuming that the concentration at a height of 50 m is representative for the mixed layer. The reference height of 4 m follows from the height at which air concentrations are measured in the LML. The above expression represents the stationary situation, assuming a height-independent deposition rate. In reality this gradient only develops at some distance (5-50 km) from a source, when there is no longer a Gaussian vertical concentration distribution and sufficient time has elapsed to lose a certain amount of material to the ground. The time constant τ by which this gradient establishes itself can be determined analogously to the time constant of a resistance parallel with a capacitor. The capacitance of the capacitor then represents the depth of the atmospheric layer:

$$\tau = (r_a(z).z)^{-1} \tag{5}$$

so that it follows from (3) and (5):

$$C(4) = C(50).(1-(1-\phi).(1-\exp(-t.\tau^{-1}))) \tag{6}$$

The loss of material between emission point and receptor is calculated in two steps, a. over a trajectory where vertical mixing is not yet complete, and b. where this is the case. Without considering further details, it can be stated that the loss is determined by integration of the product of concentration and deposition velocity over these trajectories. The deposition approach described above could be characterized as source depletion with surface correction.

2.4 Wet deposition

Although the wet deposition process is complex, an attempt has been made to use as simple a parameterization as possible in the OPS model, which could be applied more or less universally and which could yield satisfactory results for both short distances from a source and long-range transport. For short distances - where there is generally not yet interaction between smoke plume and clouds - an approach has been chosen via a washout coefficient as used by Janssen and Ten Brink, 1986):

$$\Lambda_p = \epsilon\ \lambda^0\ R^{1-\beta}\ [h^{-1}] \qquad \text{(particles)} \qquad (7)$$

en

$$\Lambda_g = \lambda^0\ D_g^{\ 1-\alpha}\ R^{1-\beta}\ [h^{-1}] \qquad \text{(readily soluble gases)} \qquad (8)$$

where ϵ is the particle size-dependent collision efficiency as given by Slinn (1977), D_g is the diffusion coefficient in air of the gas concerned ($cm^2.s^{-1}$), λ^0 and β are parameters relating to the drop-size spectrum of the rain drops, and R is the rainfall intensity ($mm.h^{-1}$).

At a greater distance from the source, where the smoke plume will (partly) penetrate the cloud base because of turbulent diffusion, a more important process concerning the loss rate begins to operate, namely, the rainout of material taken up into cloud droplets (in-cloud scavenging). At a greater distance from the source, the combined process of washout and rainout are parameterized in this model via an effective scavenging coefficient:

$$\Lambda_r = W\ R\ /\ H \quad [h^{-1}] \qquad \text{(gases and particles)} \qquad (9)$$

where H is the mixing height (m), R is the rainfall intensity (here in $m.h^{-1}$), and W is the ratio between concentrations in rainwater and in air.

The rate at which the rainout process begins to contribute to the total wet deposition process has been chosen on relatively arbitrary grounds dependent on plume height, mixing height and vertical diffusion rate.

To derive an average wet deposition velocity from the scavenging coefficients (valid during rainfall), taking into account the intermittent nature of rain, it has been assumed that the distribution of wet and dry periods over the source-receptor trajectory is of Poisson form (van Egmond, 1984):

$$\bar{\Lambda} = \frac{P}{\tau_w} \left(1 - \exp\left(-\Lambda \, \tau_w\right)\right) \quad [h^{-1}] \qquad (10)$$

where P is the rainfall probability and τ_w is the average shower duration (h). The parameters P, R, H and τ_w have been incorporated in the meteostatistics, so that the wet deposition velocity can be calculated from actual observations and differentiated according to stability and wind direction. However, it will be clear that, because of the parameterization chosen, oxidation reactions, for example, are disregarded. The reliability of differentiation according to conditions other than the average ones will therefore usually be limited.

2.5 **Conversion**

The OPS model treats the chemical conversion of the substance to a daughter product exclusively as a loss process. The rate of conversion can be made dependent on (measured) solar radiation incorporated in the meteostatistics. Like wet deposition, the model describes conversion as source depletion.

2.6 **Model limitations**

- In view of the similarity of this model to the National Model designed for local situations, its limitations are also mostly the same. This implies that the model may only be used in those situations where the influence of buildings and other ground irregularities is small. Thus, the height of the buildings will in most situations be such that the shortest distance from the source for which information may be given about concentration and deposition will be more than 50 m.

- Wet and/or heavy plumes cannot be calculated with this model.
- Although provisions have been made enabling dispersion of heavy particles (with a considerable falling speed) to be included, the diameter of the largest particles must be less than 50 μm.
- The OPS model does not allow for a possible background concentration of a particular substance; dispersion, deposition and conversion are independent of the existing or the added concentration, or of concentrations of other substances.
- Loss parameters used in this model are taken to be representative of the entire receptor area. This implies that no details can be given about typical areas such as agricultural land or forest within the receptor area.
- Since the meteoparameters are exclusively based on the Netherlands, the spatial application range is in principle limited to the Netherlands. Application in adjoining areas is only possible if it can be expected that relevant parameters, averaged over the period chosen, will be the same as in the Netherlands. In particular, when the topography deviates strongly from that in the Netherlands (hills, sea) or the precipitation pattern exhibits appreciable difference, the model results in these areas should be interpreted with due caution. An error analysis is required in these cases.
- Emissions which are fed into the model should be distributed uniformly over the chosen period (summer, winter, year). However, effects arising from variations in emissions over the day can be explicitly incorporated.

2.7 **Applications**

Model studies using the OPS model (or a provisional version of it) have been carried out in a number of research projects. A few examples are given below.

Air pollution as a result of the emission from coal-fired installations (LUK):

- Modelwise description of concentration and deposition of coal-relevant components in the Netherlands, arising from emissions in Europe (van Jaarsveld and Onderdelinden, 1986).
- Contribution from a coal-fired power station to local air concentrations and deposition levels (Potma *et al.*, 1986).

Integrated criteria documents:

- Calculation of concentrations in the Dutch atmosphere using the OPS model; Benzene and Toluene (van Jaarsveld, 1989).

Emissions from the grate boiler furnaces Project

- Dispersion and deposition of dioxins, dibenzofurans and heavy metals emitted by a municipal waste incinerator (van Jaarsveld and Onderdelinden, 1989).

Deposition North Sea

- Deposition of metals from the atmosphere into the North Sea (van Jaarsveld *et al.*, 1986).

3. Model validation

The OPS model provides information about average concentration and deposition (dry and wet) for a particular substance, for a particular period. In view of the fact that the average values are calculated by summation of the contributions from the individual sources, it might be sufficient to verify the results for a single source on different distance scales and different time-scales. In practice, the influence of an individual source cannot be identified at a large distance from that source, leaving aside tracer experiments and nuclear accidents such as Chernobyl. Furthermore, the experiments must be representative of all possible meteorological situations, which implies that they have to be performed over a relatively long period of time. For short distances from a source, the long-term influence on the environment can be determined with an intensive measuring campaign, if necessary. However, it should then be possible to recognize clearly the influence of the source in relation to the existing background concentrations and deposition levels. This is rarely the case in densely populated and industrialized areas such as the Netherlands. Consequently, a suitable set of data to check the behaviour of an individual source is not available in the Netherlands. It may be expected that dispersion models (both short-term and long-term) are the most sensitive to the choice of parameters at a very short distance from the source. Sensitivity tests performed with the National Model (Small Committee on Models, 1976) indicate, for example, that the use of the dispersion coefficients of Pasquill-Gifford (Gifford, 1961) gives a fourfold lower maximum concentration than use of the coefficients of Singer and Smith (1966).

3.1 Local scale

Since validation of the OPS model has not yet proved to be possible for short distances, this aspect is confined to a comparison with the National Model. This comparison shows that the calculated maximum concentration for a number of source heights stays within 35% of that the value calculated with the National Model, and the same is true of the position of these maxima, as shown graphically in figure 2. In general, it can be stated that, for short distances, the OPS model calculates higher maxima for low-level sources without heat content and slightly lower maxima for sources with a large heat content. These differences are chiefly caused by the difference in mixing height classification.

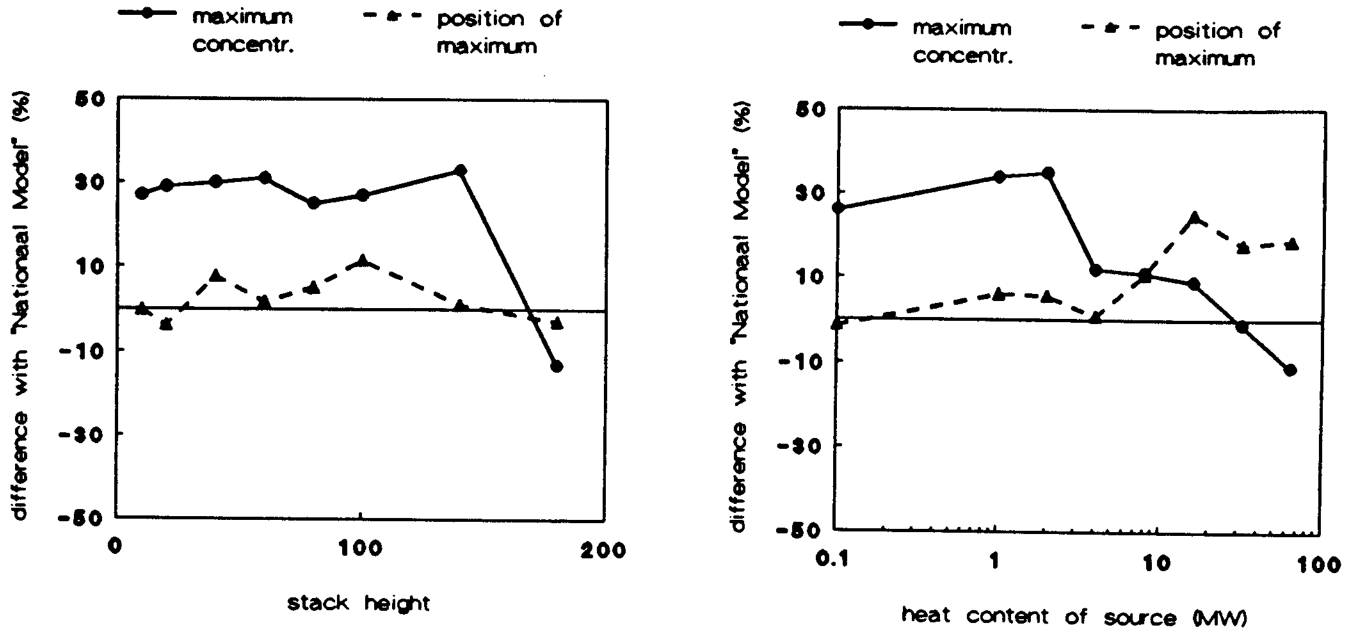


Figure 2: Comparison of the OPS model with the National Model. The relative difference in maximum concentration and the distance from the source where this maximum occurs is shown. Left: a point source with variable height, without heat content. Right: an 80 metre-high point source with variable heat content.

For verification of the plume washout mechanism incorporated in the model, the reader is referred to the plume washout experiments carried out by the ECN at the Flevo power station as part of the NOK/LUK study (Janssen and Ten Brink, 1985).

3.2 **Regional scale**

In a complex source area, where the air concentrations are caused by a number of sources especially on a local scale, possibilities for verification do exist. For example, the SO2 concentration was calculated at the locations of 30 LML monitoring stations in South-Holland (12 of which in the Rijnmond) on the basis of 5-yearly average meteorological data. A comparison with the measured values for the same period gave a calculated/measured ratio of 1.06, a spatial correlation coefficient of

0.91 and a r.m.s. value of 13% (van Jaarsveld and Onderdelinden, 1984). The emission inventory for the year 1980 was used in these calculations, as incorporated in the Air Quality Management System for the Netherlands, Belgium and part of West Germany (Veldt, 1980), supplemented with emission estimates for the rest of Europe (EMEP, 1981).

This comparison provides information about the average contribution from sources on a local scale, but not about the local maxima. It is therefore not possible to draw conclusions from this about the chosen dispersion parameters or plume rise formulae. It can here also be noted that the error made in the description of the spatial distribution is partly determined by the amount of detail in the emission file used. The fact is that the spatial resolution of the calculated concentrations can be no better than the spatial resolution of the emission description.

3.3 **National scale**

The measurements from the National Air Quality Monitoring Network and the National Rainwater Composition Monitoring Network (concentration and wet deposition) can be used for verification of the dispersion on a national scale. There is on this scale, as well as the influence of regional area sources, also a large influence of foreign area sources on the spatial distribution. Furthermore, the influence of deposition and conversion on the concentrations occurring is going to play an important role. A similar comparison as mentioned above was made for 99 so-called grid stations (van Jaarsveld and Onderdelinden, 1984). The spatial correlation coefficient found was 0.95, while the r.m.s. value of the differences was of the order of 10%. It should be noted here that the result of a comparison on this time-scale is chiefly determined by the quality and the resolution of the emission file used. To investigate to what extent the chosen stability and mixing height classifications do actually lead to a distinction between concentrations occurring during these situations, and to what extent the model also reproduces this, the concentration for the separate classes has been calculated and placed alongside the measured values.

Figure 3 shows that the average SO_2 concentration in the Netherlands is indeed related to the stability structure of the atmosphere, and that this is described very satisfactorily by the model. However, it may be expected that the distribution will be different for substances with low emission heights such as NO_x and NH_x, especially during stable conditions.

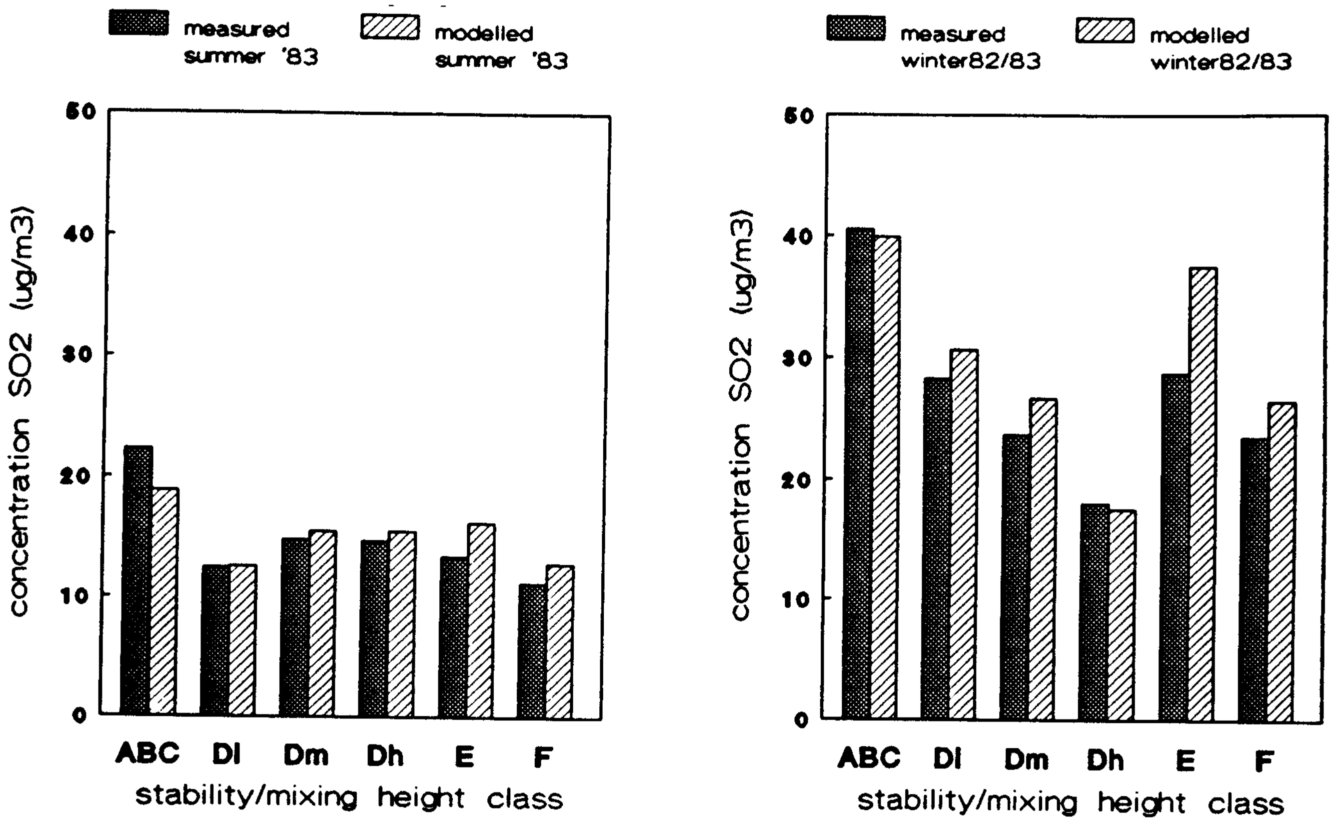


Figure 3: Comparison of measured with calculated SO_2 concentrations in the Netherlands per stability/mixing height class.

Table 2 gives the results of a number of comparisons on different time-scales, always on the basis of grid stations of the LML. To avoid the influence of changing emissions over the years on the comparison, the r.m.s. value has been determined after normalization of the calculated national average to the measured average over the period considered. As a supplement to table 2, it can be stated that the model overestimates the average SO_2concentrations in the Netherlands for the emission year 1980 by about 5% and underestimates the NO_x concentrations by about the same percentage.

Table 2. Comparison of calculated SO_2 and NO_x concentrations with measurements from the LML on the basis of 97 and 30 grid stations, respectively. Included are the spatial correlation coefficient r and the r.m.s. values of the observed differences.

time-scale	number of periods	r	median of r	r.m.s.	median of r.m.s.
SO_2:					
month	96	0.56-0.94	0.84	15-54%	25%
half year	14	0.77-0.87	0.86	23-30%	21%
year	8	0.88-0.93	0.91	15-31%	18%
long term	-	0.95	-	11%	-
NO_x:					
month	84	0.56-0.96	0.82	10-34%	21%
half year	14	0.78-0.91	0.84	9-18%	14%
year	7	0.88-0.94	0.92	11-14%	12%
long term	-	0.95	-	11%	-

In support of the data in table 2, the model's ability to describe the monthly variation is shown in figure 4. In view of the good agreement, it can be stated that the meteorological influences are correctly taken into account and that influences of sources at large distances are accurately represented. The latter is important because the contribution from sources in other countries to the concentrations in the Netherlands is generally estimated to be at least 70% (SO_2).

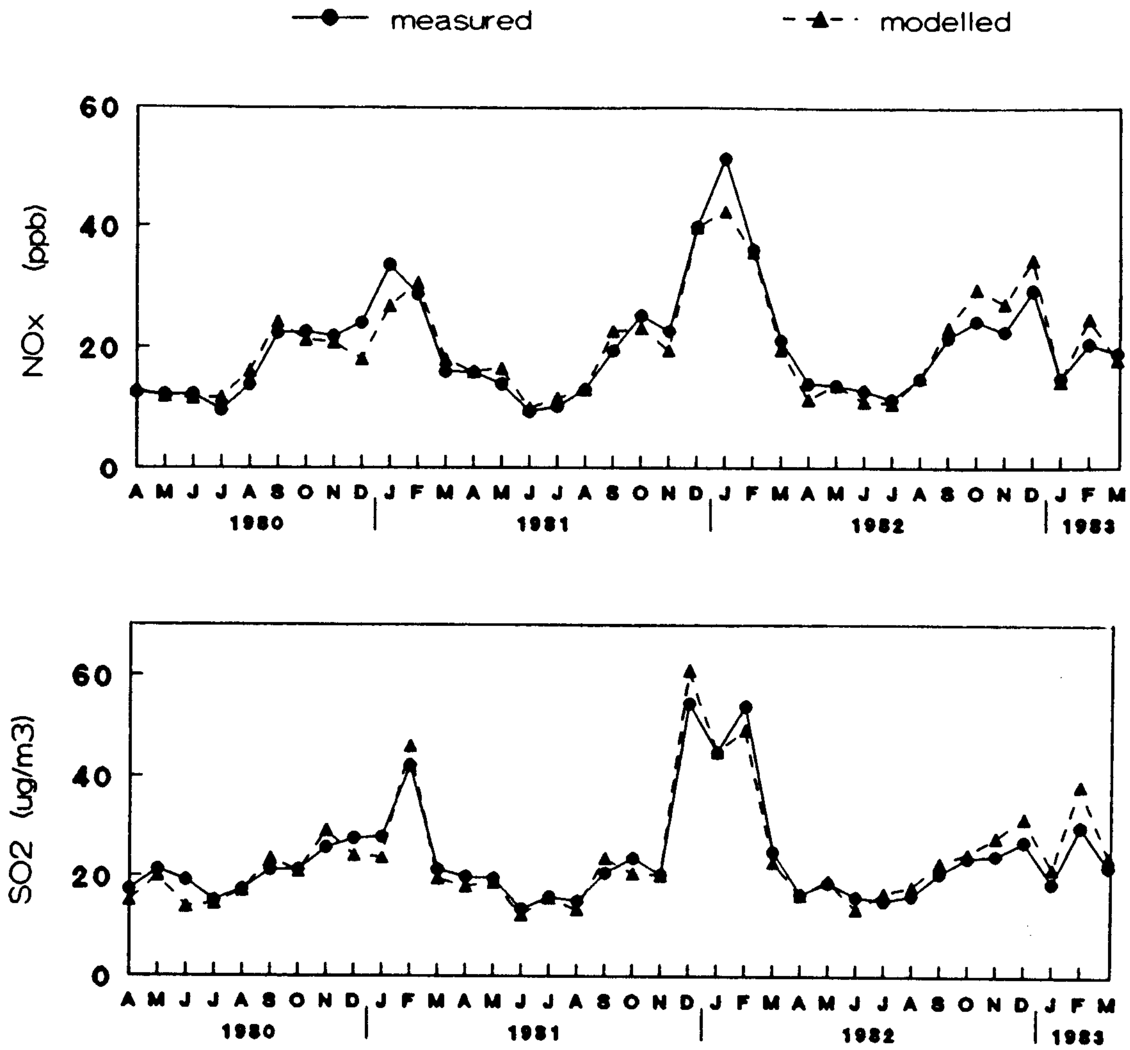


Figure 4: Monthly average SO_2 and NO_x concentrations in the Netherlands versus modelled values. The emission data used are representative of the year 1980.

Of the dry and wet deposition calculated by the model, only the wet deposition can actually be verified by measurements. In general, it was found that the wet deposition of sulphate and nitrate can be described reasonably well (Onderdelinden *et al.*, 1984; van Jaarsveld, 1988). The variations on a monthly basis are greater than for the air concentrations, but it should be noted that the uncertainty in the measured wet deposition is also greater. An important point here is that up till 1988 the National Precipitation Chemistry Network (LMR) used so-called open-top rain collectors for making measurements, which, as well as the wet deposition, also measure an unknown amount of dry deposition. A comparison with wet-only collectors showed that this contribution is of the order of 25% for sulphate (Ridder *et al.*, 1984).

Since this model does not calculate secondary components, the element lead was chosen as an example for comparison of calculated and measured wet deposition of aerosols.

Lead is believed to occur in the atmosphere in particulate form and to be derived primarily from traffic (addition of lead to petrol). Figure 5 shows the wet deposition of lead as measured at 20 measuring stations of the LMR and the calculated values for the same locations, both as averages for 1985. The remark made about the type of wet collector is here also appropriate. The calculated depositions can be qualified as reasonably good in relation to the measured values, especially when it is considered that the model assumes the same volume of precipitation for all locations in the Netherlands.

For the verification of calculated air concentrations of some heavy metals, the reader is referred to the NOK/LUK study (van Jaarsveld and Onderdelinden, 1986).

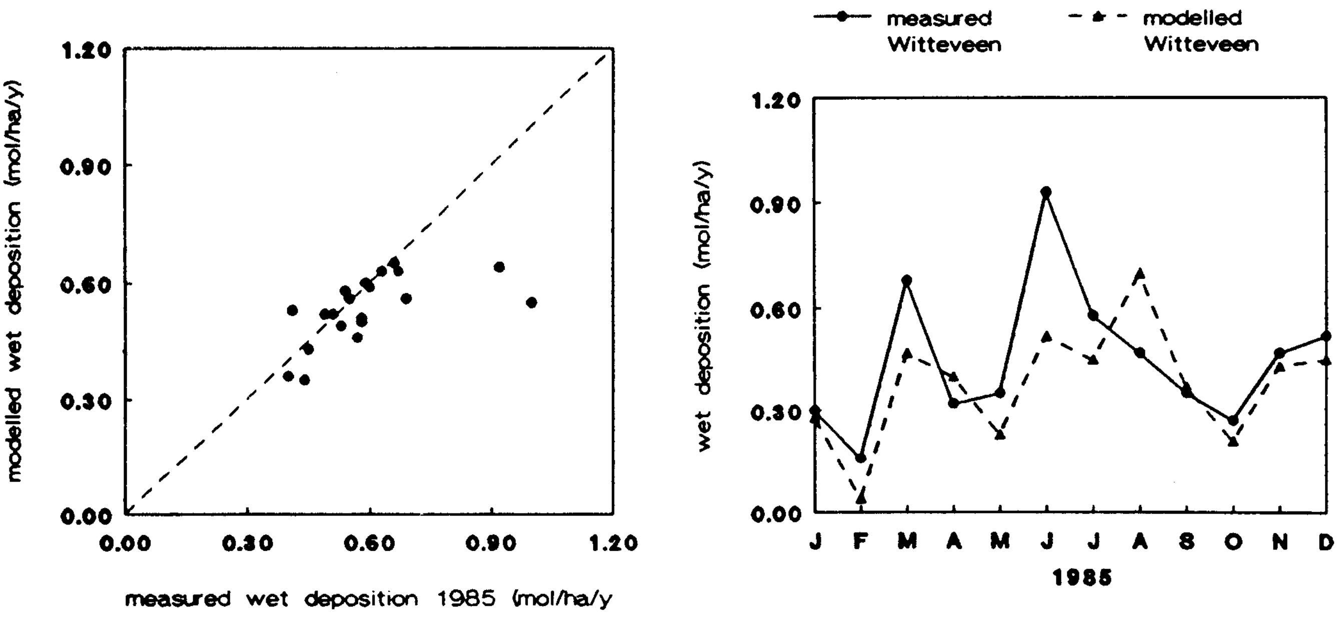


Figure 5: Comparison of calculated wet deposition fluxes of lead with observations from the LMR. Left: the annual average results from 20 stations are plotted against each other. Right: the variation over 12 months for one station (Witteveen).

3.4 Reliability of the model results

To sum up, it can be concluded that, on the basis of comparisons with measurements, the average concentrations and depositions on regional and national scales can be calculated in the case of properly chosen loss parameters and a correct emission file, with an error smaller than:

concentration:	ca 10%	deposition:	ca 15% (long term)
	ca 15%		ca 20% (specific year)
	ca 20%		ca 30% (specific summer or winter)
	ca 30%		ca 40% (specific month)

It has been assumed here that the dry deposition parameters are the same in the entire area about which information is given.
Nothing can (as yet) be said in this context about calculated maximum concentrations and concentrations close to the source, except that this maximum will vary less than 35% from the value calculated by the National Model. It may be expected, however, that in view of the sensitivity with respect to certain assumptions, the absolute deviation can easily be over 100%, independent of the averaging time. Research into this aspect is therefore needed. Possibly, results of dispersion experiments in North America can be used for this purpose, for example the EPRI measuring campaign in the vicinity of the Kincaid power station (EPRI, 1983), where extensive observations have been carried out of both air concentrations and meteorological parameters over several consecutive months.

4. Model specification

4.1 Receptor area

The area for which concentrations and depositions can be calculated is determined by the size of the area for which meteorological parameters are known. Since the climatological data set used for this model is for the principal parameters based on observations from the National Air Quality Monitoring Network, the maximum size of the receptor area becomes in effect the Netherlands and adjoining regions. To make it possible to take the influence of climatological differences within the Netherlands into account, a choice can be made from the climatological data set of:

- the whole of the Netherlands
- 6 areas within the Netherlands

The areas are shown in figure 6.

1 - Coast of Friesland-Groningen
    Northern part of North-Holland
2 - North-Holland
    South-Holland
    Zeeland-South
3 - Drente and Environs
4 - Zeeland
5 - Twente
    Gelderland
    Brabant
6 - Achterhoek
    Brabant-East
    Limburg

Figure 6: Climatological division of the Netherlands into areas

In addition to the above-mentioned area division, there is also the possibility of compiling special statistics on the basis of one or more meteostations of the LML. However, this, in view of the required files, can only be done at the RIVM. Receptor points for the calculation of concentrations and depositions can be chosen:

- in a regular (cartesian) grid, with a grid distance to be chosen (max. 65x65 grid points).
- at a number of locations to be defined by the user.
- at the locations of measuring stations of the LML with the same grouping of stations as that used within the LML (only possible within RIVM/LLO).

This model does not take into account the direct influence of obstacles (e.g. buildings) on the dispersion. The shortest distance from a source for which this model may be used has therefore been set at 50 m for flat terrain (roughness length < 0.25 m) and 100 m for greater terrain roughnesses.

4.2 **Source area**

The model describes the transport of substances over greater distances with wind fields generated from the time behaviour of the wind direction, wind speed, atmospheric stability and mixing height averaged over the Netherlands. Despite the rather rough extrapolation, it was found that the related TREND model describes the large-scale transport of SO_2 satisfactorily (see model validation, chapter 3). The source area for this model has therefore been set at a circle with a radius of 1000 km, with the Netherlands as the centre.

4.3 **Time-scale**

The OPS model basically calculates long-term average concentrations and depositions. In fact, the period of which the calculations are representative is entirely determined by the period for which the meteostatistics have been made. The observations from the LML have made it possible to make meteostatistics since 1 April 1977. To date, the following statistics have been incorporated in accordance with standard procedure:

- the consecutive period from 1-1-1979 to 1-1-1989
- the summers (April to September inclusive) in the above period
- the winters (October to March inclusive) in the above period

In addition to the standard (multi-year) averages, the OPS model can also calculate concentrations and depositions for shorter periods (specific year, season, month). Special statistics will then have to be compiled for such a period. By way of illustration: the monthly average concentration and deposition for SO_2 and NO_x in the Netherlands have been calculated with the afore-mentioned TREND model, giving good agreement with measurements (see chapter 3, figure 4).

4.4 **Sources**

The OPS model distinguishes the following source types:

a. Point sources:

- source height > 0 m
- negligible diameter
- with or without heat content

b. Area sources:

- source height > 0 m
- diameter ca 10 m - 500,000 m
- square or circular
- with or without (average) heat content
- initial spread in the vertical (from 0 m to average source height)

4.5 **Emissions**

4.5.1 **Behaviour in time**

The time-dependent emission behaviour can only be specified as a daily variation. The options are:

- continuous in time
- dependent on the (average) industrial activity over a working day
- dependent on the (average) heating activity for space heating
- dependent on traffic intensity
- dependent on a daily variation to be specified by the user (a maximum of 3 different daily variations to be defined).

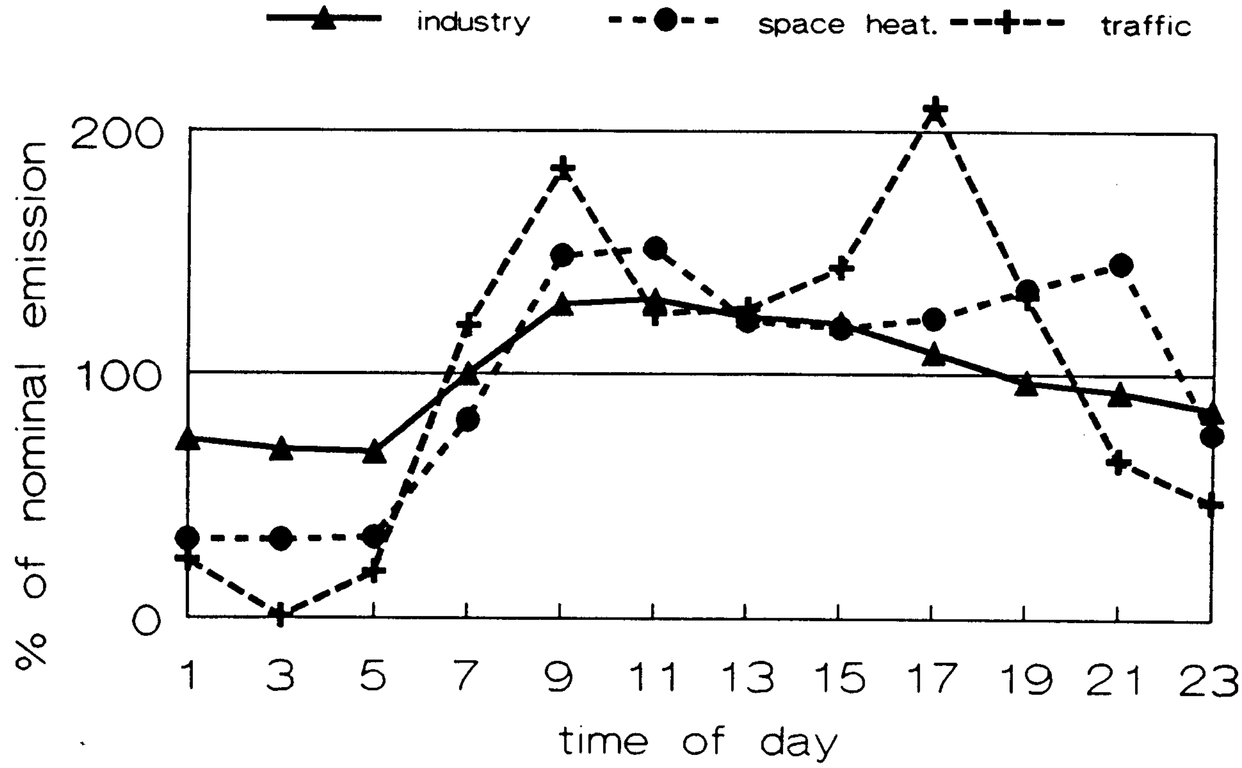


Figure 7: The average variation of the emission over the day, for three source types.

4.5.2 **Emission speciation**

The model distinguishes two types of emissions:

- gaseous emissions (no so-called heavy or wet plumes)
- particulate emissions

In the case of particulate emissions, the emission is considered to be distributed over 5 particle-size classes, namely:

< 0.95 μm 0.95 - 4 μm 4 - 10 μm 10 - 20 μm and >20 μm

The model calculates these classes separately, with specific properties for each class.

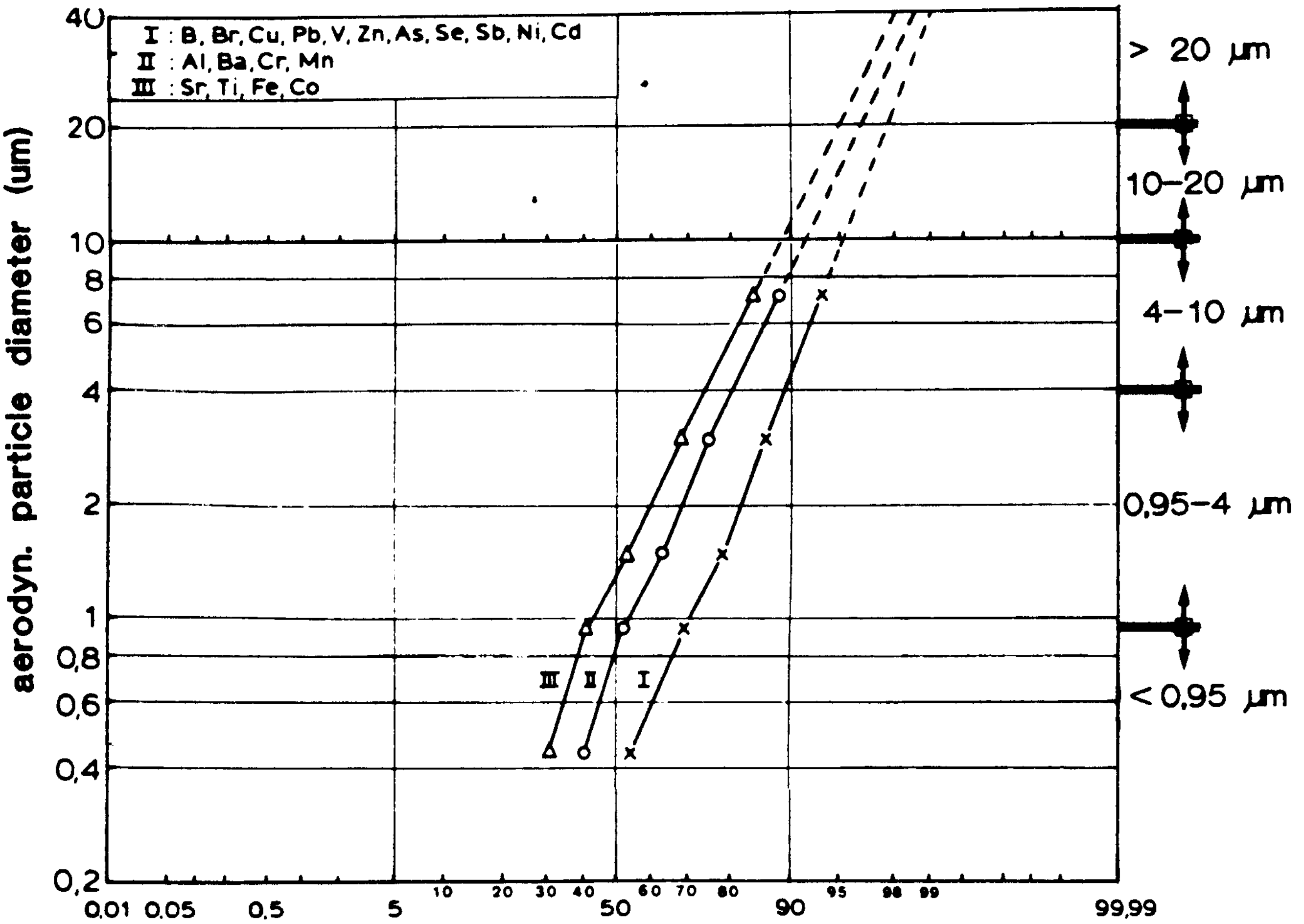


Figure 8: Particle-size distributions for a number of elements as measured in background concentrations, and classified into three groups (Potma *et al.*, 1986). After log-normal extrapolation these distributions are also taken to be representative of source emissions. The particle-size classification used in the OPS model is given on the right-hand side.

The user can choose from three standard particle-size distributions (see figure 8 and table 3), or can input a more specific distribution over the above-mentioned classes. In calculating the concentrations and depositions for the heaviest particles (> 20 μm), allowance is made for the fact that the sedimentation rate of these particles is not insignificant, so that plume descent occurs with distance.

4.6 **Loss processes**

Loss of mass over the trajectory from source to receptor occurs in this model in three ways:

- dry deposition
- wet deposition
- conversion

The material lost through dry and wet deposition is accumulated and included in the output as are also the calculated concentrations; the daughter products (e.g. sulphate) formed by conversion are here not included.

For particulate pollution, the loss parameters as a result of deposition are related to the particle-size class (van Jaarsveld and Onderdelinden, 1986) and incorporated in the model. The user cannot alter these parameters.

4.6.1 **Dry deposition**

Dry deposition is simulated in the OPS model by means of the so-called resistance model. The deposition velocity is here determined by three resistances in series:

- the aerodynamic resistance (r_a)
- the laminar boundary layer resistance (r_b)
- the surface resistance (r_c)

The deposition velocity is given by: $V_d = (r_a + r_b + r_c)^{-1}$ [m/s]

r_a and r_b are calculated when the meteostatistics for a certain period/area are made, and as such form also part of these statistics; r_c has to be specified by the user for the substance he wishes to calculate as an average over the period to be considered. As an alternative, however, the possibility is offered to input an average deposition velocity V_d, whereby the model calculates r_c using average values of r_a and r_b. In this way, the specific r_a and r_b for a particular stability class can still be used. The average V_d which can be entered in the above manner has an upper limit because of the fact that $r_c > 0$ s/m, which means in practice that V_d must be ≤ 0.034 m/s.

Dry deposition of particulate substances is entirely related to the dimensions of the particles. The deposition velocities for the particle-size classes have been determined using Sehmel's model (1980). This model predicts the deposition velocity of a particle dependent on the particle size, the roughness length of the ground surface, the density of the particles and the friction velocity u_*. The procedure yields a deposition velocity for all stability classes and particle-size classes which the OPS model distinguishes. Here, the logarithmic class mean has consistently been held as representative of all particle diameters in a class. For the class with the largest particles (> 20 μm), 40 μm has been taken as a representative value.

The user of the model only influences the effective deposition velocity through the distribution of the substance over the five particle-size classes. The deposition velocities concerned (weighted over the various stability classes) are given in table 3.

Table 3. Standard particle-size distributions (see also figure 8). For each class, the average (weighted over the various stability classes) dry deposition velocity is also given.

	1 <0.95 μm	2 0.95-4 μm	3 4-10 μm	4 10-20 μm	5 >20 μm	
fine (I)	70	20	5.5	2.5	2.0	%
medium (II)	53	28	11.5	4.2	3.3	%
coarse (III)	42	33	14.5	5.9	4.6	%
V_d :	0.00065	0.0025	0.0071	0.013	0.067	m/s

4.6.2 **Wet deposition**

In the OPS model, wet deposition is related to the following measured parameters and parameters incorporated in the meteostatistics:

- rainfall probability
- rainfall intensity
- average shower duration

Wet deposition may occur in two ways:

- washout (of readily soluble gases or particles below the cloud)
- rainout (of substances taken up into cloud droplets)

Washout of gases readily soluble in water is entirely parameterized for the user at a diffusion coefficient in air to be specified for the substance concerned (D_g in $cm^2.m^{-1}$). Washout of sparingly soluble gases is not incorporated in this model because of its small contribution to the total wet deposition. Rainout is related to a scavenging ratio to be specified, which can have been determined for a substance either empirically from the ratio of concentrations in rainwater and air or theoretically via the constant of Henry. The washout velocity calculated on the basis of an entered diffusion coefficient in air is limited by the wet deposition velocity, calculated from the specified scavenging ratio. The reason is that the last-mentioned (empirical) parameter is considered to comprise both processes. In addition to the above-mentioned wet deposition specification, a wet deposition velocity during rainfall can be specified (in $\%.h^{-1}$) as an alternative; the model then estimates the associated D_g from (Durham *et al.*, 1981):

$D_g = k\ M^{-0.5}$ where M is the molecular weight and k is a conversion constant (k=1). However, in this way the relationship with the rainfall intensity becomes lost.

4.6.3 **Chemical conversion**

The conversion rate for gaseous substances can be given as a constant and/or as a variable related to the solar radiation measured in that period. The solar radiation has been incorporated in the meteostatistics dependent on class.

In contrast with the TREND model, the conversion process is envisaged here exclusively as a removal term. Dispersion and deposition of the secondary product are consequently not included.

5. Technical aspects

The OPS model has been installed on the HP9000 computer equipped with the UNIX operating system of the Laboratory for Atmospheric Research (LLO). In addition to the version mentioned, a version has also been developed for use on an IBM PC (or compatible) running under MS-DOS. Both versions have been programmed in FORTRAN 77.
The minimum PC hardware configuration on which the model can be run is: 384 Kb storage capacity and at least one 360 Kb floppy disk drive. For efficient use of the model, however, a hard disk drive and a mathematical co-processor are to be recommended as extras. The design of the model is such that the hierarchical file organizations of UNIX or MS-DOS can be used, which is important especially in a multiple-user environment.

The total time required for a model run can be estimated as follows:

For the HP9000/550:

$$t = 8 + \#\text{receptors} * \#\text{sources} * 0.061 * [4.2]^{1)} \text{ seconds}$$

For an Olivetti M24 PC (8086 cpu) without mathematical co-processor:

$$t = 60 + \#\text{receptors} * \#\text{sources} * 4.5 * [4.2]^{1)} \text{ seconds}$$

For an Olivetti M24 PC (8086 cpu) with mathematical co-processor:

$$t = 55 + \#\text{receptors} * \#\text{sources} * 0.45 * [4.2]^{1)} \text{ seconds}$$

1) for particulate substances; for gaseous substances: 1.

5.1 Program description

The computer program can qua function be divided into three parts (see also block diagram in section 5.3):

- Input section
- Main program
- Output section

5.1.1 **Input section**

This is the section which concerns the user the most. The function is the collection in an interactive manner of all data needed to be able to execute the model run.

The design is such that the user can choose between more or less standard parameterization - with the number of parameters to be entered being as small as possible - and a more specific approach where the user himself specifies the deposition and/or conversion process in particular. It is obvious that the latter operation assumes that the user has considerable expert knowledge.

All answers to the questions posed by the program are checked for apparent errors, such as the typing in of alphanumerical characters there where the program expects numerical answers. Moreover, entered parameters are compared with a lower and an upper limit, so that the model does not become ineffective because of unreal input data. Answers found to be incorrect can still be corrected; however, going back in the question series is not possible. In the case of questions which can be answered with "yes" or "no", it is sufficient to input "j", "y", "yes", "1", or "n", "no", "njet", "0".

Schematically, the order in the question series is as follows:

general questions
|
read in source data
|
select sources
|
select receptor points
|
select climatological data set
|
select loss parameters
|
output specification

See chapter 6 for detailed descriptions of the input parameters.

5.1.2 **Main program**

Here - on the basis of the data from the input part - the actual computations are performed. The main features of the mathematical model as well as the main program loops are presented below:

```
                         reading of climatological file
                                       |
                         reading of receptor file (optional)
                                       |
                         initialisation of variables
                                       |
    ----------------->   reading of source data from file for each source
   |                                   |
   |  --------------->   per stability class (6)
   |  |                                |
   |  |  ------------>   per receptor point
   |  |  |                             |
   |  |  |                determination of climatological parameters
   |  |  |                             |
   |  |  |  --------->   per particle class (5, optional)
   |  |  |  |                          |
   |  |  |  |            calculation of concentration + summation
   |  |  |  |                          |
   |  |  |  |            calculation of deposition + summation (optional)
   |  |  |  |__________________________|
   |  |  |_____________________________|
   |  |________________________________|
   |___________________________________|
                                       |
```

5.1.3 **Output section**

This part of the program first carries out a few additional operations on the concentration and deposition fields, such as the calculation of averages and effective deposition velocities. Secondly, autoscaling is applied to obtain the figures in the fields within the 1 to 1200 range.

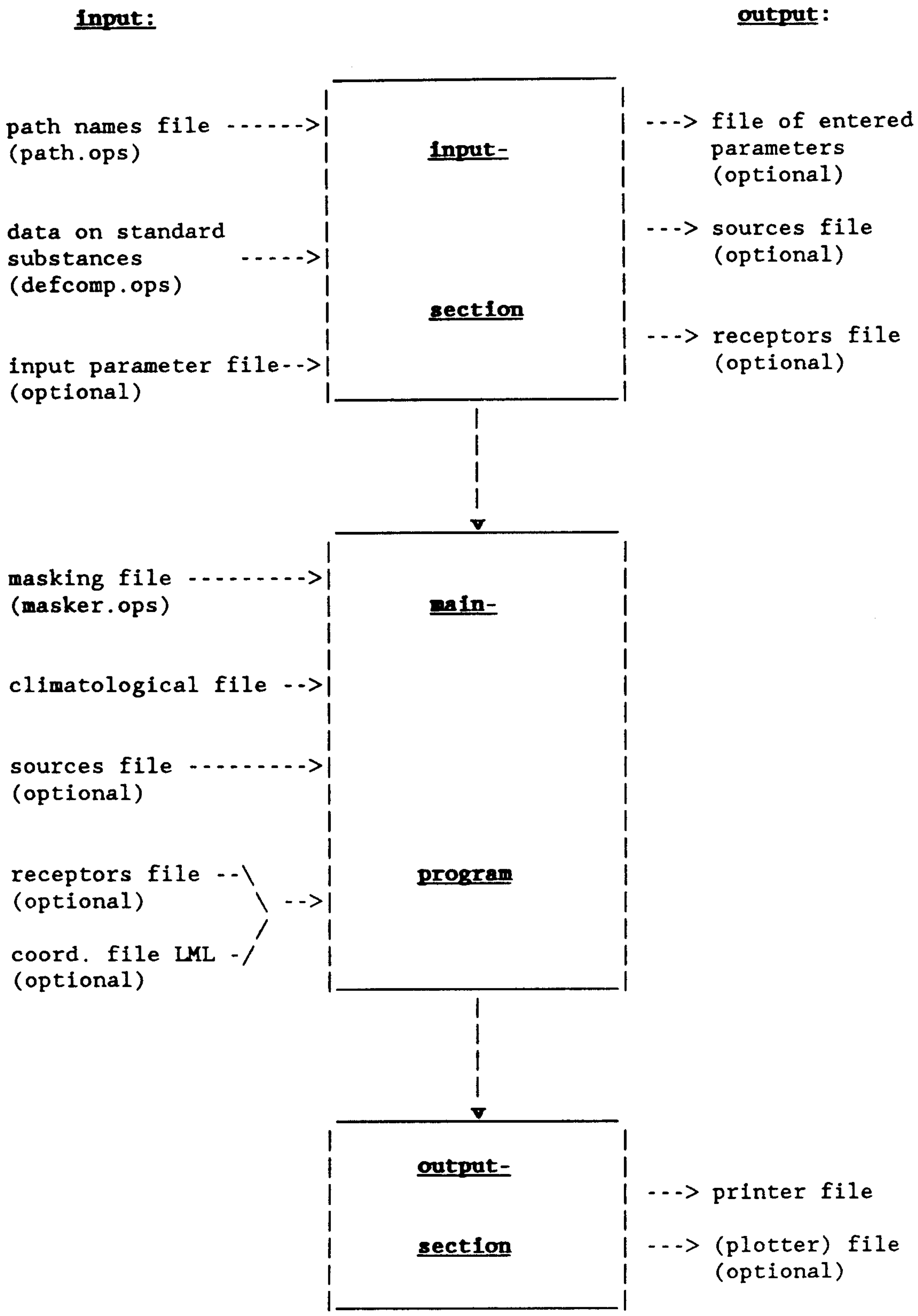
Finally, the fields together with the other relevant data are sent to a file, so that it can be printed on a printer at a later stage. Here the file is also generated which can serve as input for a plot program. Each field in this file is provided with a so-called "standard APS header", containing data on the field. See appendix 2 for a description of this header.

5.2 **Files and file names**

To structure the naming of the model's input and output in some degree, a 3-letter code is added to the file names entered by the user. This offers at the same time the possibility of keeping the basic name of the files pertaining to a model run the same. Besides, the user can also continue to use a variant file extension. The entered basic file name is limited to 8 symbols in the model. A summary of the various files, the extensions used and the default names is given below. The default names are used in the model if the user does not want to store certain data for reuse.

file	extension	default name	use
input data	.inp	stdpar.ops	storing input data for reuse
source data	.brn	stdbrn.ops	storing source data
receptor data	.rcp	----------	storing receptor data
printer output	.lpt	stdout.ops	the actual model output
(plotter) output	.plt	----------	storing results for additional operations

5.3 **Summary of the files used in conjunction with the OPS model**



6. Description of input parameters

6.1 General

In the development of the OPS computer program, an attempt has been made to limit as far as possible the number of operations required in its use, without making concessions to the possibilities for its application. For example, the user can choose as many built-in data as possible, or he can input all necessary parameters himself.

All entered data can be stored under a name which can be chosen by the user, while these parameters are printed together with the model results. In this way a model run can be unambiguously identified. To save time, an input file thus made can be altered (to a limited extent) in a text editor and subsequently used for a new model run, for example, when the user wants a more detailed calculation.

Although it is not possible to return to answers once they have been entered, a check for fulfillment of certain conditions does take place when the requested parameters are entered. The questions to be answered by the user and/or options are elucidated below. It is obvious that the number of data to be entered depends on the options chosen.

6.1.1 Selection of parameter file

The user can choose between:

a. data from existing file
b. entering data manually
c. entering data manually and storing

6.1.2 Name of input parameter file

When 6.1.1 a or c is selected: give here the name of an existing or new file respectively; a maximum of 12 characters is allowed

6.1.3 Project name

For user's administration only; a maximum of 18 characters is permitted.

6.1.4 **Substance to be modelled**

Here, a choice can be made from a list of substances for which recommended values of properties have been incorporated in the model (present in file: **defcomp.ops**).
These specific properties concern:

a - name of the substance
b - molecular weight
c - particle-size characteristic (0=gaseous)
d - dry deposition velocity, characterized by a surface resistance r_c
e - diffusion coefficient in air
f - scavenging ratio
g - conversion rate (constant in time)
h - conversion rate (proportional to solar radiation)

d, e, f, g and h for gaseous substances only.

The recommended values for the parameters are given in appendix 1.

To date, recommended values are available for the following substances:

1 - SO2 (gaseous)
2 - NOx (gaseous) (as NO2)
3 - NH3 (gaseous)
4 - HF (gaseous)
5 - F (aerosol)
6 - HCl (gaseous)
7 - Cl (aerosol)
8 - HBr (gaseous)
9 - Br (aerosol)
10 - B (gaseous)
11 - B (aerosol)
12 - Se (gaseous)
13 - Se (aerosol)
14 - Hg (gaseous)
15 - Hg (aerosol)
16 - C6H6 (gaseous) (benzene)
17 - C7H8 (gaseous) (toluene)
18 - As (aerosol)
19 - Cd (aerosol)
20 - Cr (aerosol)
21 - Cu (aerosol)
22 - Pb (aerosol)
23 - Zn (aerosol)

For substances not included in the list, or for those cases where the user wishes to deviate from the standard value, he chooses here "to be specified by user" (0). In the latter case, it is advisable to be prepared for questions referring to the above data.

6.1.5 **Name of substance**

For user's administration only (a maximum of 18 characters)

6.1.6 **Molecular weight**

This refers to the molecular weight of the substance to be modelled. The emission strength must be specified on the basis of this molecular weight.

e.g. Fluorine can be calculated as F, mol. wt.: 19. The emission must be given in $g.s^{-1}$ F and the calculated deposition will then be expressed as F in, for example, $g.s^{-1}.m^{-2}$. If the user wishes to calculate hydrogen fluoride (HF), then specify mol. wt.:20 and emission as HF, whereafter deposition is also calculated as HF.

6.1.7 **Selection of gaseous or particulate form**

If a substance occurs in both gaseous and particulate form and the user does not want to calculate this separately, then the most common form is chosen. Since the loss rates are generally higher for the gaseous than for the particulate form, the former is usually preferred. Another reason is that particulate substances are calculated in 5 separate size classes, so that the computing time is roughly a factor of 5 longer. Note that the deposition velocity must be adjusted to the mixed form, for example, by a weighted averaging of the separate rates.

6.1.8 **Particle-size distribution**

For the calculation of concentrations and depositions of particulate pollution, the OPS model assumes that the emission is divided into 5 particle-size classes. This division is necessary in order to be able to do justice to the differences in properties between larger and smaller particles. These differences manifest themselves especially in the loss rates of the particles: small particles have a lower dry deposition velocity and also a lower wet deposition velocity than their larger counterparts. The particles have been classified according to diameter as follows:

1	2	3	4	5
<0.95 μm	0.95-4 μm	4-10 μm	10-20 μm	>20 μm

The loss rates associated with the above-mentioned classes have been incorporated in the model, the dry deposition velocity having been determined on the basis of Sehmel's model (1980) and the particle size-dependent wet deposition velocity calculated analogously to the method described by Janssen and Ten Brink (1985) for washout and analogously to van Jaarsveld and Onderdelinden (1986) for rainout. The distinction between the various substances is now determined by the distribution of the emission over the 5 classes. The user of this model can choose from 3 "standard" distributions, designated "fine", "medium" and "coarse". This classification has arisen from measurements of size distributions of heavy metals made by the ECN as part of the NOK-LUK study (Potma *et al.*, 1986), see also figure 8. For these standard distributions, the emission has been distributed among the particle-size classes (in %) as follows:

	1	2	3	4	5
fine	70	20	5.5	2.5	2.0
medium	53	28	11.5	4.2	3.3
coarse	42	33	14.5	5.9	4.6

In addition to the 3 standard distributions, the user can also choose his own distribution, which he will then be asked to enter. Note that the distribution over the size classes should be the same distribution in which the substance leaves the chimney. The reason is that the atmospheric lifetime of larger particles is considerably shorter than that of small particles, so that the distribution changes in favour of the small particles with time.

6.2 **Source data**

This part of the program asks the user to specify the source data. These data can be read in from a file (made for and/or by this model), or can be entered manually. If the number of sources to be entered is more than 5, then it is generally quicker to create a file with a text editor (e.g. on the basis of an existing file, see 6.2.12). The source data to be entered are:

6.2.1 **Source strength**

The unit of source strength is $g.s^{-1}$. Here, the strength of the source is the average over the total period considered. Thus, if the user wants to calculate an annual average concentration, he must also input an annual average emission.

6.2.2 **Heat content**

The heat content of the source is used to permit calculation of the effective plume height under different climatological conditions. The unit is megawatt. When the heat content is not constant, an emission-weighted average can be chosen. Alternatively, the heat content can be calculated from:

$$Q_w = 0.0013 * V_n * (T_g - 288)$$

where Q_w = heat content of the flue gas in megawatts
V_n = volume flow of the flue gas in $Nm3.s^{-1}$
T_g = temperature of the flue gas in Kelvin

6.2.3 **Stack height**

This is the height of the physical outlet above ground. With area sources, the average emission height must be entered here.

6.2.4 **Source diameter**

The OPS model treats area sources as being square in shape, with the source diameter = side of square. It is also possible to start from a circular source by entering the diameter as a negative figure. The dimension of the stack exit should definitely not be entered as a source diameter. Although the model yields the same results for an area source with a diameter approaching zero and a point source, it is advisable to input a source diameter greater than zero only when the horizontal dimension of the source is also really of importance.

6.2.5 Source-height distribution

This parameter is only relevant with area sources. An area source is generally a collection of unspecified point sources, each of which may lie at a different height. The source height is taken to be the average stack height of sources within the area source, and the parameter asked here is the standard deviation of this average height. The initial distribution of emissions in the vertical is especially important for calculating concentrations within a surface source.

6.2.6 Emission time behaviour

This model can take account of the fact that the emissions from certain sources exhibit a characteristic daily variation.
The user can choose from the following distributions of emissions over the day:

0 - continuous variation
1 - variation according to an average industrial activity
2 - variation dependent on the average heating behaviour for space heating
3 - variation dependent on the average traffic intensity
4, 5 and 6 - daily variations to be specified by the user.

The distributions 1 to 3 incl. are given in 2-hourly classes in the following table (see also 4.5.1 and figure 7):

	0-2	3-4	5-6	7-8	9-10	11-12	13-14	15-16	17-18	19-20	21-22	23-24	hour
1:	73	69	68	100	129	131	124	121	109	97	93	86	%
2:	33	33	35	80	150	155	120	116	122	135	145	77	%
3:	24	1	19	120	185	125	127	144	210	132	65	48	%

6.2.7 Source category number

This number can be used to distinguish various categories (such as economic sectors) in the case of (especially larger) emission files. The model offers the possibility of selecting a certain category from an emission file, so that its contribution can be calculated separately.

6.2.8 Source area number

As above for source category number, but designed to make a spatial classification of the sources possible. Note that there is no connection between this source area number and the area classification which is used for the meteostatistics.

6.2.9 Source coordinates

The position of a source can be fixed in each coordinate system that is parallel to the system used in the LML (RDM). It is obvious that the receptor area still to be specified must be given in the same coordinate system. When calculating concentrations around a local source, 0.0 can here be entered.

6.2.10 Multiple sources

If desired, the points 6.2.1 to 6.2.10 inclusive can be repeated to input a number of sources. In this way a maximum of 40 sources can be entered manually. As stated under 6.2, in the case of large numbers of sources, it is more convenient to place them in a source file without the help of the model. Source files which are made with a text editor can contain an unlimited number of sources. See 6.2.12 for a source file specification.

6.2.11 Specification of daily variation of emission

When daily variations to be specified by user have been chosen under "Emission time behaviour" (6.2.6), they will have to be entered here.
The daily variation is incorporated in 12 2-hour periods, the first period beginning at 00.00 hours and ending at 02.00 hours. The user can simply

input the relative emission strength in arbitrary quantities, and the model will normalize the 12 entered values to a percentage of the daily average. The emission daily variations entered here by the user are part of the emission data, and as such are held in the emission file.

6.2.12 **Storage of source data**

The entered source data can be stored for reuse under a file name to be specified. Otherwise the source data will be sent to a file named "**stdbrn.ops**". The model does not check whether a file under the entered name already exists, so caution is required.
A copy of a small emission file is given below:

```
tb      2    4    6    8   10   12   14   16   18   20   22   24

04      0    0    0  218  218  218  218  218  109    0    0    0
05    100  100  100  100  100  100  100  100  100  100  100  100
06    100  100  100  100  100  100  100  100  100  100  100  100

ssn    x(m)     y(m)    q (g/s)   w(mw)    h(m)    d(m)   s(m)  tb   cat area

  1   80100   435000  .100E-01    .000    10.0   2000     3.0   0    1    1 substx
  2  120640   455000  .040E-01    .000    15.0   1000     1.0   1    2    1 substx
  3  110000   472500  .130E-01    .000    20.0   2000     4.0   1    2    1 substx
  4  164000   399500  .220E-01    .000    10.0  10000     3.0   4    3    1 substx
```

Space has been reserved at the beginning of the emission file for three different emission daily variations to be specified by the user. In the above file this has been done for one of the three. The emission file contains, per source:

ssn - source sequence number
x - x-coordinate (m)
y - y-coordinate (m)
q - source strength *g/s)
w - heat content (MW)
h - height (m)
d - source diameter (m)
s - vertical spread of source height (m)
tb - code for emission time behaviour (0 - 6)

cat - source category number (1-9999)
area - country or area number (1-0000)
substx - name of the substance (not essential)

The format in which a source record is written to file is:

(i4,2i8,e10.3,f6.1,i7,f6.1,3i4,2x,a)

The easiest way to prepare a source file with a text editor, without the model, is on the basis of an existing file. The file "**stdbrn.ops**" can usually serve as a starting point.

6.3 Selection of sources from file

When sources are read in from a file, or when more than one source has been entered as described under 6.2, a number of operations on the emissions in that file can here be performed before they are used for this model run. The file as such, however, remains unaltered.

6.3.1 Emission trend correction

Emissions from the entered or existing file can be multiplied by a factor to be specified. The correction factor acts on all source categories and source areas simultaneously. The file as such remains unaltered.

6.3.2 Selection of a source category

A particular category can be selected from the emission file by giving here the source category concerned. Of course, these numbers must have been filled in when compiling the emission file (see 6.2.7). Only one source category at a time can be selected in this way.

6.3.3 Selection of country or area

As 6.3.2, but designed for area selection.

6.4 Receptor points

The places for which concentrations and depositions have to be calculated can be defined as points in a regular (cartesian) grid, or as more specific places. The latter is applicable, for example, when the user wishes to compare model results with values measured at certain locations.

6.4.1 Receptor points in a regular grid

A regular grid is defined by:

- number of grid points in x direction (max. 65)
- number of grid points in y direction (max. 65)
- dimensions of a grid cell in metres (same in x and y direction)
- the coordinates of the origin of the grid (origin is here the centre of the grid)

The above quantities determine in fact the model area for a particular application. The coordinate system in which the origin of the grid is expressed should of course be the same as that in which the locations of the sources have been given. With a single source, it is advisable to use the same coordinates for grid and source and to choose an uneven number of grid points in x and y directions, so that the source comes to lie on a receptor point. The symmetry in the calculated concentration field will then be preserved when the user is going to change the grid cell dimensions.

The OPS model distinguishes one special type of grid, which is a grid designed to calculate concentrations on the scale of the Netherlands. The top left point of the grid is fixed at 1000,620000 in the RDM system. The user has to give here only the grid cell size, and the other parameters are then calculated in such a way that the grid covers the whole of the Netherlands. The smallest grid cell size for this type of grid is about 5 km.

6.4.2 Receptor points outside the Netherlands

To perform calculations for Dutch receptor points only, it is important to exclude receptor points in other countries when using a grid. For that

purpose, a routine has been incorporated into the OPS model which can determine whether a receptor point lies within or outside the frontiers. By sending a grid specified in the above way to this routine, the grid points lying outside Dutch territory (and outside the mainland) are marked. No calculations are then performed for these marked receptor points. The points concerned are indicated in the output of the model with the number: -1.
In addition to a shorter computing time, application of this procedure also offers the advantage that an area-average concentration and deposition across the Netherlands can be calculated.

6.4.3 **Special receptor points**

Special receptor points are characterized by:

- name or number of receptor point
- x- and y-coordinates (see source coordinates)

The OPS model can handle up to 700 of these special receptor points. The data on the receptor points can be derived from:

1 - a (existing) receptor file
2 - manual input
3 - National Air Quality Monitoring Network (LML) (only possible within RIVM/LLO)

In cases 1 and 2 the user will be asked for a receptor file name, to read in or store the receptor data. The receptor file meant here can of course also be made with the text editor.

The format of receptor files is: **(i4,x,a12,2i8)**

example of a receptor file:

```
   1 Bilthoven     141900  459100
   2 Rekken        246400  457000
   3 Witteveen     241400  536900
   4 Vredepeel     187300  394700
```

In case 3 (not applicable outside RIVM/LLO) the location data from measuring stations of the LML are used. This is useful especially when the user wants to test model results against measurements which are made within the LML. The measuring stations can be selected with the following characteristics:

1 - component number (ex: 1-SO_2 4-CO 5-O_3 7-NO_2)
2 - old (up to 1-4-1986) or new monitoring network configuration
3 - station selection code (ex: 0-all stations 22-grid stations only)

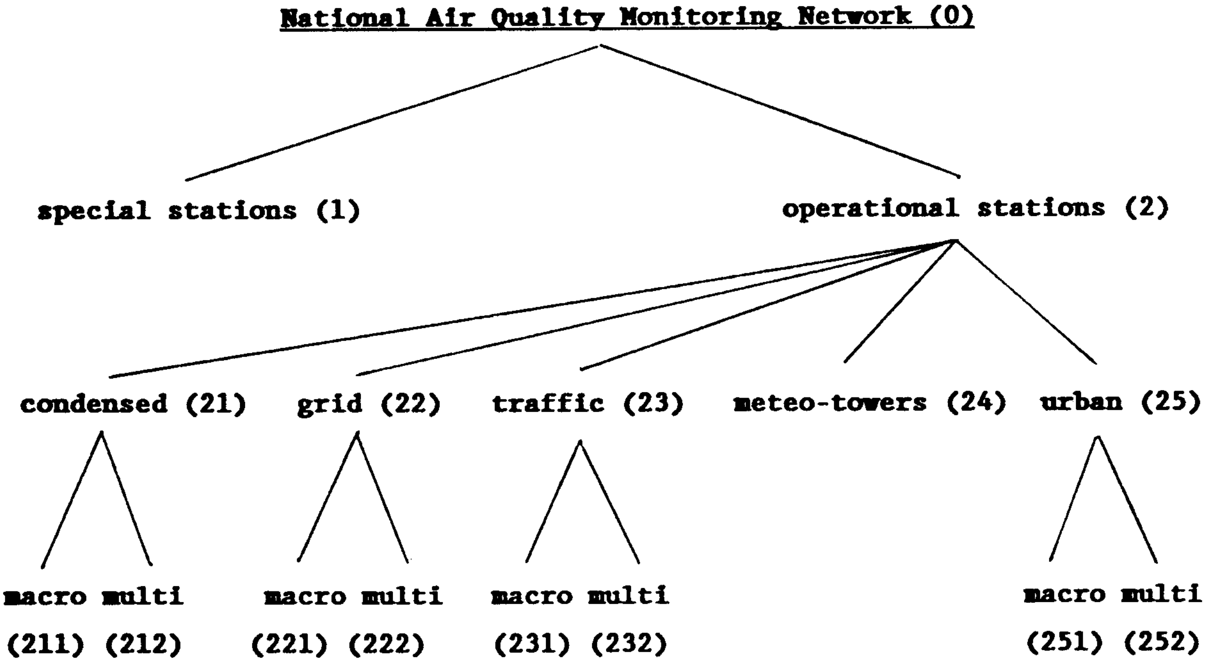


Figure 9: Summary of station selection codes of the LML

6.5 Selection of climatological data set

At present, the OPS model makes it possible to choose from the following climatological data sets:

period: - long term year
- long term summer
- long term winter

area : - the whole of the Netherlands
- 6 areas within the Netherlands (see figure 6)

area classification:

1 - Coast of Friesland-Groningen
Northern part of North-Holland
2 - North-Holland
South-Holland
Zeeland-South
3 - Drente and Environs
4 - Zeeland
5 - Twente
Gelderland
Brabant
6 - Achterhoek
Brabant-East
Limburg

As the statistics are based in all cases on data from more than one meteostation, they can be termed spatial "average" statistics. The area to be chosen is determined by the area where the source or sources are situated. If concentrations from sources spread across the Netherlands are calculated, the statistics based on meteostations throughout the Netherlands are chosen.

Apart from the above-mentioned more or less standard climatological data sets, special statistics can also be chosen, which can be statistics based on the observations from one or more specific meteostations of the LML, or statistics based on the meteorological data obtained over a period of arbitrary length (since 1 January, 1979).
These special statistics can only be made at the RIVM.

6.6 **Roughness length**

The roughness length asked for here refers to the (local) roughness of the terrain in the immediate vicinity of the source. The model only uses this roughness to influence the initial dispersion (in the same way as in the National Model).

A few representative values are (Subcommittee on Models, 1976):

- flat terrain	ca 0.03 m
- agricultural land	ca 0.10 m
- cultivated land	ca 0.30 m
- residential area	ca 1.00 m
- urban area	ca 3.00 m

The large-scale ground roughness is considered to have been taken into account in the meteostatistics used. This large-scale roughness has been set at 0.15 m for the Netherlands. Each of the various areas has a specific roughness length, which is derived from a roughness map for the Netherlands (van Dop, 1988). These roughness lengths are given below:

area:	average roughness length:
1	0.10 m
2	0.15 m
3	0.13 m
4	0.12 m
5	0.18 m
6	0.20 m

6.7 **Deposition**

6.7.1 **Dry deposition**

The dry deposition velocity is simulated in the OPS model according to the so-called resistance model:

$$V_d = (r_a + r_b + r_c)^{-1}$$

where r_a and r_b are a function of the atmospheric stability and as such have been incorporated in the meteostatistics; r_c is the resistance at the surface for the uptake of the substance.

The advantage of the above approach is that the deposition velocity can be separated into a substance-specific part and a substance-independent part. It is therefore preferable to characterize the deposition velocity of a particular substance by the surface resistance r_c, so that the deposition velocity can be differentiated according to stability class (r_a and r_b are heavily dependent on the atmospheric stability). The height for which the deposition velocity is specified in this model is 4 m.

An example of the long-term average deposition velocities associated with the stability classes used (roughness length: 0.15 m; r_c: 70 $s.m^{-1}$) is given below.

	ABC	Dl	Dm	Dh	E	F	all classes	
frequency	9.7	23.9	33.4	18.9	6.2	7.9	100	%
r_a(4m)	15	47	14	10	39	171	25	$s.m^{-1}$
r_b	19	42	15	11	34	86	47	$s.m^{-1}$
V_d(4m)	0.0096	0.0063	0.010	0.011	0.007	0.0031	0.0085	$m.s^{-1}$

When the user opts for the specification of a (average) deposition velocity, the model will estimate a corresponding r_c value using the following semi-empirical relationship:

$$r_c = V_d^{-1} - (V_d . V_d\mathrm{max})^{-0.5})$$

where $V_d$max has been set at 0.034 $m.s^{-1}$, this being the maximum achievable average deposition velocity for a source of average height and depositing in a large area.

Because of the atmospheric stability dependence of r_a and r_b, the effective deposition velocity is not the same for all source heights or source-receptor distances. Low sources, for example, produce a relatively high concentration in class F because the wind speed is low and vertical dispersion is small, while in this situation tall sources have very little influence on the local concentration on the ground because their plumes stay above the mixing layer.
The ultimate effective deposition velocity for the field of receptor points is calculated from:

$$V_d \text{ eff} = \frac{\Sigma \text{ dry deposition } (\mu g.m^{-2}.s^{-1})}{\Sigma \text{ concentration } (\mu g.m^{-3})}$$

The effective deposition velocity is included in the model output.

6.7.2 **Wet deposition**

Although the wet deposition process can be regarded as very complex, an approach has been chosen in this model in which the total process is defined by only a few substance-specific parameters. The best results can be achieved if the (measured) average ratio between rainwater concentration and air concentration of the substance to be modelled is known. The model can then relate this empirical relationship per meteoclass to: rainfall probability, rainfall intensity, shower duration, source height and mixing height.
Wet deposition may occur in two main ways:

- wash-out (from plumes below the cloud)
- rain-out (of substances taken up into cloud droplets)

In the model, wash-out occurs at a short distance from the source and rain-out at a greater distance, when the plume is situated wholly or partially in the clouds.

Wash-out is assumed to occur only for those substances which dissolve so readily in water that, when a drop passes through a plume, no saturation in the drop occurs. This is the case, for example, with HCl, HF, HNO_3 and aerosols. With less readily soluble gases, the raindrops in the cloud will become virtually saturated with the substance, so that below the cloud little more will be able to enter the drops. Wash-out of these gases is therefore not modelled separately.
Dependent on the data available to him/her, the user can specify the wet deposition velocity in three ways:

1 - As an average scavenging coefficient during rainfall ($\%.h^{-1}$).
2 - Via a scavenging ratio, this being the average ratio between rainwater concentrations and air concentrations during rainfall.
3 - Via wash-out and rain-out parameters to be given separately.

For readily soluble gases (such as halogens), the wash-out velocity D_g is calculated in the last case on the basis of a diffusion rate in air to be specified for the substance to be modelled (D_g in $cm^2.s^{-1}$) (Janssen and Ten Brink, 1985). The rain-out parameter is specified in the same way as in case 2. The model estimates the diffusion rate for cases 1 and 2 from (Durham *et al.*, 1981):

$$D_g = k\ M^{-0.5} \qquad [\ cm^2.s^{-1}]$$

where M is the molecular weight of the substance concerned and k is a conversion constant (k=1). The importance of the wash-out process is, however, assessed from the magnitude of the entered overall deposition velocity. In all cases, the wash-out velocity (averaged over the mixing height) will never be able to exceed the rain-out velocity.

The scavenging ratios which have to be fed into the model are in fact the average ratios between rainwater concentrations and air concentrations <u>during</u> showers. To enable derivation of these scavenging ratios from measurements of long-term average concentrations in rainwater and air, the following relationship has been developed (van Jaarsveld and Onderdelinden, 1986):

$$W_{emp} = \frac{H}{R \tau_w} (1 - \exp(-W \frac{R \tau_w}{H}))$$

where W_{emp} is the measured ratio between rainwater concentration and air concentration, W is the scavenging ratio during a shower, H is the mixing height (m), R is the rainfall intensity ($m.h^{-1}$), and τ_w is the average lenght of a wet period (h). This relationship has been plotted in figure 10 for average values of R, H and τ_w.

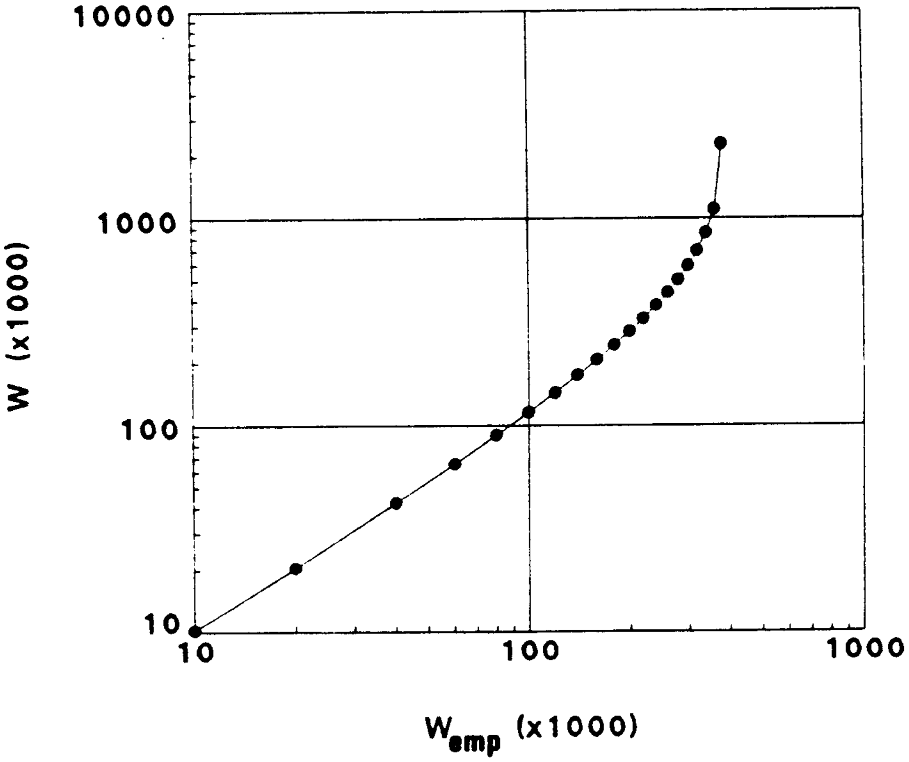
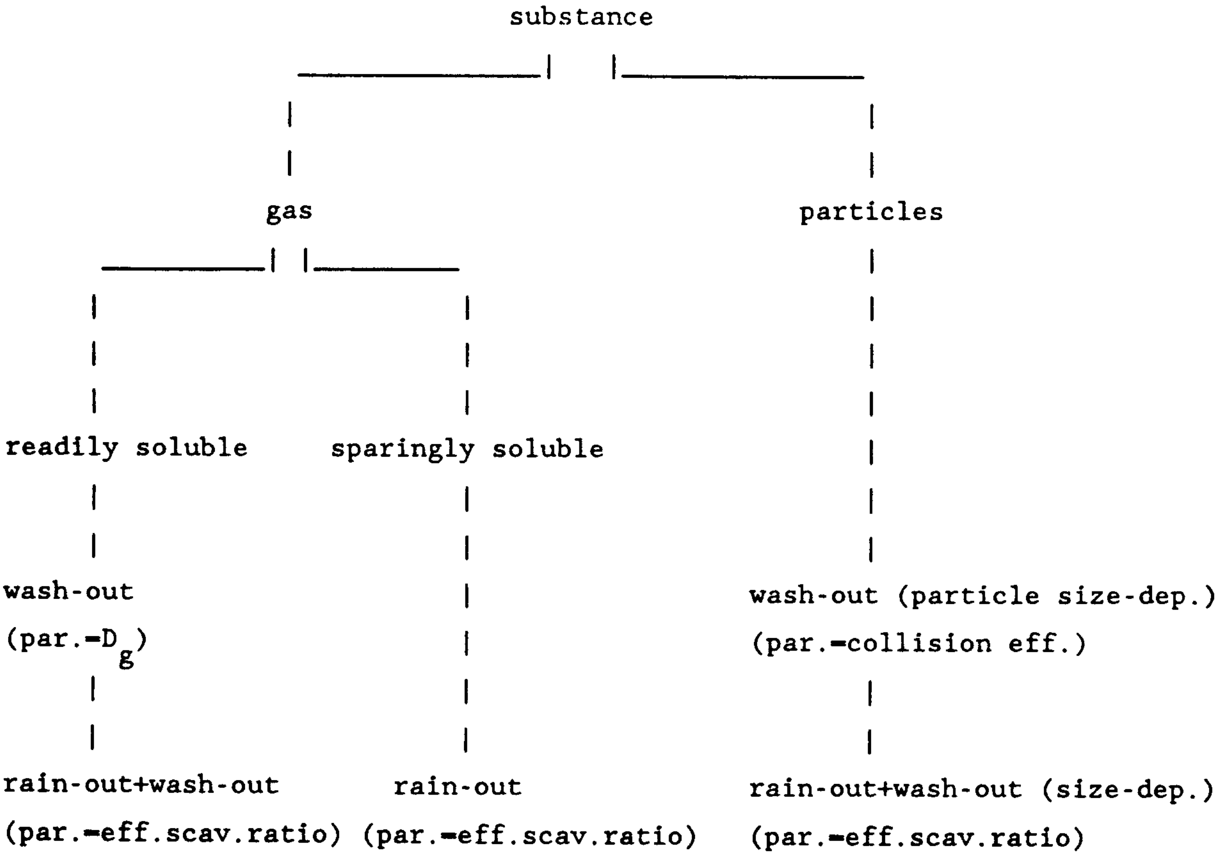


Figure 10: **Relationship between the average scavenging ratio during rainfall (W) and the scavenging ratio determined from longer term average rainwater and air concentrations (W_{emp}).**

The treatment of wet deposition by the OPS model can be represented schematically as follows:



The difference in the spatial distribution of the wet deposition between the various cases is that substances which dissolve readily in water show a maximum in the wet deposition level very close to the source, whereas the maximum for sparingly soluble substances can lie at several kilometres from the source. By way of illustration: the rainfall probability, average shower duration and rainfall intensity for the separate classes (long-term average values), as well as the resulting average wet deposition velocity for a scavenging ratio $W = 1*10^5$:

	ABC	D1	Dm	Dh	E	F	all classes	
rainfall prob.	0.6	4.3	9.0	10.0	2.0	0.9	6.0	%
shower duration	0.8	1.4	1.6	1.5	1.1	1.2	1.5	h
intensity	2.4	1.5	1.4	1.7	1.5	1.7	1.5	$mm.h^{-1}$
wet dep.velocity	0.6	2.4	2.5	1.8	1.6	0.8	2.0	$\%.h^{-1}$

6.8 Chemical conversion

This model regards conversion of the substance to be modelled into a daughter product exclusively as a loss process. The conversion rate can be given with two parameters:

a - a constant conversion rate (in $\%.h^{-1}$).
b - a variable conversion rate, dependent on the solar radiation.

b yields a conversion rate which varies from one meteoclass to another. The general expression for the conversion rate is:

$$\text{conv } [\%.h^{-1}] = a\ [\%.h^{-1}] + b\ [\%.h^{-1}.W^{-1}.m^{2}] * (\text{solar rad.})\ [W.m^{-2}]$$

The long-term average values of the solar radiation in the Netherlands are (LML, 1977-1986):

	ABC	Dl	Dm	Dh	E	F	all classes	
solar rad.	481	20	58	206	0	0	110	$W.m^{-2}$

The maximum hourly average solar radiation is about 900 $W.m^{-2}$. In view of the wind-direction dependence of the solar radiation and its variation over the day, the effective value of the conversion rate cannot be precisely determined beforehand. However, the model calculates this effective value from a mass-weighted averaging of the conversion rates of the separate classes and sources and is as such included in the model output.

6.9 Model output specification

6.9.1 Selection of unit of deposition

The unit in which calculated concentrations are given is $ug.m^{-3}$. There is no practical standard for the unit of deposition and, therefore, the possibility is offered here to choose from a number of frequently used units:

1 - mmol/m^2/s
2 - g/m^2/s
3 - mol/ha/yr
4 - kg/ha/yr
5 - mmol/m^2/yr
6 - g/m^2/yr

6.9.2 **Storage of model results**

The calculated concentration and deposition fields are incorporated into the model output in such a way that the spatial distribution becomes optically visible. This means that the figures are scaled with a certain factor in order to obtain whole figures in the 1 to 1200 range. However, these fields can also be stored separately, specifically to serve as input for further operations such as the making of maps in various shades of grey. The figures are then written to file in ASCII code in scientific notation, and each field is provided with a standard (APS) header (see appendix 2).
The following fields are stored in this manner:

1 - concentration
2 - dry deposition
3 - wet deposition
4 - total deposition

A printout of such a file has been included with the computation examples in appendix 3.
Concentrations and depositions calculated for receptor points not lying in a regular grid are written to file in another way, of which an example is given below:

```
name           x-coord y-coord     conc.  dry dep.  wet dep.  tot.dep.
                                    Lead      Lead      Lead      Lead
                     m       m     ug/m3  mol/ha/y  mol/ha/y  mol/ha/y
Vlaardingen      82000  436400  .145E+00  .167E+01  .161E+00  .183E+01
Rockanje         64500  432500  .845E-02  .432E-01  .600E-02  .492E-01
Maasdijk         75000  441800  .163E-01  .946E-01  .197E-01  .114E+00
Poortugaal       86000  430000  .183E-01  .146E+00  .250E-01  .171E+00
```

The format after the first three lines is: **(a12,2i8,4e10.3)**

6.9.3 **Printer output**

The normal model output is written to the file "**stdout.ops**" according to a standard procedure. However, the model output can also be sent to a file to be specified by the user.

N.B.: The OPS program never sends its output directly to a printer or other peripheral, but the files which have been used, including their path names, are shown on the screen. When the user is not interested in the deposition fields as such, he can leave them out in the model output. However, calculated averages and totals are always included in the output.

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Appendix 1. List of recommended parameters for substances incorporated in the model

A printout of the file "**defcomp.ops**" is shown below. This file contains the specific values of the parameters for a number of substances. Most of the substances which have been included in this list derive from earlier applications of this model or from related models such as those in the NOK/LUK project (van Egmond, 1986).

component name	sd	mol	rc	scav.rat.	dg	rev	conv(a)	conv(b)	*ref.* *)
SO2 - gas.	0	64.1	60	75000	.136	1	1.0000	.0072	*[1]*
NOx - gas.	0	46.0	600	10000	.160	0	2.0000	.0065	*[2]*
NH3 - gas.	0	17.0	30	1000000	.240	0	28.8000	.0000	*[3]*
HF(fluorine)-gas.	0	20.0	13	1000000	.230	0	.0000	.0000	*[4,5]*
F(fluorine)-aer.	1	19.0	0	0	.0	0	.0	.0	*[5]*
HCl(chlorine)-gas.	0	36.5	13	1000000	.190	0	.0000	.0000	*[4,5]*
Cl(chlorine)-aer.	1	35.5	0	0	.0	0	.0	.0	*[5]*
HBr(bromine)-gas.	0	80.9	13	1000000	.11	0	.00	.0000	*[4,5]*
Br(bromine)-aer.	1	79.9	0	0	.0	0	.0	.0	*[5]*
B(boron)-gas.	0	10.8	49	50000	.150	0	.0000	.0000	*[4,5]*
B(boron)-aer.	1	10.8	0	0	.0	0	.0	.0	*[5]*
Se(selenium)-gas.	0	79.0	49	120000	.11	0	.0000	.0000	*[5]*
Se(selenium)-aer.	1	79.0	0	0	.0	0	.0	.0	*[5]*
Hg(mercury)-gas.	0	200.6	49	120000	.071	0	.0000	.0000	*[5,7]*
Hg(mercury)-aer.	1	200.6	0	0	.0	0	.0	.0	*[5]*
C6H6(benzene)-gas	0	78.0	9999	17	.113	0	.5400	.0000	*[6]*
C7H8(toluene)-gas	0	92.0	9999	8	.104	0	2.8000	.0000	*[6]*
As(arsenic)-aer.	1	74.9	0	0	.0	0	.0	.0	*[5]*
Cd(cadmium)-aer.	1	112.4	0	0	.0	0	.0	.0	*[5]*
Cr(chromium)-aer.	2	52.0	0	0	.0	0	.0	.0	*[5]*
Cu(copper)-aer.	1	63.7	0	0	.0	0	.0	.0	*[5]*
Pb(lead)-aer.	1	207.2	0	0	.0	0	.0	.0	*[5]*
Zn(zinc)-aer.	1	65.4	0	0	.0	0	.0	.0	*[5]*

*) *references:*

[1]: Onderlinden *et al.*, 1984

[2]: van Jaarsveld, 1988

[3]: Asman and Janssen, 1987

[4]: Janssen and Ten Brink, 1985

[5]: van Jaarsveld and Onderdelinden, 1986

[6]: van Jaarsveld, 1989

[7]: See remarks about occurring Hg compounds in this appendix.

Parameters present on the list

sd : Size distribution of the aerosol, classes 1, 2 and 3. See chapter 6.1.8, table 3 and also figure 8 (sd=0 means that the substance concerned is gaseous).

mol : Molecular weight of the element or compound. See chapter 6.1.6.

If the substance is particulate, then all other deposition parameters are related to the particle size and as such implicitly present in the model. They have been marked "0" on the list for practical reasons.

rc : The surface resistance (s.m^{-1}). See chapter 6.7.1.

scav.rat. : scavenging ratio (average ratio of water concentration to air concentration at the onset of a precipitation event). See chapter 6.7.2. A scavenging ratio of 10^6 means that the wet deposition process is so efficient that the atmosphere is "washed clean" after every shower. The factor which controls the wet deposition is then the number of showers falling during a certain period.

dg : diffusion coefficient in air of the element or compound concerned (cm^2.s^{-1}). This parameter governs the washout velocity of a substance.

rev : Reversible washout or not (0=no). This parameter indicates whether material disappears again from a raindrop when this drop comes in cleaner air (e.g. below a flue gas plume).

conv(a) : Rate at which the substance is converted into a daughter product or disappears in a way other than by dry or wet deposition (%.h^{-1}); the constant fraction of this in time. See chapter 6.8.

conv(b) : As above, but the fraction of the conversion rate which can be related to the solar radiation occurring in the Netherlands. See chapter 6.8 for the use of this parameter.

Remarks concerning the list of recommended parameters.

SO_2, NO_x and NH_3

For SO_2, NO_x and NH_3, calculation of primary component only. The calculated deposition is a measure of the total deposition caused by a source of these compounds within a limited distance from the source only. It can be expected that the error is small within a distance of 20 km from the source.

NO_x

NO_x concentrations are expressed in the model as NO_2 concentrations. The emission of NO_x must therefore also be expressed in NO_2 equivalents. The parameters given are based on average ratios of NO to NO_2 in the Netherlands. In view of the fact that NO_x is initially released into the atmosphere chiefly as NO, not much value can be attached to the calculated deposition of this compound close to a source.

Hg

The parameter values given in the list are the same as those used in the NOK/LUK study (van Jaarsveld and Onderdelinden, 1986). Recent studies in Sweden (Brosset, 1986; Iverfeldt and Rodhe, 1987) suggested much lower deposition velocities. Atmospheric Hg can broadly be divided into two groups:

1. Water-insoluble Hg (metallic mercury, ($(CH_3)_2Hg$ (dimethyl mercury)).
2. Water-soluble mercury compounds (e.g. CH_3HgCl).

The compounds falling in group 2 are not very volatile and can be treated in the model as Hg aerosol. Of the water-insoluble gaseous mercury (the majority from group 1), metallic mercury can be regarded as relatively inert. Its lifetime in the atmosphere is estimated at 0.5 - 2 years (Lindqvist and Rodhe, 1985). The lifetime of dimethyl mercury is estimated to be of the order of several hours to days, its conversion into nonvolatile (water-soluble) mercury compounds or elemental mercury being the determining factor here (Iverfeldt and Lindqvist, 1986).

The above information perhaps makes clear that calculation of deposition of mercury is a precarious undertaking. The form in which the mercury is emitted, in particular, has to be known beforehand. Only then is estimation of the (wet) deposition possible. In practice, it will prove to be necessary to calculate the various compounds separately. However, this model cannot take into account the effect of conversion from one type into another.

In the practical situation it would perhaps be best - assuming an emission known exclusively as total mercury - to discount deposition losses, because elemental mercury is usually the dominant species in the emission.

Appendix 2. Description of the APS file header

To obtain an unambiguous notation of model results, the APS department of the LLO writes a standard heading above the fields in the case of model output in grid form, which gives all relevant information about the field concerned. Files thus written to disk or tape can be operated on with "standard" application programs (e.g. plot programs, grid manipulation programs).
A description of such a "standard APS header" is given below.

Described in the header are:

1. time identification
2. component identification
3. origin of the data (e.g. model version)
4. area identification

The sequence in which the data is stored in the OPS model is:

1. concentration field
2. dry deposition field
3. wet deposition field
4. total deposition field

The header comprises 120 characters. The header contains successively:

1. [i3] : year for which data is valid (if not applicable, enter the value 0)
2. [i3] : month for which data is valid (if year is not equal to zero and month=0: annual average)
3. [i3] : hour for which data is valid (if month is not equal to zero and day=0: monthly average)
4. [i3] : hour for which data is valid (if day is not equal to zero and hour=0: daily average)

(numbers 1 to 4 incl. do not apply to the OPS model)

[1x]

5. [a10] : component name

[1x]
6. [a10] : unit in which component is written to file
[1x]
7. [a10] : origin of the data (e.g. model name)
[1x]
8. [a22] : user's comments

The OPS model has used this part as follows:
[a14] : name of the quantity (concentration, dry dep., etc.)
[a8] : name of meteostatistics (file name)

[1x]
9. [a6] : format in which field is written to file (according to a standard procedure in OPS model (V1.11E): '65e9.3')
[1x]
10. [i2] : code for coordinate system:

1- amersfoort (RDM) coordinates (according to a standard procedure in OPS model)
2- geographical coordinates
3- projection onto 50 NL
4- projection onto 60 NL

[1x]
11. [f8.3] : x-coordinate top left point of the field (km)
[1x]
12. [f8.3] : y-coordinate top left point of the field (km)
13. [i3] : number of grid points in the x direction
14. [i3] : number of grid points in the y direction
[1x]
15. [f8.3] : grid cell dimension in the x direction (km)
[1x]
16. [f8.3] : grid cell dimension in the y direction (km)

Appendix 3. Calculation examples.

In this appendix three calculation examples have been worked out. The first example is a case as simple as possible, in which the user has to specify as little as possible. In the second and third case it is attempted to use the different options of the OPS model as much as possible.

A calculation example consists of:

a. problem specification
b. copies of the screen during the model run, including the interactive input session.
c. a copy of the model (printer) output
d. copies of the files generated by the model
e. when applicable: a grey scale plot of the concentration distribution made on basis of the (plotter) output file.

The data entered by the user during the interactive input part are listed in a **boldface** lettertype. Comments on details of the calculation examples have been printed in *italics*.

Calculation example 1

problem : Point source 25 m high with a heat content of 1 MW and situated in the western part of the Netherlands. This source emits continuously gaseous hydrogen fluorine (HF) with a rate of 10 g/s. Calculate the summer-average HF concentration and deposition around this source in an area of 7.5 x 7.5 km^2, with a apatial resolution of 500 m. Assume the roughness length at the source position equal to that of the climatological region. Save the calculated data in a file for possible future operations.

Copies of the screen during the use of the model are given below. Everything what is entered by the user is typed boldface.

opsmod

```
      oooooooo       oooooooo      oooooooo
    oo        oo   oo        oo   oo        oo
   oo       oo    oo       oo    oo
  oo       oo    oooooooooo      ooooooo
 oo       oo    oo                     oo
oo       oo    oo            oo       oo
 oooooooo     oo              oooooooo
```

```
This model calculates average concentrations and depositions
due to the release of a substance to ambient air by one
or more sources. Parameters which determine the dispersion
and deposition of a substance can be taken from pre-defined
values, but can also be specified by the user within wide
limits.
In all cases however, the user remains responsible for the
choice of parameters and emission strengths and the correct
interpretation of the model results.

If you accept these conditions, press "y" <cr> to continue.
```

Y

```
================================ OPS-V1.11E ================================

     ---- Welcome to the Priority Substances Model ----

A description of this model and information about the parameters
to be entered, can be found in:

     Jaarsveld J.A. van, (1990)
     An Operational atmospheric transport model for Priority Substances;
     specification and instructions for use
     Report nr. 222501002
                                        RIVM - Laboratory for Air Research
                                        P.O. Box 1
```

```
                                             3720 BA Bilthoven, The Netherlands
________________________________________________________________________________

data and parameters to run this model:

                     0 = from an (existing) input parameter file
                     1 = to be entered manually
                     2 = to be entered manually with saving
2
name of input parameter file?
examp1.inp
project name ? (max=18 char.)
calculation examp.
================================== OPS-V1.11E ==================================

which substance do you want to model?
                     0 = user specified substance
                     1 = SO2-gas.                   2 = NOx-gas.
                     3 = NH3-gas.                   4 = HF(fluorine)-gas.
                     5 = F(fluorine)-aer.           6 = HCl-gas.
                     7 = Cl-aer.                    8 = HBr(bromine)-gas.
                     9 = Br(bromine)-aer.          10 = B(boron)-gas.
                    11 = B(boron)-gas.             12 = Se(selenium)-gas.
                    13 = Se(selenium)-aer.         14 = Hg(mercury)-gas.
                    15 = Hg(mercury)-aer.          16 = C6H6(benzene)-gas
                    17 = C7H8(tolueen)-gas         18 = As(arsenic)-gas.
                    19 = Cd(cadmium)-aer.          20 = Cr(chromium)-aer.
                    21 = Cu(copper)-aer.           22 = Pb(lead)-aer.
                    23 = Zn(zinc)-aer.

4
================================== OPS-V1.11E ==================================

emission source data ?
                     0 = from an (existing) emission file
                     1 = to be specified manually
1
================================== OPS-V1.11E ==================================

source strength (annual av. in g/s)
1
heat content (MW)
1
source height (m)
25
source diameter (m) (specify 0 for point sources)

0
daily variation of the emission of this source?

                     0 = no variation (continuous emission)
                     1 = according to an av. industrial activity
                     2 = according to an av. space heating energy demand
                     3 = according to an av. traffic intensity
                     4,5 and 6 = daily variations to be specified by the user
0
source category number ? (1-9999)
1
```

```
country or area identification number ? (1-9999)
1
coordinates x and y (m) ?
0 0
enter data for another source ?
no
save the data of the source(s) in a source data file ?
yes
name of source data file ? (max. 12 characters)
exampl
================================== OPS-V1.11E ==================================

receptor points ?
                    0 = in a regular grid
                    1 = at specific positions (to be specified)
0
grid over the Netherlands (0) or special grid (1)
1
x and y coordinates of grid centre (m) ?
0 0
number of grid elements in x and y direction (max=65) ?
(normally 21 elements can be printed on one line of an A4 !)
15 15
grid resolution (m) ?
500
================================== OPS-V1.11E ==================================

selection of climatological data:

         1   111111
        11    1111333          0 = The Netherlands: total area
        11    3333333
        222 2333355            1 = N-Holland, N-Friesland, N-Groningen
       2222 33555556           2 = Randstad, W-Brabant, E-Zeeland
      22222255556666           3 = Drente, S-Friesland, S-Groningen
     42222255556666            4 = W-Zeeland, ZH-Islands
    4444225555566              5 = Mid-Brabant, Veluwe, Twente
   444222555556666             6 = S-Limburg, E-Brabant, Achterhoek
  444422      6666
              66               7 = Special climatological datafile
              666

climatological area ?
2
================================== OPS-V1.11E ==================================

selection of climatological period:

                    0 = Year............(1979-1989)
                    1 = Summer period...(1979-1989)
                    2 = Winter period...(1979-1989)

climatological period ?
1
roughness length in the source area (m) ?

                    0 = equal to roughness length in receptor area
0
```

```
================================== OPS-V1.11E ==================================

select the unit of deposition:

                    1 =  mmol/m2/s
                    2 =  g/m2/s
                    3 =  mol/ha/y
                    4 =  kg/ha/y
                    5 =  mmol/m2/y
                    6 =  g/m2/y
3
================================== OPS-V1.11E ==================================

save the model results in a [.plt] file ?
yes
name of this file ?
exampl
special printer output file ? (default=stdout.ops   )
yes
name of printer output file ?
exampl
include deposition grids also in printer output file ?
yes
```

The screen below appears after the parameter input session, sources are treated one by one.
The progress of a calculation is made visible by an activity indicator.

```
================================== OPS-V1.11E ==================================


     ========== end of input specification, start of calculations ==========

reading file with climatological data ....

statistiek van periode: 79  4  1 tot 88 10  1

initialization and reading source data ......

ssn:  1    q=.100E+02 g/s   h= 25 m  hc= 1.00 MW  d=    .0 km  HF(fluor  100%

average HF(fluorine)-gas. concentration: .88E+00 ug/m3

name of input parameter file    :exampl.inp
name of source data file        :exampl.brn
data to (plotter) file          :exampl.plt
name of printer output file     :exampl.lpt
```

end of the modelrun

Contents of the printer output file 'exampl.lpt':

```
Project: calculation examp.  subst.: HF(fluorine)-gas.    date: 07-12-90  13:22
==================================== OPS-V1.11E ===================================

concentration distribution of HF(fluorine)-gas.: ( .1E-01 ug/m3)

 20  22  24  27  31  35  40  45  50  56  57  55  55  52  49

 21  24  27  31  35  42  49  56  63  70  72  69  66  62  55

 23  26  30  34  41  49  60  70  83  91  90  88  81  71  62

 26  29  33  39  48  58  76  91 113 124 122 113  95  83  70

 30  33  39  45  55  70  92 121 159 180 168 138 116  94  78

 33  38  46  54  64  78 104 159 244 276 220 172 131 101  80

 36  43  53  65  81  94  98 148 422 397 266 183 135 105  82

 40  48  60  77 102 137 147   0 364 363 249 173 126  96  76

 42  51  65  82 112 162 215 169 286 260 197 147 114  90  72

 42  52  66  86 113 151 177 185 224 197 161 127 101  81  65

 43  52  64  80 102 121 133 139 152 146 126 105  87  72  60

 42  49  59  72  84  94 100 103 109 109  98  86  73  63  54

 40  46  54  61  68  74  77  79  83  82  77  69  62  54  48

 38  43  47  52  56  60  61  62  65  64  62  57  52  47  43

 35  39  42  45  47  49  50  50  52  51  50  48  45  41  38

grid cell dimension  :   .500 km
number of grid points:  15x15
top left coordinates :   -3.500,    3.500 km

average HF(fluorine)-gas. concentration: .88E+00 ug/m3
```

```
Project: calculation examp.  subst.: HF(fluorine)-gas.    date: 07-12-90  13:22
================================== OPS-V1.11E =================================

dry deposition distribution (as HF(fluorine)-gas.): ( .1E+01 mol/ha/y )

 36  41  47  54  66  79  94 107 121 138 144 151 150 143 133

 40  45  53  62  77  96 117 137 157 180 190 195 187 173 155

 44  51  60  72  87 114 148 179 216 246 261 256 235 208 183

 51  57  68  83 105 138 190 244 312 354 369 338 291 252 215

 60  69  81  97 125 165 242 345 476 564 526 442 368 300 241

 68  82 101 124 149 198 290 500 813 906 741 576 426 318 248

 78  96 122 158 207 260 308 52115161434 910 605 424 314 242

 90 114 148 200 282 414 499   013361220 800 541 386 288 223

 97 122 162 220 320 508 717 5931005 850 615 435 324 248 195

 98 125 165 224 310 433 538 578 721 610 474 365 282 223 176

 98 124 157 203 265 330 371 397 451 430 361 292 236 193 159

 95 115 142 177 213 242 263 278 304 307 272 233 195 164 140

 89 105 126 147 169 183 194 203 219 222 208 184 161 140 121

 82  95 108 122 133 143 148 154 165 165 162 148 133 119 106

 75  83  93 100 107 113 117 121 128 128 127 121 112 101  92

grid cell dimension   :   .500 km
number of grid points:  15x15
top left coordinates :   -3.500,    3.500 km

average dry deposition             :  .25E+03 mol/ha/y
effective dry deposition velocity :    1.822 cm/s (calc. from dry dep. and conc.
total dry deposition               :  .91E+00 g/s  (in the selected field)
```

```
Project: calculation examp.  subst.: HF(fluorine)-gas.    date: 07-12-90  13:22
================================== OPS-V1.11E ==================================

wet deposition distribution (as HF(fluorine)-gas.): ( .1E+01 mol/ha/y )

   6   6   7   9   9  11  13  14  16  18  19  18  18  17  15

   6   6   7   9  10  13  15  17  19  21  23  21  20  18  16

   5   6   7   9  11  13  17  20  24  27  26  25  22  19  15

   5   6   7   9  11  14  21  26  31  35  32  28  21  18  16

   5   6   7   8  11  16  26  35  44  46  39  28  23  18  15

   5   5   6   8  10  17  31  55  75  62  40  29  22  17  15

   4   5   6   8  11  17  35 111 130  62  38  27  21  19  15

   4   5   5   7   9  15  30   0 113  55  35  25  20  16  14

   4   4   5   6   8  12  25  55  57  41  29  22  18  16  14

   3   4   5   6   8  12  20  27  26  27  23  19  16  14  12

   3   4   5   6   8  11  16  17  16  17  17  16  14  13  11

   3   4   5   6   8  10  12  13  12  12  13  13  12  11  10

   4   4   5   6   7   9  10  10  10  10  10  10  11  10  10

   4   4   5   6   7   8   8   8   9   8   8   9   9   9   9

   4   4   5   6   6   7   7   7   8   7   7   8   8   8   8

grid cell dimension  :   .500 km
number of grid points:  15x15
top left coordinates :   -3.500,     3.500 km

average wet deposition         :  .17E+02 mol/ha/y
effective wet deposition rate:     2.322 %/h   (mass weighted)
total wet deposition           :  .59E-01 g/s   (within selected field)
annual precipitation amount    :       699 mm   (av. in climatological area)
```

<u>Remark</u> 1: *From the emitted 10 g/s HF, 0.91 g/s will be deposited in the selected area and 0.059 g/s as wet deposition.*

<u>Remark</u> 2: *The selected grid cell dimension of 500 m is obviously too large to determine the wet deposition maximum. For substances which are well water soluble this maximum will be situated very close to the source. Wet deposition maxima as calculated with this model and reported, have always been specified as the average of an area of 1x1 km^2.*

```
Project: calculation examp.  subst.: HF(fluorine)-gas.    date: 07-12-90  13:22
================================== OPS-V1.11E =================================

emission source data:

ssn    x(m)     y(m)    q  (g/s) hc(MW)  h(m)   d(m)   s(m)  tb cat area subst.
--- ------- ------- --------- ------ ----- ------ ----- --- --- ---- --------
  1       0       0 .100E+02  1.000  25.0      0    .0   0   1    1 HF(fluorine


z0   : .15 m    seasonal temp. corr.: .34    emission trend corr.:1.00

climatological area   : 2 = Randstad, W-Brabant, E-Zeeland
climatological period: 1 = Summer period...(1979-1989)

name of input parameter file      :exampl.inp
name of emission data file        :exampl.brn
name of climatological data file :\usr\hans\ops\meteosta\k2zolt
data to (plotter) file            :exampl.plt
name of printer output file       :exampl.lpt

HF(fluorine)-gas. considered as gaseous

average dry HF(fluorine)-gas. deposition: .25E+03 mol/ha/y
average wet HF(fluorine)-gas. deposition: .17E+02 mol/ha/y

eff. chem. conv. rate :  .00 %/h
eff. wet dep. rate    : 2.32 %/h
eff. dry dep. velocity: 1.82 cm/s

mean diurnal concentration distribution HF(fluorine)-gas. in ug/m3 :

     1- 2       3- 4       5- 6       7- 8       9-10      11-12
    -----      -----      -----      -----      -----      -----
  .81E+00    .82E+00    .94E+00    .10E+01    .90E+00    .85E+00

    13-14      15-16      17-18      19-20      21-22      23-24
    -----      -----      -----      -----      -----      -----
  .86E+00    .84E+00    .86E+00    .98E+00    .89E+00    .82E+00
```

```
Project: calculation examp.  subst.: HF(fluorine)-gas.    date: 07-12-90  13:22
================================ OPS-V1.11E =================================

input parameters:                 (file=exampl.inp        )

j                   *acceptance of user conditions
0                   *save input parameters
exampl.inp           name of input parameter file
calculation examp.   project name
 4                  *substance to model (0=user spec. 1=SO2 2=NOx 3=NH3)
1                   *emission data (0=from data file 1=manually entered)
.100E+02             source strenght (g/s)
  1.000              heat content (MW)
  25.0               source height (m)
      0             *source diameter (m)
0                    daily var. of emiss. (0=cont. 1=ind. 2=sp.h. 3=tr. 4,5,6=o
   1                 source category number
   1                 country or area identification number
 0000000  0000000    coordinates x and y (m)
0                   *enter another source ?
1                   *save the data of the source(s) in a source data file ?
exampl.brn           name of source data file ?
0                   *gridded receptor points(=0) or spec. positions(=1) ?
1                   *grid over the Netherlands(=0) or special grid(=1) ?
 0000000  0000000   *x and y coordinates of grid centre (m) ?
 15 15               number of grid elements in x and y direction
   500               grid resolution (m)
 2                   climatological area (0 t/m 7)
 1                   climatological period (0 t/m 2)
 .000                roughness length in m (0=equal to receptor area)
3                    select the unit of deposition
1                   *save the model results in a [.plt] file ?
exampl.plt           file name for saving conc. and dep. grids?
1                   *special printer output file ?
exampl.lpt           name of printer output file ?
1                    deposition grids also in printer output file ?


warning: when re-using this input file, do not change the parameters
         marked with a * !
```

The (plotter) file 'exampl.plt':

```
 0  0  0  0 HF(fluorin      ug/m3 OPS-V1.11E concentration k2zolt   65e9.3  1   -3.750    3.750 15 15     .500      .500
.195E+00 .216E+00 .243E+00 .274E+00 .307E+00 .354E+00 .400E+00 .451E+00 .505E+00 .559E+00 .571E+00 .554E+00 .546E+00 .52
.214E+00 .236E+00 .268E+00 .307E+00 .351E+00 .420E+00 .485E+00 .557E+00 .634E+00 .696E+00 .723E+00 .690E+00 .661E+00 .61
.234E+00 .262E+00 .295E+00 .345E+00 .411E+00 .490E+00 .603E+00 .705E+00 .829E+00 .908E+00 .898E+00 .876E+00 .811E+00 .71
.262E+00 .291E+00 .333E+00 .390E+00 .479E+00 .580E+00 .756E+00 .914E+00 .113E+01 .124E+01 .122E+01 .113E+01 .950E+00 .82
.296E+00 .334E+00 .386E+00 .451E+00 .549E+00 .697E+00 .921E+00 .121E+01 .159E+01 .180E+01 .168E+01 .138E+01 .116E+01 .94
.325E+00 .379E+00 .457E+00 .545E+00 .638E+00 .780E+00 .104E+01 .159E+01 .244E+01 .276E+01 .220E+01 .172E+01 .131E+01 .10
.364E+00 .433E+00 .528E+00 .650E+00 .805E+00 .941E+00 .984E+00 .148E+01 .422E+01 .397E+01 .266E+01 .183E+01 .135E+01 .10
.397E+00 .483E+00 .603E+00 .774E+00 .102E+01 .137E+01 .147E+01 .000E+00 .364E+01 .363E+01 .249E+01 .173E+01 .126E+01 .96
.425E+00 .512E+00 .648E+00 .823E+00 .112E+01 .162E+01 .215E+01 .169E+01 .286E+01 .260E+01 .197E+01 .147E+01 .114E+01 .89
.422E+00 .516E+00 .657E+00 .856E+00 .113E+01 .151E+01 .177E+01 .185E+01 .224E+01 .197E+01 .161E+01 .127E+01 .101E+01 .80
.426E+00 .521E+00 .637E+00 .798E+00 .102E+01 .121E+01 .133E+01 .139E+01 .152E+01 .146E+01 .126E+01 .105E+01 .868E+00 .71
.418E+00 .494E+00 .594E+00 .724E+00 .839E+00 .935E+00 .997E+00 .103E+01 .109E+01 .109E+01 .980E+00 .856E+00 .731E+00 .62
.401E+00 .463E+00 .543E+00 .615E+00 .682E+00 .735E+00 .770E+00 .790E+00 .826E+00 .822E+00 .773E+00 .691E+00 .616E+00 .54
.380E+00 .430E+00 .474E+00 .520E+00 .562E+00 .597E+00 .610E+00 .623E+00 .649E+00 .636E+00 .616E+00 .572E+00 .523E+00 .47
.355E+00 .385E+00 .417E+00 .447E+00 .468E+00 .487E+00 .496E+00 .504E+00 .521E+00 .512E+00 .504E+00 .481E+00 .446E+00 .41
 0  0  0  0 HF(fluorin  mol/ha/y  OPS-V1.11E dry dep.      k2zolt   65e9.3  1   -3.750    3.750 15 15     .500      .500
.357E+02 .406E+02 .467E+02 .538E+02 .663E+02 .793E+02 .938E+02 .107E+03 .121E+03 .138E+03 .144E+03 .151E+03 .150E+03 .14
.396E+02 .453E+02 .528E+02 .619E+02 .767E+02 .959E+02 .117E+03 .137E+03 .157E+03 .180E+03 .190E+03 .195E+03 .187E+03 .17
.437E+02 .507E+02 .596E+02 .715E+02 .872E+02 .114E+03 .148E+03 .179E+03 .216E+03 .246E+03 .261E+03 .256E+03 .235E+03 .20
.511E+02 .574E+02 .679E+02 .832E+02 .105E+03 .138E+03 .190E+03 .244E+03 .312E+03 .354E+03 .369E+03 .338E+03 .291E+03 .25
.599E+02 .693E+02 .813E+02 .970E+02 .125E+03 .165E+03 .242E+03 .345E+03 .476E+03 .564E+03 .526E+03 .442E+03 .368E+03 .30
.683E+02 .823E+02 .101E+03 .124E+03 .149E+03 .198E+03 .290E+03 .500E+03 .813E+03 .906E+03 .741E+03 .576E+03 .426E+03 .31
.779E+02 .965E+02 .122E+03 .158E+03 .207E+03 .260E+03 .308E+03 .521E+03 .152E+04 .143E+04 .910E+03 .605E+03 .424E+03 .31
.898E+02 .114E+03 .148E+03 .200E+03 .282E+03 .414E+03 .499E+03 .000E+00 .134E+04 .122E+04 .800E+03 .541E+03 .386E+03 .28
.967E+02 .122E+03 .162E+03 .220E+03 .320E+03 .508E+03 .717E+03 .593E+03 .100E+04 .850E+03 .615E+03 .435E+03 .324E+03 .24
.980E+02 .125E+03 .165E+03 .224E+03 .310E+03 .433E+03 .538E+03 .578E+03 .721E+03 .610E+03 .474E+03 .365E+03 .282E+03 .22
.982E+02 .124E+03 .157E+03 .203E+03 .265E+03 .330E+03 .371E+03 .397E+03 .451E+03 .430E+03 .361E+03 .292E+03 .236E+03 .19
.946E+02 .115E+03 .142E+03 .177E+03 .213E+03 .242E+03 .263E+03 .278E+03 .304E+03 .307E+03 .272E+03 .233E+03 .195E+03 .16
.886E+02 .105E+03 .126E+03 .147E+03 .169E+03 .183E+03 .194E+03 .203E+03 .219E+03 .222E+03 .208E+03 .184E+03 .161E+03 .14
.820E+02 .948E+02 .108E+03 .122E+03 .133E+03 .143E+03 .148E+03 .154E+03 .165E+03 .165E+03 .162E+03 .148E+03 .133E+03 .11
.747E+02 .835E+02 .931E+02 .100E+03 .107E+03 .113E+03 .117E+03 .121E+03 .128E+03 .128E+03 .127E+03 .121E+03 .112E+03 .10
 0  0  0  0 HF(fluorin  mol/ha/y  OPS-V1.11E wet dep.      k2zolt   65e9.3  1   -3.750    3.750 15 15     .500      .500
.552E+01 .626E+01 .733E+01 .866E+01 .944E+01 .115E+02 .128E+02 .144E+02 .162E+02 .178E+02 .190E+02 .178E+02 .178E+02 .16
.553E+01 .637E+01 .736E+01 .875E+01 .970E+01 .125E+02 .146E+02 .167E+02 .191E+02 .210E+02 .226E+02 .211E+02 .198E+02 .18
.538E+01 .624E+01 .735E+01 .867E+01 .109E+02 .133E+02 .172E+02 .201E+02 .237E+02 .267E+02 .257E+02 .246E+02 .220E+02 .18
.517E+01 .590E+01 .702E+01 .868E+01 .109E+02 .143E+02 .214E+02 .255E+02 .312E+02 .347E+02 .324E+02 .281E+02 .214E+02 .18
.496E+01 .571E+01 .672E+01 .817E+01 .111E+02 .158E+02 .260E+02 .352E+02 .444E+02 .461E+02 .391E+02 .278E+02 .226E+02 .18
.468E+01 .548E+01 .640E+01 .810E+01 .105E+02 .170E+02 .307E+02 .547E+02 .750E+02 .620E+02 .397E+02 .287E+02 .219E+02 .17
.445E+01 .507E+01 .603E+01 .760E+01 .108E+02 .170E+02 .353E+02 .111E+03 .130E+03 .621E+02 .381E+02 .268E+02 .210E+02 .18
.400E+01 .461E+01 .548E+01 .691E+01 .946E+01 .147E+02 .296E+02 .000E+00 .113E+03 .549E+02 .352E+02 .254E+02 .196E+02 .16
.379E+01 .403E+01 .465E+01 .558E+01 .767E+01 .120E+02 .253E+02 .546E+02 .568E+02 .407E+02 .291E+02 .223E+02 .183E+02 .15
.332E+01 .381E+01 .452E+01 .569E+01 .765E+01 .122E+02 .202E+02 .270E+02 .259E+02 .272E+02 .230E+02 .189E+02 .160E+02 .13
.337E+01 .393E+01 .450E+01 .567E+01 .780E+01 .114E+02 .158E+02 .174E+02 .163E+02 .170E+02 .174E+02 .157E+02 .143E+02 .12
.339E+01 .393E+01 .467E+01 .587E+01 .771E+01 .952E+01 .120E+02 .127E+02 .118E+02 .122E+02 .126E+02 .131E+02 .122E+02 .11
.352E+01 .412E+01 .483E+01 .593E+01 .733E+01 .856E+01 .975E+01 .100E+02 .961E+01 .968E+01 .102E+02 .102E+02 .107E+02 .10
.365E+01 .416E+01 .491E+01 .580E+01 .664E+01 .791E+01 .835E+01 .847E+01 .869E+01 .805E+01 .830E+01 .877E+01 .926E+01 .91
.365E+01 .422E+01 .490E+01 .551E+01 .637E+01 .717E+01 .737E+01 .741E+01 .759E+01 .698E+01 .719E+01 .765E+01 .772E+01 .80
 0  0  0  0 HF(fluorin  mol/ha/y  OPS-V1.11E total dep.    k2zolt   65e9.3  1   -3.750    3.750 15 15     .500      .500
.412E+02 .468E+02 .541E+02 .624E+02 .757E+02 .907E+02 .107E+03 .122E+03 .137E+03 .155E+03 .163E+03 .169E+03 .168E+03 .15
.451E+02 .516E+02 .601E+02 .707E+02 .864E+02 .108E+03 .132E+03 .153E+03 .177E+03 .201E+03 .212E+03 .216E+03 .207E+03 .19
.491E+02 .569E+02 .669E+02 .802E+02 .980E+02 .127E+03 .166E+03 .199E+03 .239E+03 .272E+03 .287E+03 .281E+03 .257E+03 .22
.563E+02 .633E+02 .750E+02 .919E+02 .116E+03 .152E+03 .212E+03 .269E+03 .343E+03 .388E+03 .401E+03 .366E+03 .313E+03 .27
.649E+02 .750E+02 .880E+02 .105E+03 .136E+03 .181E+03 .268E+03 .380E+03 .521E+03 .610E+03 .565E+03 .470E+03 .390E+03 .31
.730E+02 .878E+02 .108E+03 .132E+03 .159E+03 .215E+03 .321E+03 .554E+03 .888E+03 .968E+03 .781E+03 .605E+03 .448E+03 .33
```

```
.823E+02 .102E+03 .128E+03 .165E+03 .218E+03 .277E+03 .343E+03 .632E+03 .165E+04 .150E+04 .948E+03 .632E+03 .445E+03 .33
.938E+02 .118E+03 .153E+03 .207E+03 .291E+03 .428E+03 .529E+03 .000E+00 .145E+04 .127E+04 .836E+03 .566E+03 .406E+03 .30
.100E+03 .126E+03 .167E+03 .226E+03 .328E+03 .520E+03 .743E+03 .648E+03 .106E+04 .890E+03 .645E+03 .458E+03 .342E+03 .26
.101E+03 .128E+03 .170E+03 .230E+03 .317E+03 .445E+03 .558E+03 .605E+03 .747E+03 .637E+03 .497E+03 .384E+03 .298E+03 .23
.102E+03 .128E+03 .161E+03 .208E+03 .273E+03 .342E+03 .387E+03 .414E+03 .468E+03 .447E+03 .378E+03 .308E+03 .250E+03 .20
.980E+02 .119E+03 .147E+03 .183E+03 .221E+03 .252E+03 .275E+03 .291E+03 .316E+03 .319E+03 .284E+03 .246E+03 .207E+03 .17
.921E+02 .109E+03 .131E+03 .153E+03 .176E+03 .192E+03 .204E+03 .213E+03 .229E+03 .231E+03 .218E+03 .195E+03 .172E+03 .15
.857E+02 .990E+02 .113E+03 .128E+03 .139E+03 .151E+03 .157E+03 .163E+03 .173E+03 .173E+03 .170E+03 .157E+03 .142E+03 .12
.783E+02 .877E+02 .981E+02 .106E+03 .114E+03 .121E+03 .124E+03 .128E+03 .135E+03 .135E+03 .134E+03 .129E+03 .119E+03 .10
```

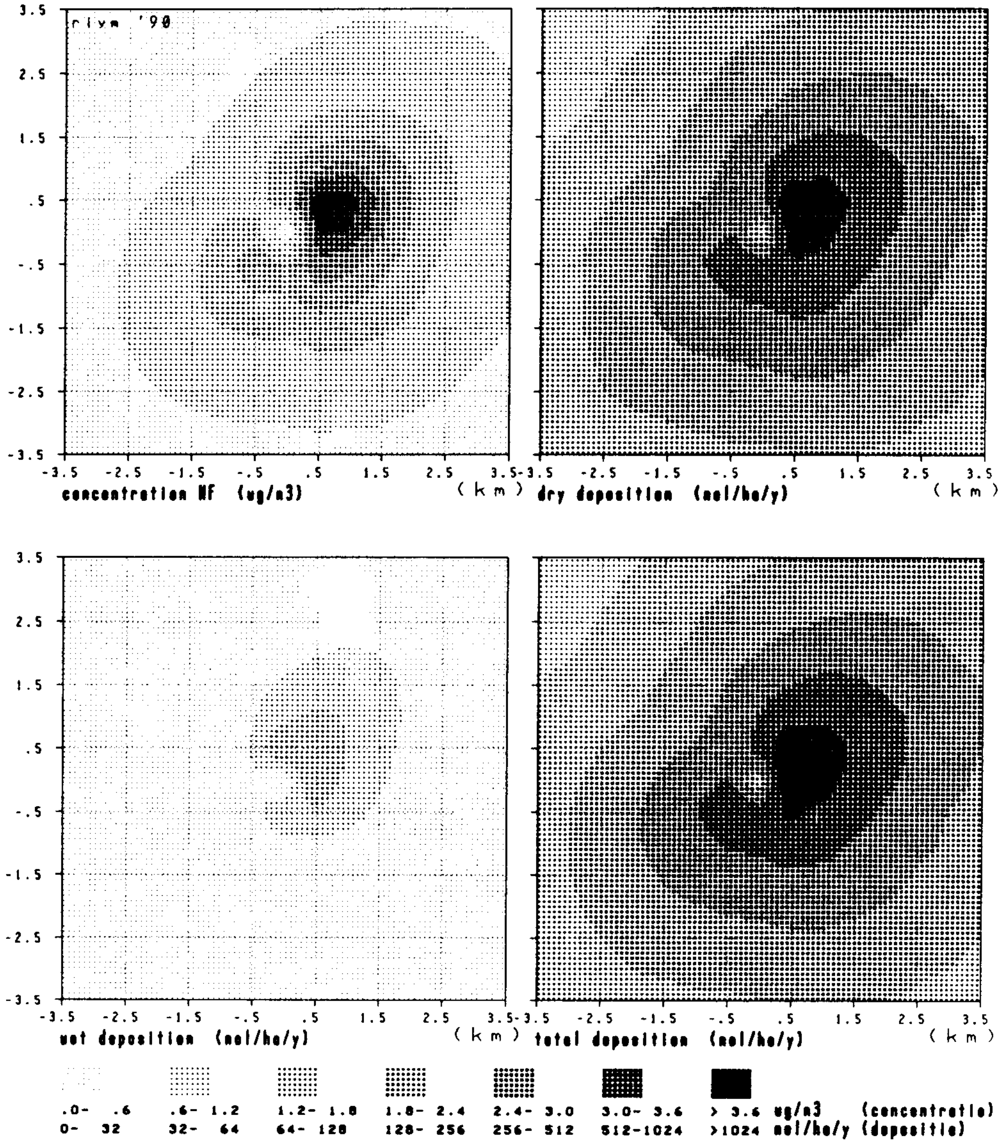
The emission data file exampl.brn':

```
tb   2   4   6   8  10  12  14  16  18  20  22  24

04 100 100 100 100 100 100 100 100 100 100 100 100
05 100 100 100 100 100 100 100 100 100 100 100 100
06 100 100 100 100 100 100 100 100 100 100 100 100

 ssn    x(m)    y(m)   q (g/s) hc(MW)  h(m)    d(m)  s(m)  tb cat area

   1       0       0  .100E+02  1.000  25.0       0    .0   0   1    1 HF(fluorine)-g
```



Graphic representation of results of example 1

Calculation example 2

problem : Area source of ammonia (NH_3) situated in Drente, 5 x 5 km^2 (square), mean heigth 1 m and vertical distribution of emissions (sd) 0 m. The emission rate of this source in on average 5 g/s, but is during the day about three times higher than during the night. The surface resistance r_c in this area is 20 s/m, the scavenging ratio of NH_3 is estimated in this case at 3.10^5 and the diffusion velocity in air at 0.23 $cm^2.s^{-1}$. The conversion rate of NH_3 to NH_4^+ is estimated to be 20 $\%.h^{-1}$ continuously plus a radiation dependent part of 10 $\%.h^{-1}$.

Calculate the yearly average NH_3-concentration and -deposition around this source in an area of 9 x 9 km^2, with a spatial resolution of 500 m. Assume the roughness length at the source position equal to that of the climatological region. Save the calculated data in a file for possible future operations.

Copies of the screen during the use of the model are given below. Everything what is entered by the user is typed boldface.

```
opsmod
--------------------------------------------------------------------------
                       oooooooo      oooooooo      oooooooo
                     oo       oo   oo       oo   oo       oo
                    oo       oo   oo       oo   oo
                   oo       oo   oooooooooo      ooooooo
                  oo       oo   oo                     oo
                 oo       oo   oo            oo       oo
                  oooooooo    oo              oooooooo
--------------------------------------------------------------------------

      This model calculates average concentrations and depositions
      due to the release of a substance to ambient air by one
      or more sources. Parameters which determine the dispersion
      and deposition of a substance can be taken from pre-defined
      values, but can also be specified by the user within wide
      limits.
      In all cases however, the user remains responsible for the
      choice of parameters and emission strengths and the correct
      interpretation of the model results.

      If you accept these conditions, press "y" <cr> to continue.

Y

================================ OPS-V1.11E ================================

         ---- Welcome to the Priority Substances Model ----
```

```
A description of this model and information about the parameters
to be entered, can be found in:

      Jaarsveld J.A. van, (1990)
      An Operational atmospheric transport model for Priority Substances;
      specification and instructions for use
      Report nr. 222501002
                                    RIVM - Laboratory for Air Research
                                    P.O. Box 1
                                    3720 BA Bilthoven, The Netherlands
______________________________________________________________________________

data and parameters to run this model:

                    0 = from an (existing) input parameter file
                    1 = to be entered manually
                    2 = to be entered manually with saving
2
name of input parameter file?
examp2
project name ? (max=18 char.)
calculation examples
================================= OPS-V1.11E =================================

which substance do you want to model?
                    0 = user specified substance
                    1 = SO2-gas.                      2 = NOx-gas.
                    3 = NH3-gas.                      4 = HF(fluorine)-gas.
                    5 = F(fluorine)-aer.              6 = HCl-gas.
                    7 = Cl-aer.                       8 = HBr(bromine)-gas.
                    9 = Br(bromine)-aer.             10 = B(boron)-gas.
                   11 = B(boron)-gas.                12 = Se(selenium)-gas.
                   13 = Se(selenium)-aer.            14 = Hg(mercury)-gas.
                   15 = Hg(mercury)-aer.             16 = C6H6(benzene)-gas
                   17 = C7H8(tolueen)-gas            18 = As(arsenic)-gas.
                   19 = Cd(cadmium)-aer.             20 = Cr(chromium)-aer.
                   21 = Cu(copper)-aer.              22 = Pb(lead)-aer.
                   23 = Zn(zinc)-aer.

0
================================= OPS-V1.11E =================================

name of the substance? (max=18 char.)
NH3
molecular weight of  NH3 ?
17
 NH3 to consider as ?
                    0 = particle bounded
                    1 = gaseous
1
================================= OPS-V1.11E =================================

emission source data ?
                    0 = from an (existing) emission file
                    1 = to be specified manually
1
```

```
================================ OPS-V1.11E ================================

source strength (annual av. in g/s)
5
heat content (MW)
0
source height (m)
1
source diameter (m) (specify 0 for point sources)
5000
std. dev. of emission heights within area source (m)
0
daily variation of the emission of this source?

                    0 = no variation (continuous emission)
                    1 = according to an av. industrial activity
                    2 = according to an av. space heating energy demand
                    3 = according to an av. traffic intensity
                    4,5 and 6 = daily variations to be specified by the user
4
source category number ? (1-9999)
1
country or area identification number ? (1-9999)
1
coordinates x and y (m) ?
0 0
enter data for another source ?
no
specify daily emission variation nr. 4 in 12 (2 hourly) steps
   2   4   6   8  10  12  14  16  18  20  22  24
  21  17  42  83 145 166 187 187 145 104  62  42
save the data of the source(s) in a source data file ?
yes
name of source data file ? (max. 12 characters)
examp2
================================ OPS-V1.11E ================================

receptor points ?
                    0 = in a regular grid
                    1 = at specific positions (to be specified)
0
grid over the Netherlands (0) or special grid (1)
1
x and y coordinates of grid centre (m) ?
0 0
number of grid elements in x and y direction (max=65) ?
(normally 21 elements can be printed on one line of an A4 !)
19 19
grid resolution (m) ?
500
```

```
================================== OPS-V1.11E =================================

selection of climatological data:

         1   111111
        11    1111333     0 = The Netherlands: total area
        11    3333333
        222 2333355       1 = N-Holland, N-Friesland, N-Groningen
       2222 33555556      2 = Randstad, W-Brabant, E-Zeeland
      22222255556666      3 = Drente, S-Friesland, S-Groningen
     42222255556666       4 = W-Zeeland, ZH-Islands
    4444225555566         5 = Mid-Brabant, Veluwe, Twente
   444222555556666        6 = S-Limburg, E-Brabant, Achterhoek
  444422     6666
              66          7 = Special climatological datafile
              666

climatological area ?
3
================================== OPS-V1.11E =================================

selection of climatological period:

                    0 = Year............(1979-1989)
                    1 = Summer period...(1979-1989)
                    2 = Winter period...(1979-1989)

climatological period ?
0
roughness length in the source area (m) ?

                    0 = equal to roughness length in receptor area
0
account also for deposition and conversion ?
1
================================== OPS-V1.11E =================================

specify dry deposition through:
                    1 = a deposition velocity (vd)
                    2 = a surface resistance (rc)

2
surface resistance (s/m) ?
20
================================== OPS-V1.11E =================================

specification of wet deposition through:
                    1 = an average scavenging coeff. during prec. events
                    2 = an average scavenging ratio (conc.in prec./conc.in air)
                    3 = a wash-out and a rain-out process separately specified

3
average ratio conc.in prec./conc.in air ?

300000
diffusion coefficient in air of  NH3 (cm2/s) ?

>>> this diff. coeff. determines the rate of the
```

```
>>> wash-out process close to the source

.23
is the wash-out process reversible ?

>>> the wash-out process is considered either as
>>> fully irreversible (most of the substances) or
>>> fully reversible (eg. SO2).
>>> In case of reversible wash-out it is assumed
>>> that there is no wash-out when the plume causes
>>> no concentration at ground-level

no
================================= OPS-V1.11E =================================

conversion rates a and b of  NH3 in air according to:

conv. [%/h] = a [%/h] + b [%/h/W.m2] * glob.rad. [W/m2]

>>> glob. rad. at noon in the Netherlands, max. :~ 900 W/m2
>>> glob. rad. in the Netherlands, long term av.:~ 108 W/m2

20 .09
================================= OPS-V1.11E =================================

select the unit of deposition:

                    1 =  mmol/m2/s
                    2 =  g/m2/s
                    3 =  mol/ha/y
                    4 =  kg/ha/y
                    5 =  mmol/m2/y
                    6 =  g/m2/y
3
================================= OPS-V1.11E =================================

save the model results in a [.plt] file ?
yes
name of this file
examp2
special printer output file ? (default=stdout.ops  )
yes
name of printer output file ?
examp2
include deposition grids also in printer output file ?
yes
```

```
================================= OPS-V1.11E =================================
```

The screen below appears after the parameter input session, sources are treated one by one.
The progress of a calculation is made visible by an activity indicator.

```
     ========== end of input specification, start of calculations ==========

reading file with climatological data ....

statistiek van periode: 79  1  1 tot 89  1  1

initialization and reading source data ......

ssn:   1    q=.500E+01 g/s   h=  1 m  hc=  .00 MW  d=   5.0 km   NH3      100%

average  NH3 concentration: .99E+00 ug/m3

name of input parameter file   :examp2.inp
name of source data file       :examp2.brn
data to (plotter) file         :examp2.plt
name of printer output file    :examp2.lpt
```

```
Project: calculation examp.  subst.:  NH3                  date: 07-12-90  13:29
================================== OPS-V1.11E ==================================

concentration distribution of  NH3: ( .1E-01 ug/m3)

  6   7   8   9  10  12  14  15  17  18  19  20  18  18  17  16  15  14  12

  7   8  10  11  13  16  19  21  23  25  26  26  24  24  22  20  18  16  14

  8  10  13  15  18  22  27  32  34  37  39  36  34  32  29  26  23  18  15

  8  11  15  22  27  35  44  54  60  65  65  58  54  49  43  38  27  21  17

  9  12  17  27  98 143 186 236 230 241 243 236 212 190 153  44  30  23  18

 10  14  20  32 130 214 273 314 319 303 330 292 304 266 192  51  34  25  19

 12  15  22  37 155 264 268 279 324 302 297 294 288 297 219  58  37  27  20

 12  16  24  41 179 233 271 271 308 300 280 275 287 308 243  63  40  29  22

 12  17  24  41 164 236 264 266 273 298 262 286 300 330 242  70  43  29  22

 13  17  25  42 163 222 236 251 265 287 293 300 306 313 254  70  41  28  21

 12  17  25  42 161 236 253 258 270 329 268 299 326 330 245  64  38  26  20

 12  16  24  40 173 234 231 255 281 322 301 271 301 311 250  58  35  24  18

 12  16  22  37 151 214 238 264 284 314 298 288 274 300 201  49  30  22  17

 11  14  20  32 130 200 244 252 295 306 310 296 286 232 160  40  26  18  14

 10  13  18  28 109 140 162 194 205 232 212 208 179 156 115  32  21  16  12

  9  12  16  25  30  34  39  44  51  53  52  46  43  38  33  26  18  14  11

  8  10  14  17  19  22  24  26  29  30  30  27  25  24  21  19  15  12  10

  7  10  11  13  14  16  17  19  19  20  20  19  18  17  15  14  13  10   8

  7   8   9  10  11  12  12  14  14  15  15  15  13  13  12  11  10   9   7

grid cell dimension  :   .500 km
number of grid points:  19x19
top left coordinates :   -4.500,    4.500 km

average  NH3 concentration: .99E+00 ug/m3
```

```
Project: calculation examp.  subst.:  NH3              date: 07-12-90  13:29
================================= OPS-V1.11E =================================

dry deposition distribution (as  NH3): ( .1E+01 mol/ha/y )

  16  19  21  24  27  33  40  45  52  57  60  62  61  61  59  56  51  47  44

  18  22  26  30  35  43  52  61  70  77  81  83  82  80  75  69  63  57  48

  20  25  33  40  47  60  75  90 102 113 119 119 114 108 100  90  80  63  53

  22  28  39  57  71  94 122 151 174 192 197 188 178 162 146 127  91  71  59

  24  32  44  69 254 381 509 659 662 703 716 745 682 622 506 148 104  80  64

  27  35  50  81 337 578 743 874 915 876 973 918 974 871 633 170 115  88  68

  30  39  56  94 400 713 740 766 910 867 912 924 925 961 717 192 126  93  70

  32  43  62 104 460 607 738 755 860 858 858 867 909 987 788 209 137  97  73

  34  46  65 108 431 639 704 725 770 848 808 886 9431022 758 224 140  98  73

  35  46  67 110 423 592 650 708 764 811 861 899 935 970 801 224 135  94  70

  34  46  65 109 414 628 669 702 723 849 785 882 9711010 758 205 124  87  66

  33  44  62 102 435 603 614 663 742 823 819 801 894 942 758 182 112  78  59

  31  41  58  94 381 549 601 678 740 796 799 794 817 901 608 152  96  69  54

  29  38  53  83 332 493 606 642 729 769 793 806 799 690 480 122  80  59  47

  27  35  48  72 267 346 402 488 502 581 538 559 487 433 339  97  66  50  40

  25  31  41  62  74  86  99 111 125 131 132 123 115 104  92  79  55  43  35

  22  28  36  43  49  55  61  66  72  75  75  72  69  65  60  53  46  37  30

  20  25  28  32  36  40  43  46  49  50  51  50  48  46  43  39  35  31  26

  18  21  23  26  29  31  33  35  36  37  37  38  36  35  33  30  28  26  23

grid cell dimension    :    .500 km
number of grid points:   19x19
top left coordinates :    -4.500,     4.500 km

average dry deposition              : .28E+03 mol/ha/y
effective dry deposition velocity :   1.540 cm/s (calc. from dry dep. and conc.)
total dry deposition                : .14E+01 g/s  (in the selected field)
```

```
Project: calculation examp.  subst.:  NH3                date: 07-12-90  13:29
================================== OPS-V1.11E ==================================

wet deposition distribution (as  NH3): ( .1E+01 mol/ha/y )

  1   2   2   2   3   3   4   5   5   6   6   7   6   6   7   6   6   5   5

  1   2   2   3   3   4   5   5   6   7   7   8   7   8   7   7   6   6   5

  1   2   2   3   3   4   6   7   7   8   9   9   9   9   8   7   7   6   5

  1   2   2   3   4   5   7   9  10  11  12  11  11  10   9   8   7   6   5

  1   2   2   3   4   7  11  15  16  16  18  17  16  13  12   8   7   6   5

  1   2   2   3   5   7  12  16  16  16  18  16  17  14  12   8   7   6   5

  1   2   2   3   4   8  10  13  16  15  15  16  15  14  13   9   7   6   5

  1   1   2   2   4   5   8  11  15  15  14  14  13  14  13   9   7   6   5

  1   1   2   2   4   5   7   9  12  14  12  12  13  14  13   9   7   6   5

  1   1   1   2   2   4   6   8  10  13  12  12  12  12  11   8   6   5   4

  1   1   1   2   3   4   5   7   8  14  11  11  12  11  11   7   5   5   4

  1   1   1   2   2   3   4   6   8  12  10   9  10  10  10   6   5   4   3

  1   1   1   1   2   3   4   5   7  10   9   8   8   8   7   5   4   4   3

  1   1   1   1   2   3   4   5   7   9   9   7   7   6   5   4   3   3   3

  1   1   1   1   2   2   3   4   6   7   7   6   5   5   4   3   3   3   2

  1   1   1   1   2   2   2   2   3   4   4   3   3   3   3   3   2   2   2

  1   1   1   1   1   2   2   2   3   3   3   3   2   2   2   2   2   2   2

  1   1   1   1   1   1   2   2   2   2   2   2   2   2   2   2   2   2   2

  1   1   1   1   1   1   1   2   2   2   2   2   2   2   2   2   2   2   2

grid cell dimension  :   .500 km
number of grid points:  19x19
top left coordinates :   -4.500,    4.500 km

average wet deposition        :  .56E+01 mol/ha/y
effective wet deposition rate:    2.627 %/h      (mass weighted)
total wet deposition          :  .27E-01 g/s     (in the selected field)
annual precipitation amount   :      735 mm      (in climatological area)
```

Remark: *from the emitted 50 g/s NH3, 14 g/s will be dry deposited in the selected field and 0.027 g/s wet deposited*

```
Project: calculation examp.  subst.:  NH3                 date: 07-12-90  13:29
================================== OPS-V1.11E ==================================

emission source data:

ssn    x(m)    y(m)    q (g/s) hc(MW)  h(m)   d(m)  s(m)  tb cat area subst.
--- ------- ------- --------- ------ ----- ------ ----- --- --- ---- --------
  1       0       0 .500E+01   .000   1.0   5000    .0   4   1    1  NH3


z0   : .13 m    seasonal temp. corr.:1.01    emission trend corr.:1.00

climatological area   : 3 = Drente, S-Friesland, S-Groningen
climatological period: 0 = Year...........(1979-1989)

name of input parameter file      :examp2.inp
name of emission data file        :examp2.brn
name of climatological data file :\usr\hans\ops\meteosta\k3jalt
name of printer output file       :examp2.lpt

 NH3 considered as gaseous

average dry  NH3 deposition: .28E+03 mol/ha/y
average wet  NH3 deposition: .56E+01 mol/ha/y

eff. chem. conv. rate :33.41 %/h  (mass weighted av. of all conv. rates)
eff. wet dep. rate    : 2.63 %/h  (mass weighted av. of all wet dep. rates)
eff. dry dep. velocity: 1.54 cm/s (calc. from av. dry dep. and av. conc.)

mean diurnal concentration distribution  NH3 in ug/m3 :

     1- 2      3- 4      5- 6      7- 8      9-10     11-12
    -----     -----     -----     -----     -----     -----
  .40E+00   .31E+00   .71E+00   .10E+01   .12E+01   .12E+01

    13-14     15-16     17-18     19-20     21-22     23-24
    -----     -----     -----     -----     -----     -----
  .13E+01   .13E+01   .13E+01   .13E+01   .10E+01   .79E+00
```

Dry and wet deposition of the secundary formed ammonium (NH4) are not calculated by the OPS model and consequently not included in the presented deposition data. In this particular case of a limited area, however, the deposition of NH4 would be small compared to the deposition of NH3.

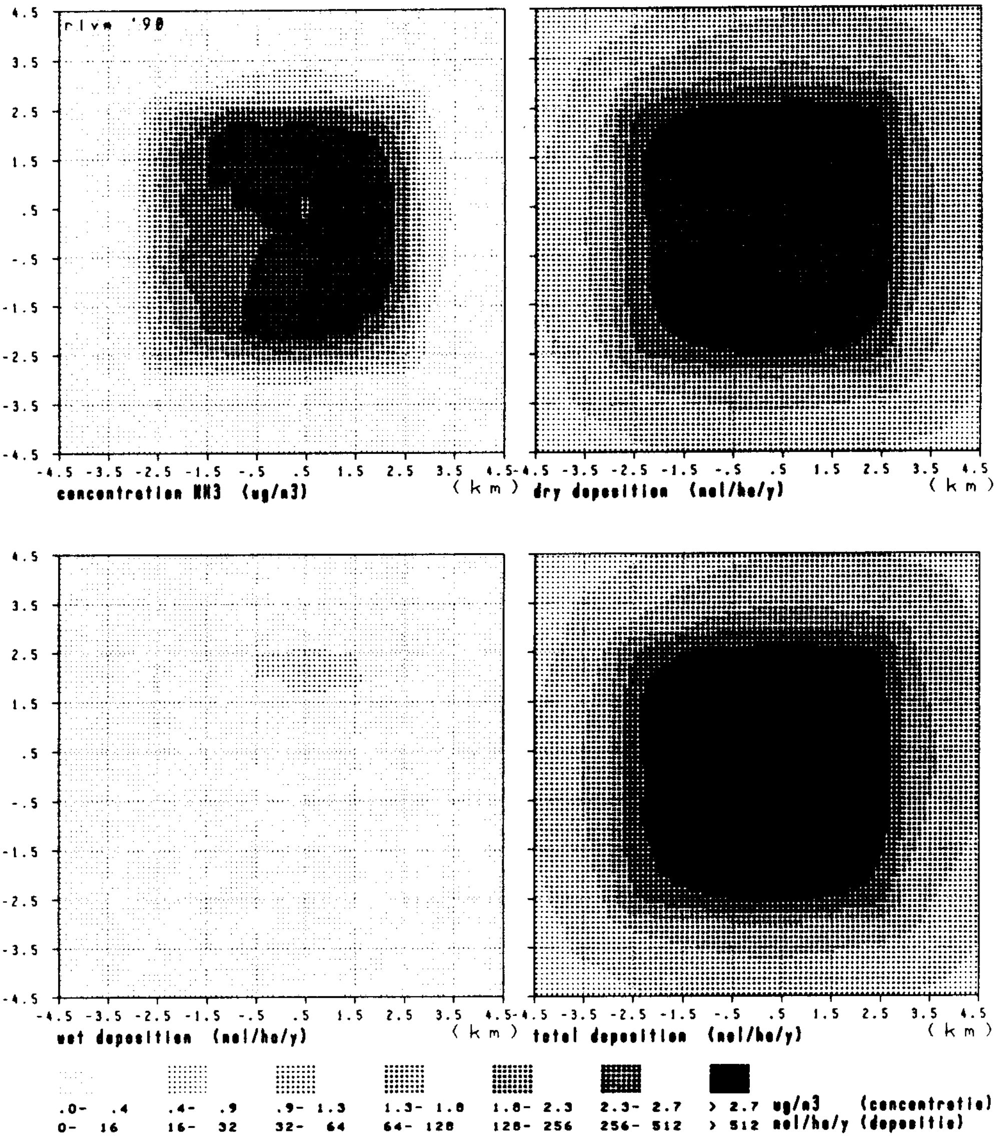
```
Project: calculation examp.  subst.:  NH3              date: 07-12-90  13:29
================================ OPS-V1.11E ================================

input parameters:               (file=examp2.inp        )

j                    *acceptance of user conditions
0                    *save input parameters
examp2.inp            name of input parameter file
calculation examp.    project name
 0                   *substance to model (0=user spec. 1=SO2 2=NOx 3=NH3)
 NH3                  name of the substance
 17.0                 molecular weight
1                    * gaseous=1 particle bounded=0
1                    *emission data (0=from data file 1=manually entered)
.500E+01              source strenght (g/s)
   .000               heat content (MW)
   1.0                source height (m)
   5000              *source diameter (m)
    .0                std. dev. emission heights)
4                     daily var. of emiss. (0=cont. 1=ind. 2=sp.h. 3=tr. 4,5,6=o
   1                  source category number
   1                  country or area identification number
 0000000  0000000     coordinates x and y (m)
0                    *enter another source ?
  021  017  042  083  145  166  187  187  145  104  062  042   daily emis. var
1                    *save the data of the source(s) in a source data file ?
examp2.brn            name of source data file ?
0                    *gridded receptor points(=0) or spec. positions(=1) ?
1                    *grid over the Netherlands(=0) or special grid(=1) ?
 0000000  0000000    *x and y coordinates of grid centre (m) ?
 19 19                number of grid elements in x and y direction
   500                grid resolution (m)
 3                    climatological area (0 t/m 7)
 0                    climatological period (0 t/m 2)
 .000                 roughness length in m (0=equal to receptor area)
1                    *account also for deposition and conversion ?
2                    *dry deposition specification (1=vd 2=rc)
    20.0              surface resistance (s/m)
3                    *spec. of wet dep. (1=sc.coeff. 2=sc.ratio 3=other)
 300000               conc.in prec./conc.in air
   .230               diff. coeff. in air
0                     reversible wash-out process
 20.0000   .0900      conversion rates a and b
3                     select the unit of deposition
0                    *save the model results in a [.plt] file ?
1                    *special printer output file ?
examp2.lpt            name of printer output file ?
1                     deposition grids also in printer output file ?


warning: when re-using this input file, do not change the parameters
         marked with a * !
```

The files 'examp2.plt' and 'examp2.brn' are not listed.
For the structure of these files see calculation example 1.



Graphic representation of results example 2

Calculation example 3

problem : Point source emitting lead (Pb) and situated in the Rijnmond area. Stack height 40 m, no heat content. This source emits at an average rate of 1 g/s and shows a typical industrial diurnal emission cycle. The particle-size distribution of the lead as emitted by this source deviates from what is usually found in ambient air: 40% < .95 lm, 60% < 4 lm, 80% < 10 lm en 90% < 20 lm. The roughness length in the neighbourhood of the source is 0.5 m.

Calculate de long-term average lead concentration and deposition due to this source of lead on four locations in the Rijnmond area: Vlaardingen, Rockanje, Maasdijk en Poortugaal. Store the coordinates of these four sites in a receptor file.

Copies of the screen during the use of the model are given below. Everything what is entered by the user is typed boldface.

opsmod

```
                        oooooooo      oooooooo      oooooooo
                      oo       oo   oo       oo   oo       oo
                     oo       oo   oo       oo   oo
                    oo       oo   oooooooooo      ooooooo
                   oo       oo   oo                     oo
                  oo       oo   oo            oo       oo
                   oooooooo    oo              oooooooo
```

```
      This model calculates average concentrations and depositions
      due to the release of a substance to ambient air by one
      or more sources. Parameters which determine the dispersion
      and deposition of a substance can be taken from pre-defined
      values, but can also be specified by the user within wide
      limits.
      In all cases however, the user remains responsible for the
      choice of parameters and emission strengths and the correct
      interpretation of the model results.

      If you accept these conditions, press "y" <cr> to continue.
Y

================================== OPS-V1.11E =================================

         ---- Welcome to the Priority Substances Model ----

A description of this model and information about the parameters
to be entered, can be found in:
```

```
      Jaarsveld J.A. van, (1990)
      An Operational atmospheric transport model for Priority Substances;
      specification and instructions for use
      Report nr. 222501002
                                    RIVM - Laboratory for Air Research
                                    P.O. Box 1
                                    3720 BA Bilthoven, The Netherlands
______________________________________________________________________________

data and parameters to run this model:

                    0 = from an (existing) input parameter file
                    1 = to be entered manually
                    2 = to be entered manually with saving
2
name of input parameter file?
examp3
project name ? (max=18 char.)
calculation examp.
================================ OPS-V1.11E ================================

which substance do you want to model?
                    0 = user specified substance
                    1 = SO2-gas.                2 = NOx-gas.
                    3 = NH3-gas.                4 = HF(fluorine)-gas.
                    5 = F(fluorine)-aer.        6 = HCl-gas.
                    7 = Cl-aer.                 8 = HBr(bromine)-gas.
                    9 = Br(bromine)-aer.       10 = B(boron)-gas.
                   11 = B(boron)-gas.          12 = Se(selenium)-gas.
                   13 = Se(selenium)-aer.      14 = Hg(mercury)-gas.
                   15 = Hg(mercury)-aer.       16 = C6H6(benzene)-gas
                   17 = C7H8(tolueen)-gas      18 = As(arsenic)-gas.
                   19 = Cd(cadmium)-aer.       20 = Cr(chromium)-aer.
                   21 = Cu(copper)-aer.        22 = Pb(lead)-aer.
                   23 = Zn(zinc)-aer.

0
================================ OPS-V1.11E ================================

name of the substance? (max=18 char.)
Lead
molecular weight of Lead ?
207.2
Lead to consider as ?
                    0 = particle bounded
                    1 = gaseous
0
particle size distribution ?
                    1 = standard distribution fine
                    2 = standard distribution medium
                    3 = standard distribution coarse
                    4 = user specified distribution
4
specify the distribution for the following particle-size classes:
<0.95 um  0.95-4 um   4-10 um   10-20 um  and >20 um
40 20 20 10 10
```

```
================================ OPS-V1.11E ================================

emission source data ?
                     0 = from an (existing) emission file
                     1 = to be specified manually
1
================================ OPS-V1.11E ================================

source strength (annual av. in g/s)
1
heat content (MW)
0
source height (m)
40
source diameter (m) (specify 0 for point sources)

0
daily variation of the emission of this source?

                     0 = no variation (continuous emission)
                     1 = according to an av. industrial activity
                     2 = according to an av. space heating energy demand
                     3 = according to an av. traffic intensity
                     4,5 and 6 = daily variations to be specified by the user
1
source category number ? (1-9999)
1
country or area identification number ? (1-9999)
1
coordinates x and y (m) ?
80000 435000
enter data for another source ?
no
save the data of the source(s) in a source data file ?
yes
name of source data file ? (max. 12 characters)
examp3
================================ OPS-V1.11E ================================

receptor points ?
                     0 = in a regular grid
                     1 = at specific positions (to be specified)
1
================================ OPS-V1.11E ================================

receptor location data ?
                     0 = from a (existing) receptor data file
                     1 = to be entered manually (data will be saved in a file)
                     2 = from the National Air Quality Monitoring Network (LML)
1
name of receptor data file ? (max. 12 char.)
examp3
name or number of receptor point:  1 (max. 12 char.) ?
Vlaardingen
coordinates x and y (m) ?
82000 436400
enter data for another receptor point ?
yes
```

```
name or number of receptor point:  2 (max. 12 char.) ?
Rockanje
coordinates x and y (m) ?
64500 432500
enter data for another receptor point ?
Y
name or number of receptor point:  3 (max. 12 char.) ?
Maasdijk
coordinates x and y (m) ?
75000 441800
enter data for another receptor point ?
Y
name or number of receptor point:  4 (max. 12 char.) ?
Poortugaal
coordinates x and y (m) ?
86000 430000
enter data for another receptor point ?
no
================================== OPS-V1.11E ================================

selection of climatological data:

         1   111111
        11    1111333    0 = The Netherlands: total area
        11    3333333
        222 2333355      1 = N-Holland, N-Friesland, N-Groningen
       2222 33555556     2 = Randstad, W-Brabant, E-Zeeland
      22222255556666     3 = Drente, S-Friesland, S-Groningen
     42222255556666      4 = W-Zeeland, ZH-Islands
    4444225555566        5 = Mid-Brabant, Veluwe, Twente
   444222555556666       6 = S-Limburg, E-Brabant, Achterhoek
  444422     6666
              66         7 = Special climatological datafile
              666

climatological area ?
4
================================== OPS-V1.11E ================================

selection of climatological period:

                    0 = Year...........(1979-1989)
                    1 = Summer period...(1979-1989)
                    2 = Winter period...(1979-1989)

climatological period ?
0
roughness length in the source area (m) ?

                    0 = equal to roughness length in receptor area
0.5
```

```
================================== OPS-V1.11E ==================================

select the unit of deposition:

                        1 =  mmol/m2/s
                        2 =  g/m2/s
                        3 =  mol/ha/y
                        4 =  kg/ha/y
                        5 =  mmol/m2/y
                        6 =  g/m2/y
3
================================== OPS-V1.11E ==================================

save the model results in a [.plt] file ?
yes
name of this file ?
examp3
special printer output file ? (default=stdout.ops  )
yes
name of printer output file ?
examp3
================================== OPS-V1.11E ==================================
```

The screen below appears after the parameter input session, sources are treated one by one.
The progress of a calculation is made visible by an activity indicator.

```
     ========== end of input specification, start of calculations ==========

reading file with climatological data ....

statistiek van periode: 79  1  1 tot 89  1  1

initialization and reading source data ......

ssn:   1    q=.100E+01 g/s   h= 40 m  hc=  .00 MW  d=    .0 km  Lead       100%

average Lead concentration: .47E-01 ug/m3

name of input parameter file   :examp3.inp
name of source data file       :examp3.brn
name of receptor data file     :examp3.rcp
data to (plotter) file         :examp3.plt
name of printer output file    :examp3.lpt
```

The printer output file 'examp3.lpt':

```
Project: calculation examp.  subst.: Lead                 date: 07-12-90  13:33
================================== OPS-V1.11E ==================================


Concentrations and depositions Lead calculated for some specific locations

 nr      name       x-coord y-coord      conc.  dry dep.  wet dep.  tot.dep.
                      (m)     (m)        ug/m3  mol/ha/y  mol/ha/y  mol/ha/y
                                           x        x         x         x
                                        .1E-02    .1E-01    .1E-01    .1E-01

  1  Vlaardingen     82000  436400        145       167        16       183
  2  Rockanje        64500  432500          8         4         1         5
  3  Maasdijk        75000  441800         16         9         2        11
  4  Poortugaal      86000  430000         18        15         3        17

average Lead concentration: .47E-01 ug/m3
```

```
Project: calculation examp.  subst.: Lead                 date: 07-12-90  13:33
================================== OPS-V1.11E ==================================

emission source data:

ssn    x(m)    y(m)    q (g/s) hc(MW)  h(m)   d(m)  s(m)  tb cat area subst.
--- ------- ------- --------- ------ ----- ------ ----- --- --- ---- --------
  1   80000  435000  .100E+01   .000  40.0      0    .0   1   1    1 Lead


z0   : .50 m    seasonal temp. corr.:1.01    emission trend corr.:1.00

climatological area   : 4 = W-Zeeland, ZH-Islands
climatological period: 0 = Year............(1979-1989)

name of input parameter file     :examp3.inp
name of emission data file       :examp3.brn
name of receptor data file       :examp3.rcp
name of climatological data file :\usr\hans\ops\meteosta\k4jalt
data to (plotter) file           :examp3.plt
name of printer output file      :examp3.lpt

Lead considered as aerosol; size distribution: 4

<0.95 um: 40 %   0.95-4 um: 20 %   4-10 um: 20 %   10-20 um: 10 %   >20 um: 10 %

average dry Lead deposition: .49E+00 mol/ha/y
average wet Lead deposition: .53E-01 mol/ha/y

eff. chem. conv. rate :  .00 %/h
eff. wet dep. rate    : 2.07 %/h
eff. dry dep. velocity:  .68 cm/s

mean diurnal concentration distribution Lead in ug/m3 :

     1- 2      3- 4      5- 6      7- 8      9-10     11-12
    -----     -----     -----     -----     -----     -----
  .45E-01   .42E-01   .41E-01   .52E-01   .54E-01   .46E-01

    13-14     15-16     17-18     19-20     21-22     23-24
    -----     -----     -----     -----     -----     -----
  .40E-01   .41E-01   .44E-01   .51E-01   .56E-01   .53E-01
```

```
Project: calculation examp.  subst.: Lead                  date: 07-12-90  13:33
================================= OPS-V1.11E =================================

input parameters:                  (file=examp3.inp        )

j                    *acceptance of user conditions
0                    *save input parameters
examp3.inp            name of input parameter file
calculation examp.    project name
 0                   *substance to model (0=user spec. 1=SO2 2=NOx 3=NH3)
Lead                  name of the substance
207.2                 molecular weight
0                    * gaseous=1 particle bounded=0
4                    *size distribution
  .400  .200  .200  .100  .100   size distribution
1                    *emission data (0=from data file 1=manually entered)
.100E+01              source strenght (g/s)
   .000               heat content (MW)
  40.0                source height (m)
      0              *source diameter (m)
1                     daily var. of emiss. (0=cont. 1=ind. 2=sp.h. 3=tr. 4,5,6=o
   1                  source category number
   1                  country or area identification number
 0080000  0435000     coordinates x and y (m)
0                    *enter another source ?
1                    *save the data of the source(s) in a source data file ?
examp3.brn            name of source data file ?
1                    *gridded receptor points(=0) or spec. positions(=1) ?
1                    *receptor data (0=from file 1=manual 2=LML)?
examp3.rcp            naam receptorfile
Vlaardingen           name of receptor point
 0082000  0436400     coordinaten x en y (m)
1                    *enter another receptor point ?
Rockanje              name of receptor point
 0064500  0432500     coordinaten x en y (m)
1                    *enter another receptor point ?
Maasdijk              name of receptor point
 0075000  0441800     coordinaten x en y (m)
1                    *enter another receptor point ?
Poortugaal            name of receptor point
 0086000  0430000     coordinaten x en y (m)
0                    *enter another receptor point ?
 4                    climatological area (0 t/m 7)
 0                    climatological period (0 t/m 2)
 .500                 roughness length in m (0=equal to receptor area)
3                     select the unit of deposition
1                    *save the model results in a [.plt] file ?
examp3.plt            file name for saving conc. and dep. grids?
1                    *special printer output file ?
examp3.lpt            name of printer output file ?


warning: when re-using this input file, do not change the parameters
         marked with a * !
```

The (plotter) file 'examp3.plt':

```
name          x-coord y-coord    conc.   dry dep.  wet dep.  tot.dep.
                                  Lead      Lead      Lead      Lead
                    m       m    ug/m3 mol/ha/y  mol/ha/y  mol/ha/y
Vlaardingen     82000  436400 .145E+00  .167E+01  .161E+00  .183E+01
Rockanje        64500  432500 .845E-02  .432E-01  .600E-02  .492E-01
Maasdijk        75000  441800 .163E-01  .946E-01  .197E-01  .114E+00
Poortugaal      86000  430000 .183E-01  .146E+00  .250E-01  .171E+00
```

The emission data file 'examp3.brn':

```
tb   2   4   6   8  10  12  14  16  18  20  22  24

04 100 100 100 100 100 100 100 100 100 100 100 100
05 100 100 100 100 100 100 100 100 100 100 100 100
06 100 100 100 100 100 100 100 100 100 100 100 100

 ssn     x(m)     y(m)    q (g/s)  hc(MW)   h(m)    d(m)   s(m)   tb cat area

   1    80000   435000   .100E+01    .000   40.0       0     .0    1   1    1  Lead
```

The receptor data file 'examp3.rcp':

```
   1 Vlaardingen     82000  436400
   2 Rockanje        64500  432500
   3 Maasdijk        75000  441800
   4 Poortugaal      86000  430000
```