



Airviro Specification

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} = \frac{1}{\rho} \frac{\partial}{\partial z} \left[\rho \left(K_z \frac{\partial c}{\partial z} + w_s c \right) \right] + \frac{Q}{\rho}$$

Airviro Specification v6.00

Part II: Appendices

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Amendments

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Appendix E: Models and Formulae Used in the Airviro Modules

E1 Statistical Models

E1.1 The Stepwise Regression Scheme

The stepwise regression scheme is based on the Forward Selection principle and can be explained as follows:

Assume that you have decided to set up a model:

$$Y = b_0 + b_1X_1 + b_2X_2 + \dots + b_5X_5 + \varepsilon$$

and have chosen the 5 predictors as well as the predictand among the data in the Time Series Database. When you ask for the regression the following will happen:

The stepwise regression routine looks at all predictors to find out the single one of the five X_1 to X_5 that best describes the variation in the predictand Y . Let us assume that X_1 is the one. Thereafter the parameters b_0 and b_1 are optimised in the equation:

$$Y = b_0 + b_1X_1 + \varepsilon_1$$

so that the error ε_1 is minimised. This is called a first order model (or model size 1) because it involves just one predictor. Verification scores are determined for this model size.

The next step is to find and include the second best predictor (assume that this is X_2) and determine the parameters b_0 , b_1 and b_2 in the equation:

$$Y = b_0 + b_1X_1 + b_2X_2 + \varepsilon_2$$

so that the error ε_2 is minimised. Verification scores are determined for this model size.

This procedure continues until there is no meaning in including an additional predictor because the improvement of the model is not significant. At this moment you know which of the original predictors should be included in the regression model and you know which model size is the best one to use.

A criterion is needed for the meaning of a *significant improvement*. For this reason there is the possibility to set the two criteria **F-in** and **F-out**. These represent the risk (as a percentage) that you are willing to take to *not include* a predictor that should be in the equation or to *exclude* a predictor already in the equation.

E1.2 Validation of the Regression Model

The usual problem when dealing with regression models is the consequence of overfitting. If the data is sparse and knowledge of how to formulate a proper regression model is poor, then it is likely that the regression parameters will be well fitted to the current period of data, but not relevant to other periods.

To avoid this problem a cross validation procedure is provided. The cross validation procedure means that all original data are divided into 10 subsets. For each model size the parameter will be estimated using 9 of the 10 subsets (basic data). Verification scores will then be estimated on the remaining subset (independent data or test data). The original data are permuted 10 times so that each subset is used as a test data period against the remaining 9 subsets. The verification scores are averaged and presented for different model sizes. Simply explained, the original data will be used both as basic data as well as test data. This method is useful in many cases and gives a distinct message concerning what model size should be used.

E1.3 Factor Analysis

The purpose of factor analysis is to identify typical structures within a collection of data samples. The technique which it uses is the extraction of the eigenvalues and eigenvectors from the matrix of correlation.

Given time series measurements $x_1(t)$, $x_2(t)$, ..., $x_K(t)$, the indices 1-K represent any measured data variable in the time series database. The index (t) represents the time dimension, i.e. it could represent the index for measurement of a specific hour, day, etc.

In the concept of Factor Analysis the user is interested in investigating to what extent a number of series have similar or different behaviour. The first step is to standardise the original time series $x_1 - x_K$. The reason for this is to find the covariation of the time series and not the different sizes of the individual variations. Assume that 10 series $x_1 - x_{10}$ are chosen for a period of 100 values, i.e. $t = 1, 2, 3, \dots, 100$. The standardisation means that for each series the time mean value and the standard deviation are determined, i.e.:

$$m_i = \frac{1}{M} \sum_1^M x_i \quad \text{and} \quad s_i = \frac{1}{M-1} \sum_1^M (x_i - m_i)^2$$

where $M=100$. Thereafter the standardised variables $z_i(t)$ are constructed as follows:

$$z_i(t) = \frac{x_i(t) - m_i}{\sigma_i}$$

i. e. all the variables z_i have the same mean value (0) and the same standard deviation (1).

We now transform our standardised variables into an orthonormal set of factors as follows:

$$z_i(t) = \sum_{n=1}^N f_n(t) \cdot h_n(i) \quad \text{for } i=1, 2, \dots, K \text{ (i.e. the total number of initial variables (10))}$$

The $f_n(t)$ denote the factors and the $h_n(i)$ the eigenvectors corresponding to the factor f_n . The original standardised variables have been transformed to a number of new variables f_n and the contribution of each factor f_n to the original series is described by the eigenvector $h_n(i)$

In the decomposition of the original data into factors a constraint of fastest possible convergence is applied. This is the same as saying that the first factor chosen is the one that alone can explain as much variation of the original variables as possible. Normally the number of factors are the same as the number of original variables ($N=K$). If the original variables are extremely well correlated, then the calculation will probably end up with a number of factors that are less than the original number of variables ($N<K$).

The most valuable help that can be provided by the factor analysis is that it will structure your data, find the typical variation among all your data series, try to compress the common variation into a number of factors and describe to what extent the factors could explain the variation in each original time series.

E1.4 Principal Component Analysis

Principal Component Analysis is similar to Factor Analysis but no standardisation is made on the original variables, i.e. a decomposition

$$zx_i(t) = \sum_{n=1}^N a_n(t) \cdot g_n(i) \text{ for } i = 1, 2, \dots, K$$

is performed.

E2 Formulae Used for Time and Temperature Dependent Calculations in the EDB

E2.1 Point, Area and Grid Source Emissions

In the Airviro EDB, emissions can be calculated as a function of the hour, day, weekday, month and as a function of the outdoor temperature. In order to identify non-working days when they appear in the middle of the week (e.g. when New Years Day appears on a Wednesday) the concept of day types is introduced, i.e.

Day type (index)	Meaning	Relative occurrence during a year
Monday-Thursday type (0)	Ordinary working day	4/7
Friday type (5)	Day before non working day	1/7
Saturday type (6)	Non working day - Saturday	1/7
Sunday type (7)	Non working day - Sunday	1/7

The following variables and functions are defined:

dt	= day type index = {0,5,6,7}
w(dt)	= relative occurrence of day type dt
m	= index for month m= {1, 2, ..., 12}
w(m)	= relative occurrence of month m (approximated as 1/12)

h	= hour during the day = {1, 2, ..., 24}, e.g. h=12 corresponds to mean value between 11 and 12
s	= scenario index
T	= outdoor temperature = {T1-T2, T2-T3, ..., T29-T30}. By default -30°C<T<30 with a class width of 2°C.
w(T)	= relative occurrence of temperature interval T.
E₀	= mean emission during the year (g/s)
E_{max}	= maximum emission at any hour during a year
E(h,dtty,m,s)	= estimated emission for any hour, day-type and month for the scenario s
TabS(s)	= is a table defining the variation with different scenarios and is not normalised.

TabM(m), **TabD (dtty,h)** and **TabT(T)** are the tables defined in the EDB Time and Temperature formulae giving the variation for months, for all hours and all day types and outdoor temperatures. A normalisation constant **k** is calculated so that the following condition is fulfilled:

$$k \times \frac{1}{12} \sum_m TabM(m) \times \left\{ \frac{1}{24} \sum_h \sum_{dtty} w(dtty) \times TabD(dtty, h) + \sum_T w(T) \times TabT(T) \right\} = 1 \quad (\text{eq E2.1.1})$$

The emission can be calculated in two different ways, i.e.:

$$E(h, dtty, m, s) = E_0 \times TabS(s) \times k \times TabM(m) \times \{TabD(dtty, h) + TabT(T)\} \quad (\text{eq E2.1.2})$$

$$E(h, dtty, m, s) = TabS(s) \times E_{\max} \times Amp \quad (\text{eq E2.1.3})$$

$$\text{where } Amp = TabM(m) \times [TabD(dtty, h) + TabT(T)] \quad \text{if } Amp < 1 \quad (\text{eq E2.1.4})$$

else $Amp = 1$

The difference between equation E2.1.2 and E2.1.3 will become obvious when you work with the formulae. Equation E2.1.3 represents an upper limit restricted emission, i.e. the maximum emission is $E_{\max}$ for all hours during the year. If you describe the emission as originating from an oil-burning power plant, then the energy production rate and consequently the emissions would depend on the load. There is however an upper limit in the production rate, restricted by the maximum capacity of the boiler. *Equation E2.1.3 is used for the emission estimation in the EDB when you choose emission estimation based on **Fuel**.*

In equation E2.1.2 there is no such restriction. E_0 represents the total emission during a year if we convert the units from grams/second to tons/year. The factor **k** ensures that the mean emission from the source for the whole year is the figure E_0 . The figures in TabM, TabD and TabT just give the variation within the year. *Equation E2.1.2 is used for the emission estimation in the EDB when you choose emission estimation based on Substances (or Substance group) and yearly emission figures.*

Consequently, equation E2.1.2 permits the user to prescribe a scenario in which all pollutants coming from a source are concentrated to a few hours.

E2.2 Road Source Emissions

The following variables and functions are defined:

dtv	= day type index = {0,5,6,7}
w(dty)	= relative occurrence of day type dty
m	= index for month m= {1, 2, ..., 12}
w(m)	= relative occurrence of month m (approximated as 1/12)
h	= hour during the day = {1, 2, ..., 24}, e.g. h=12 corresponds to mean value between 11 and 12
s	= scenario index
l	= length of the road
n	= average number of vehicles per day on the road
corr	= correction factor for the road
E(speed,h,dty,m,s)	= estimated emission for any speed, hour, day-type and month for the scenario s
TabS(s,v)	is the table defining the variation with different scenarios and is not normalised.
TabR(speed,v)	is the table defining the absolute emission from the vehicle with index v for different speeds.

TabM(m,v) and **TabD(dty,h,v)** are the tables defined in the formulae giving the variation for months, during the hours for all existing day types for a vehicle with index v. For each vehicle in a road type the normalisation constant **k(v)** is calculated so that the following condition is fulfilled:

$$k(v) \times \frac{1}{12} \sum_m TabM(m,v) \times \frac{1}{24} \sum_h \sum_{dty} w(dty) \times TabD(dty,h,v) = 1 \quad (\text{eq E2.2.5})$$

The emission for a road is then calculated as:

$$E(speed,h,dty,m,s) = corr \times n \times 1 \times \sum_v (TabS(s,v)) TabR(speed,v) \times k(v) TabM(m,v) \times TabD(dty,h,v) \quad (\text{eq E2.2.6})$$

E3 Models Available for Use With the Dispersion Module

E3.1 The Wind Model - Calculation of the Wind Fields

E3.1.1 Principles of Wind Field Calculations

The wind field calculation is based on the concept first described by Danard (1976), where mesoscale winds are generated by using:

- horizontal momentum equation
- pressure tendency equation
- first thermodynamic equation

This concept assumes that small scale winds can be seen as a local adaptation of large scale winds (free winds) due to local fluxes of heat and momentum from the sea or earth surface. Any non-linear interaction between the scales is neglected. Danard assumes that the adaptation process is very fast, 1.5 hours for model resolutions of 10*10 km. It is also

assumed that horizontal processes can be described by non-linear equations while the vertical processes can be parametrised as linear functions.

The large scale winds as well as vertical fluxes of momentum and temperature are estimated from profile measurements in one or several meteorological masts (called principal masts). When the topography is relatively smooth, without dominating ridges or valleys, the free wind is assumed to be horizontally uniform.

For deep bi-directional valleys, this is not possible. A channel flow approach has been used to include the governing effects on the free winds in deep valleys.

For larger areas or for areas with complex meteorological situations (such as sea breezes) information from more than one meteorological station is needed. The data from these stations will then pass through a mesoscale interpolation (see E3.1.4 “Stability and Turbulence Estimation - Preprocessing of Meteorological Data”) before entering the wind model.

E3.1.2 Wind Model Equations

The equations below are solved in a terrain-following coordinate system (s-coordinates):

$$\frac{\partial V_s}{\partial t} = -V_s \cdot \nabla V_s - (g \nabla Z_s + R T_s \nabla \ln p_s) - f K \times V + F + K_m \nabla^2 V \quad (\text{eq E3.1.1})$$

$$\frac{\partial \Theta_s}{\partial t} = -V \cdot \nabla \Theta_s + K_t \nabla^2 \Theta_s + Q / C_p \quad (\text{eq E3.1.2})$$

$$\frac{\partial p_s}{\partial t} = \frac{g}{R \Theta_s T_s} \cdot \int_0^H \frac{\partial \Theta}{\partial t} dz \quad (\text{eq E3.1.3})$$

V = horizontal wind

$$\Theta = T_s \left(\frac{P_0}{P_s} \right)^{\frac{R}{C_p}} = \text{potential temperature}$$

$$F = c \cdot C_D \cdot \frac{V^2}{H} = \text{friction, the drag coefficient: } C_D = \left[\frac{\kappa}{\ln \left(\frac{z}{z_0} \right)} \right]^2$$

p = air pressure

H = boundary layer height

(all variables with index s refer to the surface, i.e. 10m above ground)

E3.1.3 Initialisation

Boundary scaling parameters are determined from one or several profile measurements in the area, giving estimates of boundary layer heights (H), diabatic heating (Q) and potential temperature distribution at ground level (Θ_s). Physiographical information (surface characteristics) are used for areal interpolation of H , Q and Θ_s . A free wind, i.e. an estimate of a wind at the location of the mast, at the level (H) where the wind is not affected by surface

fluxes of heat and momentum, is estimated based on the profile measurements and extrapolation procedures suggested by Holtslag (1984). The free wind field is estimated according to one of the methods suggested in E3.1.1 “Principles of Wind Field Calculations”.

When the free wind field is estimated, the initial surface pressure field is determined in accordance with a geostrophic balance. The initial wind field at the surface is estimated by running the first equation (E3.1.1) until two successive estimations of the average wind component do not differ by more than 2%.

E3.1.4 Stability and Turbulence Estimation - Preprocessing of Meteorological Data

Stability and turbulence conditions in the boundary layer are evaluated at the locations of the principal masts, i.e. where information about both the temperature gradient and the wind speed at one or two levels is available. These data are used to calculate the boundary layer scaling parameters.

The two most important parameters for the scaling of the atmospheric stability and turbulence in the surface boundary layer are the vertical heat flux H and the friction velocity u^* . From these, a characteristic length scale - the Monin-Obukhov length - can be calculated:

$$L = \frac{\bar{T}}{g} \cdot \frac{u^3 \rho c_p}{\kappa H}$$

where T is the average surface air temperature, g is gravity, κ is the von Kármán constant and ρc_p is the specific heat capacity. In the Airviro dispersion models, the Monin-Obukhov length is extensively used as a discriminator of different meteorological regimes.

There are two ways of calculating the Monin-Obukhov length (L): The profile method and the resistance method. The two are described below.

The profile method:

The determination of the Monin-Obukhov length (L) follows the profile method discussed by Berkowicz and Prahm (1982). With measured values of potential temperature difference (Δq) close to the ground and wind speed (U) at one or two levels, L is calculated with an iterative method. The local value of the ground roughness length z_0 must also be estimated (see tabulated values in textbooks, i.e. Panofsky and Dutton (1984), Table 5.1 and 5.2). For the case that two temperatures and one or two velocities are available, it is possible to calculate two other scaling variables u^* (friction velocity) and T^* (temperature scale):

$$u = \frac{\kappa (U_{z2} - U_{z1})}{\ln \left(\frac{z_{u2}}{z_{u1}} \right) - \Psi_{m2} + \Psi_{m1}}$$

$$T = \frac{H}{\rho c_p u} = \frac{\kappa \Delta \theta}{\ln \left(\frac{z_{t2}}{z_{t1}} \right) - \Psi_{H2} + \Psi_{H1}}$$

The measurement heights are z_{u2} , z_{u1} , z_{t2} and z_{t1} . If wind is measured at only one level (z_{u2}), z_{u1} is set equal to z_0 and U_{z1} to 0.

The resistance method:

The determination of the Monin-Obukhov length (L) follows the resistance method discussed by Berkowicz and Prahm (1982). With measured values of temperature at one level, cloudiness, relative humidity, wind speed and optionally global radiation. L is calculated with an iterative method. The local value of the ground roughness length z_0 must also be estimated (see tabulated values in textbooks, i.e. Panofsky and Dutton (1984), Table 5.1 and 5.2). With these measurements it is possible to calculate two scaling variables u_* (friction velocity) and T^* (temperature scale):

$$u = \frac{\kappa U_z}{\ln\left(\frac{z_u}{z_0}\right) - \Psi_{mu} + \Psi_{m0}}$$

$$T = \frac{H}{\rho c_p u}$$

Where Heat Flux (H) is estimated from net radiation, aerodynamic resistance, surface resistance, humidity and temperature. Net radiation is estimated from solar elevation, cloud cover and albedo unless global radiation is measured. In that case also the measured global radiation is included in the calculation, Nielsen et al. (1981).

For both methods:

The similarity functions Ψ_m and Ψ_H are functions of (z/L) . For stable conditions ($L > 0$) we can use (Dyer, 1974):

$$\Psi_m = -5 \cdot \frac{z}{L}$$

$$\Psi_H = -5 \cdot \frac{z}{L}$$

For unstable conditions ($L < 0$) Paulson (1970) proposes

$$\Psi_m = \ln \left[\left(\frac{1+x^2}{2} \right) \left(\frac{1+x}{2} \right)^2 \right] - 2 \arctan(x) + \frac{\pi}{2}$$

where

$$x = \left(1 - \frac{16z}{L} \right)^{\frac{1}{4}}$$

and

$$\Psi_H = 2 \ln \left[\frac{1}{2} \left(1 + \sqrt{1 - \frac{16z}{L}} \right) \right]$$

The calculated Monin-Obukhov length (L) is further used to classify the stability conditions. The depth of the boundary layer (Z_i) is a key parameter, since the pollutants released close to ground will be more or less trapped inside this layer.

For stable conditions ($L > 0$) the Zilitinkevich (1972) estimation is used:

$$Z_i = 0.4 \sqrt{\frac{u_*}{f}} L$$

Note that this estimate relies on the assumption that the inversion is caused by local cooling. It will not serve for cases with (relatively high) inversions that are caused by advective air masses.

The corresponding expression for neutral and unstable conditions ($L < 0$) is (Panofsky and Dutton, 1984):

$$Z_i = 0.3 \left(\frac{u_*}{f} \right)$$

In practice the mixing height (mixh) often cannot be set equal to the boundary layer height (Z_i). Here the relationship between these two heights is given in a resource file, by default

$$\text{mixh} = 50 + 10 \times \sqrt{Z_i + 1}$$

This empirical relationship was obtained from a data set for Göteborg (see Indic, 1990).

It is possible as an option to set Z_i equal to mixh.

Direct measurements of velocity fluctuations may be used to evaluate the dispersion coefficients σ_y and σ_z that regulate lateral and vertical diffusion of the Gaussian plume. The measured quantities are the standard deviation of wind direction (σ_α) and vertical wind speed (σ_w). The technique suggested by Draxler (1976) is as follows:

$$\sigma_y = \sigma_\alpha X \frac{1}{\left[1 + 0.9 \sqrt{\left(\frac{X}{UT_i} \right)} \right]}$$

where T_i is a Lagrangean time scale (see Table below for values recommended by Draxler). X is downstream distance (from source), U is horizontal wind velocity and σ_α the standard deviation of the horizontal wind direction.

Current models of atmospheric diffusion are generally satisfactory for near-neutral stabilities. On the stable side, boundary layer parameters and diffusion are well-defined only for slightly stable conditions when there is sufficient mechanical turbulence generated to assure that the atmosphere is well-mixed. Vertical turbulence and diffusion rates are small and as a consequence of the three-dimensional nature of small scale turbulence, diffusion due to small scale eddies in three dimensions is reduced.

However, two-dimensional mesoscale horizontal eddies are not suppressed by vertical stability forces and are produced by gravity waves, terrain interactions etc.. The effect on the plumes is usually a slow meandering of the plume, i. e., the instantaneous plume may be thin but over a time period of an hour or more it may meander over a wide angel (Hanna, S.R., (1983): Lateral turbulence intensity and plume meandering during stable conditions. J. Clim. Appl. Met. 22, 1424-1430).

For stable conditions (Monin Obukov length scale greater than zero) and weak wind speed, u_* (ustar) less than 0.5 m/s, the horizontal diffusion parameter due to meandering is,

$$\sigma_{y_meandering} = 0.5 * X / U_{ref}$$

Where X is downstream distance from the source and U_{ref} is the wind speed at plume level.

This diffusion component is added to the ordinary sigma_y-value in the following way.

$$\sigma_y = \sqrt{(\sigma_y^2 + \sigma_{y_meandering}^2)}$$

A similar expression is used for the vertical coefficient:

$$\sigma_z = \frac{\sigma_w}{U} X \left[\frac{1}{1 + 0.9 \sqrt{\left(\frac{X}{UT_i} \right)}} \right]$$

where σ_w is the standard deviation of the vertical wind speed.

Recommended values of T_i according to Draxler (1976). Sources higher than 30 m are considered as elevated.

	Surface Sources		Elevated Sources	
	stable	unstable	stable	unstable
Lateral	300	300	1000	1000
Vertical	50	100	100	500

Note that all calculated meteorological parameters should be valid for simulation of one-hour values.

E3.1.5 Mesoscale Interpolation

Influence areas

Each grid point belongs to an influence type area and within each area the meteorological conditions are considered as similar. The influence areas can be for example sea, sea close to land, land, land close to sea, urban, suburban, and so on. There can be several different areas of the same kind, for instance two separate valleys. These influence areas must exist in a resource file with names and type numbers.

Observation places

Each observation place must be classified with an influence type number. The influence from every observation place on different areas must be stated with a real number $\alpha_k(n)$, in the interval [0,1], where k is an index for the observation and n the area type number.

Analysis method

Each grid point should be classified with an influence type number, say nn (see appendix D3.3). For every grid point (i,j) a value is interpolated from all observation places:

$$value(i, j) = \frac{\sum_k obs(k) \times weight(i, j, k)}{\sum_k weight(i, j, k)}$$

where

$$weight(i, j, k) = \frac{\alpha_k(nn)}{d_k(i, j)}$$

$d_k(i, j)$ = distance between the grid point (i, j) and the observation place k.

The resulting grid will thus be affected by the observations and to some extent also by different influence type areas.

L, u*, T*, w*, Z_i and mixh

The Monin-Obukhov length (L), friction velocity (u*), temperature scale (T*), convective velocity scale (w*), boundary layer (Z_i) and mixing height (mixh) are treated in much the same way.

The input data is taken from the pre-processor: L, u*, T*, w* and Z_i. It is also possible for Z_i to be measured directly, for instance from a SODAR.

If no principal station data exists within a zoomed area then data from the nearest principal mast is used as a constant value over the whole area.

The *heat island effect* is taken into account by adjusting stable conditions to neutral conditions over urban areas. The areas of distribution for which this correction is to be applied is defined in a grid - see *Appendix D3.3*.

The location of this effect is given in a grid, see *Appendix D3.3*.

Surface temperature

The input data are temperature observations from all places with at least two sensors in the vertical and in addition an analysed grid of L, u*, T* and Z_i from above.

With this information a surface temperature T_s and T_{init}, which assumes a surface zero heat flux flow, is computed for every observation.

If data are missing within a zoomed area the main mast is used as a constant value over the whole area.

Free wind

Input data are all wind observations and the analysed grid of L.

The wind speed is first extrapolated to 150 m with help of a power law and the wind direction is twisted according to empirical data (Holtslag).

If there is no principal mast data available within a zoomed area then data from the nearest principal mast is used as a constant value over the whole area.

E3.1.6 Procedures for Solving the Wind Model Equations

When the initial conditions have been estimated, the thermodynamic equation (eq. E3.1.2) is used to estimate the local change in potential temperature. The tendency equation (eq. E3.1.3) is then utilised in order to estimate the local pressure tendency due to temperature effects. The change in local pressure at ground level is then used in the momentum equation (eq. E3.1.1) to estimate a wind tendency. Thereafter, the slightly changed wind field is used to estimate the tendency in the surface potential temperature and so on.

By iterating in this way, a quasi-steady-state condition will usually be reached within a few time steps (10-20). According to the initial assumptions, the length of the time steps is not allowed to be larger than a few seconds, in order to have an adaption process within a few minutes. The Danard concept is to some extent a contradiction. The concept is a diagnostic model, trying to identify the small scale variations in the wind field due to the forcing at the surface. To do this, prognostic equations are applied, but for periods so short that the large scale transient effects such as wind rotation due to the Coriolis force are filtered out. Consequently, it is not possible to describe the evolution of a sea breeze, but to diagnose the sea breeze if relevant input data (mast data) is present.

It is worthwhile observing that the model is not mass conservative.

E3.1.7 Numerical Methods

Generally, centred time and space differences have been used, i.e. the so-called leapfrog method. An upstream formula has been used for the advection terms.

The length of the time steps (Δt) depends upon the resolution of the grid (Δs) and the wind speed of the large scale wind (V_g), i.e.

$$\Delta t = \frac{(0.125 \times \Delta s)}{V_g}$$

Normally, for a 250*250 m resolution and a typical large scale wind of 5 m/s, the length of the time steps would be 6 seconds. The total number of time steps has a maximum of 40. Consequently, the total adaption period in this case is 4 minutes.

E3.2 The Gauss Model

This model is used to simulate the distribution of ground concentrations of pollutants over urban or industrial areas with a typical scale of one or a few tenths of kilometres. The size of the application area is limited from below by the fact that the Gauss model coefficients are not valid close to the source (distances below approximately one hundred metres). The upper limit is given by the fact that more or less stationary conditions should prevail for the time it takes for an air parcel to be advected through the area. One hour mean values are simulated, as it is known that the wind may be more or less constant during such a period (daily averages would not be sufficient). With wind speeds of 2 - 5 m/s, an air parcel would travel 7 - 18 km within one hour. This limitation of the Gauss model should be kept in mind while performing simulations on scales larger than 20 km.

In order to avoid using the model on too large areas, producing unrealistically long plumes, the Gauss model plume length is limited. The maximum plume length is defined in a resource file and depends upon the actual stability and the persistency of different weather conditions.

The Gauss model does not resolve individual buildings. Instead, surface structures like houses and trees enter the model through local roughness values and, as a consequence, through the

wind field (see *E3.1 “The Wind Model - Calculation of the Wind Fields”*). Buildings give a rougher surface, more friction means a lower wind speed, which influences the dispersion, and so on.

The default setting for the calculation height is 2 m, but the user may specify any other value. The height at which the simulated concentration values are valid will coincide with the calculation height above ground in open areas (i.e. in the countryside). Over a city area, the simulation will reflect the concentrations at the specified height above the roof height. The default setting will thus give concentrations at roof height, not the concentration at street level. The blocking effects of buildings surrounding a street which lead to raised concentration levels can be studied separately (See *E3.4 “The Street Canyon Model”*).

Note that the Gaussian dispersion model simulates steady states of pollution concentrations. Accumulation of polluted air throughout various days can not be studied with this model.

These are the restrictions of the Lagrangean/Gaussian model, but there are advantages to be gained from using it too. State-of-the-art articles (e.g. Hanna et al, 1982) mention, among other things, the following points:

- It produces results that agree with experimental data just as well as any other model.
- It is fairly easy to perform mathematical operations on this equation.
- It is appealing conceptually.
- It is consistent with the random nature of turbulence.

Usually Gaussian plume models are applied to a horizontally homogenous wind field, while the model in Airviro will take into account a realistic wind field. This means that the effect of topography, roughness distribution and horizontal variations in surface heating/cooling will enter the dispersion calculation.

Clearly there are important cases where this model is not an ideal choice such as when the accumulation of pollutants is of interest and a time sequence must be simulated, or when the horizontal scales grow from an urban/local to a regional scale. Neither will dispersion in an application area with complicated topography - e.g. a narrow and deep valley - be satisfactorily treated with the Gaussian approach. For these cases, the Airviro user should choose the advection/diffusion Grid model (see *Appendix E3.3*).

E3.2.1 Source Type Definitions

The source emission data may be described as coming from a point, a road or an area or from the EDB. From a model point of view, these are all treated as point emissions (except EDB sources): A road will be treated as a number of points distributed along a line segment, and an area as a number of points equally distributed over a horizontal rectangle.

If the emission data is obtained from the EDB, then the area, road and grid layers are collected together on an emission grid at ground level.

A source specified as a point emitter can take into account an initial plume rise calculation, relevant for chimney stacks. Area sources assume a dispersion height prescribed by the user, while the road source is assumed to be identical with traffic emissions from roads (at ground level).

E3.2.2 Plume Rise Formulation

The plume rise calculation closely follows the recommendation made by Hanna et al. (1982) (if no other reference is given):

The release height, i.e. stack height, is denoted by h_s . Due to momentum (exhaust gas velocity) and buoyancy (exhaust gas temperature excess over the ambient temperature), the plume will rise considerably over the release height. Close to the source (typically within a horizontal distance of a few hundred metres), the rise and curve of the plume is more or less independent of turbulence and stratification in the ambient air. Later the atmospheric conditions become more important, and the final plume height is determined by the stability conditions.

The initial plume path height may be described as a function of horizontal distance from the source (X):

$$h_p = h_s + \left(\frac{3M_0}{\alpha^2 u_s^2} X + \frac{3F_0}{2\beta^2 u_s^2} X^2 \right)^{\frac{1}{3}}$$

where M_0 is the initial momentum flux and F_0 the initial buoyancy flux. Note the convention of the way the initial exhaust gas volume flux is defined: $V_0 = w$ (internal stack radius)², which means that a factor π is left out. Hence we get:

$$M_0 = wV_0$$

$$F_0 = \frac{g}{T_s} (T_s - T_a) V_0$$

where w is the (vertical) exhaust gas velocity, g is the gravitational acceleration, T_s is the exhaust gas temperature and T_a the air temperature (in °C).

The wind speed at stack height is denoted u_s . The empirical coefficients α and β are set to:

$$\alpha = 0.4 + \frac{u_s}{w} \quad \text{and} \quad \beta = 0.4$$

Here initial values of both momentum and buoyancy are used. When the plume mixes with ambient air, its lifting potential will decrease and it will reach the final plume height somewhat later than what the curve expression above states.

The final plume height ($h_e = h_s + \Delta h$) depends on stability conditions. For stable situations ($0 < L < 100$) the so called bent-over plumes are to be expected:

$$\Delta h = 2.6 \left(\frac{F_0}{u_m s} \right)^{\frac{1}{3}}$$

where s describes the atmospheric stability:

$$s = \frac{g}{T_a} \left(\frac{\Delta T_a}{\Delta z} + 0.01 \right)$$

The wind speed (u_m) - an average between stack height and final plume height - is estimated iteratively. The power law is used for extrapolating the wind velocity from the 10 m wind field value, using a power $p = 0.55$.

For very low wind speeds, the expression above may yield unrealistically large plume heights, hence an upper limit is calculated as (originally from Briggs, recommended by Omstedt, 1984):

$$\Delta h = 5 \frac{F_0^{0.24}}{s^{0.375}}$$

$$h_e'' = h_s + \Delta h$$

where h_e'' is the intermediate final plume height.

The calculated plume height may be higher than the mixed layer depth $mixh$, i.e. the plume penetrates the inversion. For a calculated plume height (h_e'') within 2 times the mixed layer depth, a fraction ($frac$) of the plume is reflected back below the inversion:

$$frac = \frac{mixh}{h_e''} - 0.5$$

Weil and Brower (1982) suggests this fraction should be treated as a plume that is dispersed within the mixed layer at a height (Δh) above the stack height (h_s). The calculated plume height then becomes:

$$h_e' = h_s + (0.62 + 0.38(1.0 - frac))(h_e'' - h_s)$$

The fraction that remains above the inversion will not influence ground pollution concentrations.

The final plume rise for unstable situations ($-68 < L < 0$) is calculated with the break-up model. The final rise is not limited by any inversion, instead its buoyancy is diluted by ambient turbulence until it stops rising (originally from Briggs, recommended by Omstedt, 1984):

$$\Delta h = 4.3 \left(\frac{F_0}{u_m} \right)^{0.6} H_*^{-0.4}$$

with
$$H_* = \frac{gH}{c_p \rho T_a}$$

and u_m as the mean wind speed between stack height and plume height. As before the vertical wind profile is extrapolated with the power law, here with $p = 0.15$.

As an upper limit of the plume rise during unstable conditions, we use an expression suggested by Weil (1979):

$$\Delta h = 0.62(mixh - h_s)$$

where, as before, h is the mixed layer depth and h_s the stack height. The plume height in this case is:

$$h_e' = h_s + \Delta h$$

There remain the neutral or near neutral cases ($L > 100$ or $L < -68$), when stronger wind speeds may be expected. For this stability class, the plume rise may be influenced by downdraft (effects of lee wake of the stack or of nearby buildings). The plume rise will also be lowered due to entrainment caused by downwind turbulence created by the stack (or the plume jet itself). According to Nielsen et al. (1986):

$$\Delta h = 1.54 \left(\frac{F_0}{u_p \cdot u_*^2} \right)^{\frac{2}{3}} (h_s + \Delta h_d)^{\frac{1}{3}} + \Delta h_e + \Delta h_m$$

where u_p - the wind speed at plume height - is extrapolated with a power $p = 0.25$, and u_* is the friction velocity.

The plume downdraft Δh_d is:

$$\Delta h_d = -2 \left(\frac{w}{u_s} - 1.5 \right) D$$

for wind speeds $u_s > 1.5w$, D being the outer diameter of the stack. The plume entrainment is calculated as

$$\Delta h_e = -0.25 \sqrt{DX_*}$$

with $X_* = 6.49 F_0^{\frac{2}{5}} \Delta h_d^{\frac{3}{5}}$ (Nielsen et al, 1986). The initial momentum contribution is

$$\Delta h_m = 3D \left(\frac{w}{u_s} - 1 \right)$$

and $h_e' = h_s + \Delta h$

For all stabilities, the plume height to be used is then the minimum value of the plume path h_p (close to the stack) expression and the final plume height estimate, that is:

$$h_e = \min(h_p, h_e').$$

E3.2.3 Building Downwash

So far it has been assumed that the plume is not influenced by nearby buildings or other obstacles. We repeat that the downdraft Δh_d calculated earlier was due to a pressure drop created by the stack itself.

Concerning the building downwash, Briggs (1973) has given some recommendations that are found in most textbooks, e.g. in Lyons and Scott (1990). These recommendations have been followed:

We consider only neutral or near neutral cases ($L > 100$ or $L < -68$), i.e. downwash will not occur for stable or unstable conditions.

Define a typical height H_b and a typical width W_b of the building/buildings near to - or under - the stack. What is to be considered as “near” is within a radius of about twice the stack height. For buildings with asymmetric dimensions in the horizontal, an equivalent “width” may be estimated as

$$W_b = \sqrt{length \cdot width}$$

(actually it is the crosswind width that is of importance, but we simplify this to a typical width). The relevant length scale (ξ) to estimate the downwash effects of the building is the minimum of the height and width scales

$$\xi = \min(H_b, W_b)$$

There are 3 regimes where the buildings influence the final plume height h_e :

a) The case when the plume is totally out of the building influence

$$h_s + \Delta h_d > H_b + 1.5\xi \Rightarrow h_e = h_e \text{ (from above, } \min(h_p, h_e') \text{)}$$

b) The case when the plume is within the influence area but still higher than the building:

$$H_b + 1.5\xi > h_s + \Delta h_d > H_b \Rightarrow h_e = 2(h_s + \Delta h_d) - (H_b + 1.5\xi) \quad (1)$$

c) The case when the plume is below the building height:

$$h_s + \Delta h_d < H_b \Rightarrow h_e = h_s + \Delta h_d - 1.5\xi \quad (1)$$

The plume is considered to be trapped within the cavity if the calculated h_e is less than 0.5ξ , and the final plume height will then be set to $0.5H_b$. The lateral spreading will be proportional to ξ (think of the plume as being spread out over the lee wall of the building).

E3.2.4 The Gaussian Plume Model

If we deal with a point, road or area emission, the model will treat this as one or several point emissions, to be dispersed at a certain plume height. Depending on the emission characteristics, we estimate an initial distribution of the pollutant defined by the initial (at $X = 0$) values of σ_y and σ_z :

For point sources introduced either as individual point sources or through the EDB, σ_y and σ_z at $X = 0$ are set equal to external stack radius.

For area sources introduced individually the initial σ_y is set to $\frac{dxy}{2}$ where

$$dxy = \sqrt{width^2 + length^2}$$

¹¹ It is important to note that the calculation of these h_e 's does not take the initial thermal and momentum lift into account. The transition from a plume height affected by thermal and momentum lift to a moderate plume height affected by buildings can therefore cause drastic changes in the calculated concentration field.

σ_z is defined with an empirical formula for neutral conditions, $\sigma_z = 0.22 \times dxy^{0.78}$.

For road sources introduced individually, σ_y is set to $\frac{dxy}{2}$ and in open areas σ_z is set to 3.57-0.53U.

However, in built up areas where the Gauss model calculations are evaluated at roof level, σ_y is set to 0.667*building height. The building heights are specified in a grid, see *Appendix D3.3*.

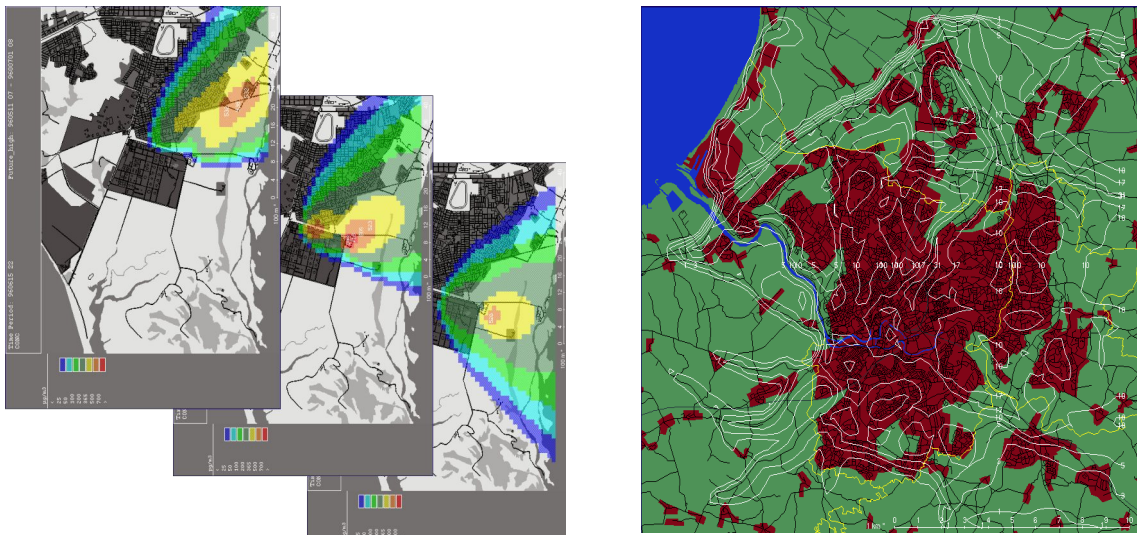
For area sources, road sources and grid layers specified in the EDB the emissions will enter the model in the form of an emission grid with grid size Δxy_{em} . The corresponding values of σ_y will be $0.5 \times \Delta xy_{em}$ and $0.5 \times \Delta xy_{em} \sigma_z$ is set to $\max[(3.57 - 0.53U), (0.667 \times \text{building height})]$.

The advection of the polluted air will follow trajectories in the wind field. For each emission point source, such a trajectory will constitute the plume centre line, i.e. a transformation to a Lagrangean coordinate system is taken place. The Gaussian plume equation is solved along the trajectories (the standard plume model may be found in any textbook on atmospheric dispersion, e.g. Hanna et al., 1982):

$$C = \frac{Q}{2\pi\sigma_y\sigma_zU} e^{-\frac{y^2}{2\sigma_y^2}} \left[e^{-\frac{(z-h_e)^2}{2\sigma_z^2}} + e^{-\frac{(z+h_e)^2}{2\sigma_z^2}} + e^{-\frac{(z+h_e-2h)^2}{2\sigma_z^2}} \right]$$

where the second and third exponential term within the brackets are due to reflection at the ground and top of mixed layer, respectively. For low inversions, there will be repeated reflections between the ground and the top mixed layer. The desired ground concentrations are found by setting $z = 2m$. The contribution of each individual (trajectory) plume is summed up on a calculation grid, where the grid concentrations are the true contributions over each grid area according to the curvature of the plume concentration distribution as a function of the distance from the plume centerline.

Output from Gaussian dispersion calculations are different types of maps, iso-lines or coloured grid, iso-colour, or as text grid files. There are also several post processing possibilities for dispersion calculation results in the Airviro Dispersion module.



Example-Gaussian plume time step sequence Example-Gaussian time average field

Necessary basic information for the Gaussian model

Physiographic information

GIS information is used to create physiographic parameters like land use classification, surface roughness (z_0), topography, house heights or other map based information like “heat island areas” and “influence zones”. The map resolution (GIS) information should at least be 50 x 50 meter.

Meteorological pre-processed input data

Hourly data from meteorological station (–s). Basic measurements are wind speed and wind direction, ground temperature and vertical temperature difference, standard deviations of vertical wind speed and horizontal wind direction. In a built in meteorological pre-processor, boundary layer parameters representative for the station (–s) location are calculated.

Meso-scale analysis

The meteorological pre-processed input data and other available meteorological data are via similarity profile methods transformed up to the level of free wind conditions and then interpolated/ extrapolated over the calculation area in order to get fields of free wind and temperature.

Wind modelling (2D)

Output from the meso-scale analysis, see above, and the ground surface conditions, are used as inputs to the wind model. The wind model generates a two-dimensional wind field representative for ten meters above ground.

Emission estimation

Emissions inputs are all factors influencing the emissions and source specific emission data (chimney height, annual emissions, traffic intensity etc). The emissions data are stored in an emissions database (EDB). When a dispersion calculation is started, an emissions modelling, appropriate for the simulation problem (substance, time, area for example), is made, i.e. a search in the EDB for the chosen emission scenario. The search result, a two dimensional emissions field and point emissions, is input data for the dispersion calculation.

E3.3 The Grid Model

The Eulerian Advection-Diffusion grid dispersion model built into Airviro is especially designed to meet the requirements given by areas with a complicated topography, e.g. valleys. The model has some additional advantages compared to the standard Gaussian dispersion approach:

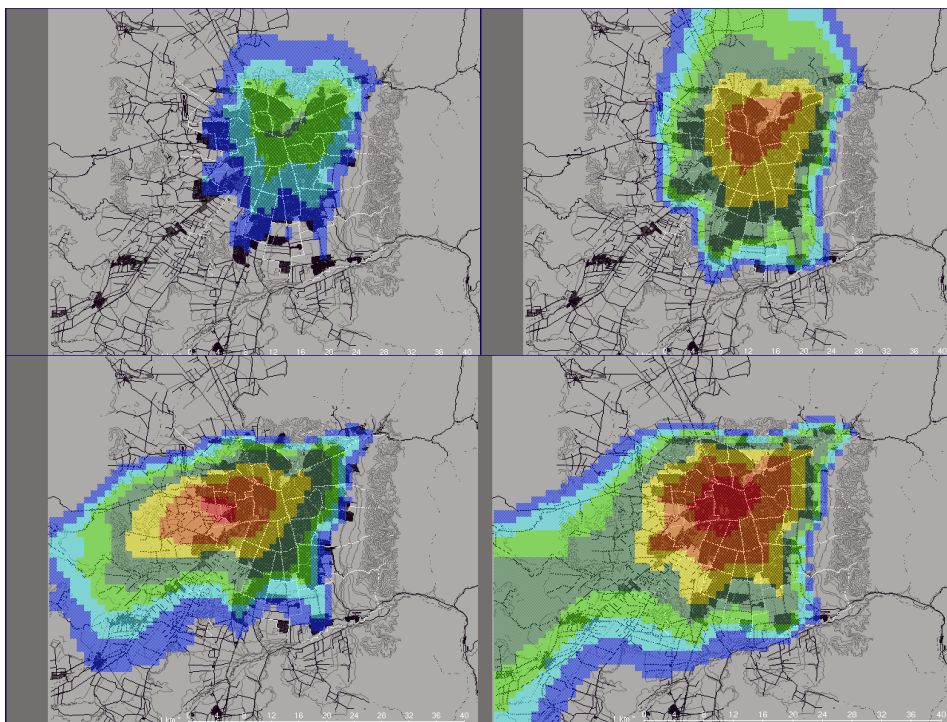
- It allows transient simulations and may simulate accumulation of pollutants during calm wind events.
- Boundary conditions (such as deposition) as well as particle characteristics (such as settling) may be introduced.

The Grid model does not resolve individual buildings. Instead, surface structures like houses and trees enter the model through local roughness values and, as a consequence, through the wind field (see E3.1 “The Wind Model - Calculation of the Wind Fields”). Buildings give a more rough surface, more friction means a lower wind speed which influences the dispersion, and so on.

The default setting for the calculation height is 2 m, but the user may specify any other value. The height at which the simulated concentration values are valid will coincide with the calculation height above ground in open areas (i.e. in the countryside). Over a city area, the simulation will reflect the concentrations at the specified height above the roof height. The default setting will thus give concentrations at roof height, not the concentration at street level. The blocking effects of buildings surrounding a street which lead to raised concentration levels can be studied separately (See E3.4 “The Street Canyon Model”).

The Grid model is designed for use on larger areas. It is not suitable for use with small scale calculations and therefore a minimum limit of 100m has been set for the size of the sides of the grid boxes used for calculations.

Output from GRID dispersion calculations are different types of maps, iso-lines or coloured grid, or text grid files. There are also several post processing possibilities in the Airviro Dispersion module. The user can step through the output result hour by hour, and optionally display the wind fields and concentrations on several levels.



Example-Distribution of NOx levels in Santiago de Chile, July 2-3 of 1995.
Simulation area 50 km x 60 km.

Necessary basic information for the Grid model

Physiographic information

GIS information is used to create physiographic parameters like land use classification, surface roughness (z_0), topography, house heights or other map based information like “heat

island areas” and “influence zones”. The map resolution (GIS) information should at least be 50 x 50 meter.

Meteorological pre-processed input data

Hourly data from meteorological station (-s). Basic measurements are wind speed and wind direction, ground temperature and vertical temperature difference, standard deviations of vertical wind speed and horizontal wind direction. In a built in meteorological pre-processor, boundary layer parameters representative for the station (-s) location are calculated.

Mesoscale analysis

The meteorological pre-processed input data and other available meteorological data are via profile methods transformed up to the level of free wind conditions and then interpolated/ extrapolated over the calculation area in order to get fields of free wind and temperature.

Wind modelling (3D, only with Grid Model)

The input is the 2-D wind field (10 m) from “Wind modelling (2D)”. Interpolation of wind fields in vertical layers, result in 3-D wind fields.

Dispersion modelling (3D, Grid)

The input is 3-D wind field (free wind), 2-D emission field for a predefined time sequence. The output is 2-D concentration fields on different levels displayed overlaid on a map in isolines and/or coloured grid or iso-colour.

E3.3.1 Formulation of the Grid Model

The model is based on the three-dimensional advection-diffusion equation for a certain substance. The substance could be one passive substance, a scalar, a chemically active substance or a suspension of non-interacting particles with or without deposition properties. The model for a chemically active substance includes in principle an advection-diffusion equation for each of the interacting “mother” and “daughter” substances. The model equation (see for example Pielke (1984)) is:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} = \frac{1}{\rho} \frac{\partial}{\partial z} \left[\rho \left(K_z \frac{\partial c}{\partial z} + w_s c \right) \right] + \frac{Q}{\rho}$$

where

c= concentration, mass of substance per unit volume/ mass of air per unit volume

ρ= density of air, a function of height

u,v,w= wind velocity components

x,y,z= cartesian coordinates

w_s= particle settling velocity

Q= sources

K_z= vertical turbulent diffusion coefficient

The equation is solved on a three-dimensional numerical grid. Two successive coordinate transformations of the equation are made. The necessary three-dimensional wind field (u,v,w) is produced by using the two-dimensional surface wind field, obtained with the wind model, combined with similarity profiles for the boundary layer and the constraint of mass continuity.

E3.3.2 Numerical Methods

The transport equation is solved with an operator splitting method and the method of fractional steps (Yanenko (1971), Marchuk (1975)). A decomposition of the operators in the transport equation is made (see also McRae et al (1982)). Note that here the operators have not been specified in the time domain:

$$c^{t+1} = A_x A_y A_z (A_c A_c) A_z A_y A_x c^{t-1}$$

A_x and A_y are the advection operators in the horizontal directions. A_z is the vertical advection, diffusion, deposition and (chemically passive) source/sink operator. A_c is the chemical sink/source operator. Principally, we then have the following principal sequence of equations to solve:

$$\begin{aligned} c^* &= A_x c^{t-1} \\ c^{**} &= A_y c^* \\ c^{***} &= A_z c^{**} \\ c^t &= (A_c A_c) c^{***} \\ c^{t+*} &= A_z c^t \\ c^{t+**} &= A_y c^{t+*} \\ c^{t+1} &= A_x c^{t+**} \end{aligned}$$

We are then solving several one-dimensional equations instead of one three-dimensional equation. The basic idea with the splitting method is that it is faster to solve the sequence of triangular matrices associated to the equations above, than to invert a large ordinary non-triangular matrix associated with the nonsplitted transport equation.

To solve the equations on the numerical grid, they are reformulated with different numerical techniques depending on the type of operator. In the horizontal directions a finite element scheme is used, a Galerkin method with linear basis functions (see Long and Pepper (1976), McRae et al (1982), Chock and Dunker (1983), van Stijn et al (1987), Pielke (1984), for example). In the vertical direction and for the chemical step a finite difference scheme is applied. In the time domain, a Crank-Nicholson approach is used in the horizontal directions and for the chemical operator. Fully implicit time stepping is applied in the vertical direction.

In the horizontal a non-linear implicit numerical filter is applied after each time step in order to remove the shortwave noise produced by the approximate numerical method (Pielke (1984)). The filter also acts, together with numerical diffusion, as an artificial horizontal diffusion. Modelling of the physical horizontal turbulent diffusion has so far not been introduced in the model.

E3.3.3 Boundary Conditions

At the lateral boundaries constant inflow and gradient outflow conditions are applied (see Pielke (1984)). A Laplacian filter is applied at the lateral boundaries at each time step.

At the lower boundary, the surface, zero wind velocity is introduced through the wind fields. The dry deposition rate is the lower boundary condition for the turbulent transport.

E3.3.4 The Numerical Grid, Coordinate Transformations

Basically the transport equation is formulated in a Cartesian co-ordinate system. In order to make the dispersion calculations in a proper topographical and numerical space environment, two space co-ordinate transformations are made.

The topographical properties of the terrain in the calculation domain are considered by a co-ordinate transformation to a terrain following co-ordinate system (Pielke (1984)). The vertical co-ordinate is transformed according to,

$$\sigma = \frac{z - z_g}{z_{top} - z_g}$$

where z_{top} is the top level of the calculation domain, z_g is the terrain height and z is the vertical co-ordinate.

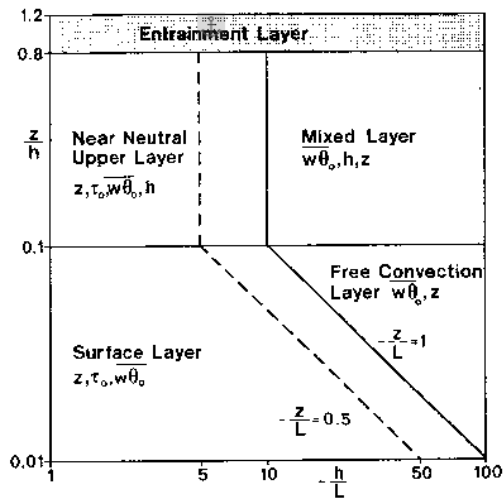
The staggered vertical co-ordinate σ is transformed to a logarithmic-linear vertical co-ordinate.

$$\zeta(\sigma) = a \left[\frac{1}{K} \ln \left(\left(\frac{\sigma + z_0}{z_0} \right) + \frac{\sigma}{b} \right) \right] + 1$$

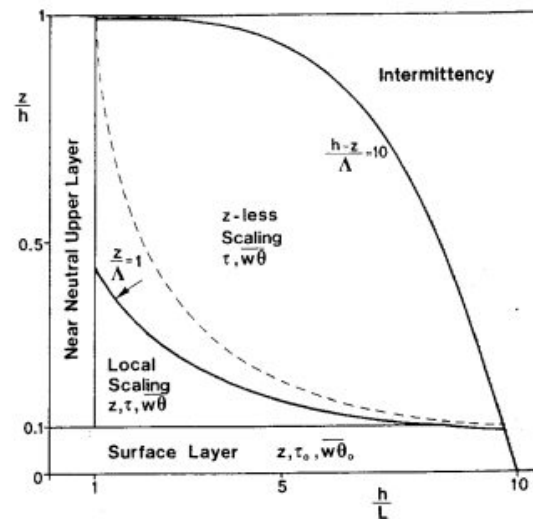
where z_0 is the surface roughness. For a certain choice of the coefficient a , the ζ -system is adjusted in an iterative way so that the distance between the grid points ($\Delta\zeta$) is close to unity for a given number of grid points. With the coefficient b , the resolution of the log-lin scale is tuned. The spacing between the levels is normally much finer close to the surface than higher up.

E3.3.5 The Turbulent Exchange Coefficient

The parameterisation of the vertical turbulent exchange coefficient is done according to a state of the art approach. A classification of different scaling regimes in the boundary layer, shown in Figures 1 and 2 below for unstable and stable conditions, respectively, has been introduced. In the figures z is distance above ground, h is the height of the boundary layer and L is the Monin-Obukov length scale, a parameter characterising the atmospheric stability. Negative L 's means unstable conditions while positive L 's indicate stable conditions. Stable conditions do suppress the vertical turbulent mixing, typical clear night conditions. Small values of h/L indicate close to neutral conditions, i.e. the vertical turbulent mixing is of mechanical origin only, thermal forces are more or less absent (Holtslag, A.A., and F.T. Nieuwstadt (1986): Scaling the atmospheric boundary layer. *Boundary -Layer Meteor.*, 36:201-209).



Definition of scaling regions in the unstable ABL ($L < 0$). Basic scaling parameters for the turbulence are indicated. Holtslag, 1987.



Definition of scaling regions in the stable ABL ($L > 0$). Basic scaling parameters for the turbulence are indicated, Holtslag 1987.

Figure 1.

Figure 2.

Convective Boundary Layer ($L < 0$)

Surface layer

$$kz(ix, iy, iz) = 0.4 * ustar * z / Fih(z, lmo)$$

Free convection layer

$$kz(ix, iy, iz) = wstar * z$$

Nearly neutral upper layer

$$kz(ix, iy, iz) = 0.4 * ustar * mixh / Fih(hs, lmo)$$

Mixed layer

$$kz(ix, iy, iz) = 0.1 * wstar * mixh$$

Layer above

$$kz(ix, iy, iz) = 0.1 * 0.4 * ustar * mixh / Fih(hs, lmo)$$

or

$$kz(ix, iy, iz) = 0.1 * 0.1 * wstar * mixh$$

Stable Boundary Layer ($L > 0$)

Surface layer

$$kz(ix, iy, iz) = 0.4 * ustar * z / Fih(z, lmo)$$

Nearly neutral upper layer

$$kz(ix, iy, iz) = 0.4 * ustar * mixh / Fih(hs, lmo)$$

Layer above

$$kz(ix, iy, iz) = 0.1 * 0.4 * ustar * mixh / Fih(hs, lmo)$$

or

Surface layer

$$kz(ix, iy, iz) = 0.4 * ustar * z / Fih(z, lmo)$$

Nearly neutral upper layer

$$kz(ix, iy, iz) = 0.4 * ustar * mixh / Fih(hs, lmo)$$

Local scaling layer

$$kz(ix, iy, iz) = 0.4 * ustarl * z / Fih(z, lmo)$$

z-less scaling layer

$$kz(ix, iy, iz) = 0.4 * ustarl * lmo$$

Intermittency layer

$$kz(ix, iy, iz) = 0.1 * 0.4 * ustar * mixh / Fih(hs, lmo)$$

Layer above

$$kz(ix, iy, iz) = 0.1 * 0.4 * ustar * mixh / Fih(hs, lmo)$$

 $Fih = 0.74 / \sqrt{1 - 9.0 * z / lmo}$; $Lmo < 0$; $z / Lmo > 1$; unstable

 $Fih = 0.74 + 4.7 * z / lmo$; $Lmo > 0$; stable

 $ustar = \text{friction velocity} (= \sqrt{\frac{\tau_0}{\rho}})$
 $ustarl = \text{local ustar} (= ustar * (1.0 - z / hs) ** 0.75)$

$$wstar = \text{convective velocity scale} \left(\left(g \cdot mixh \cdot \frac{H_0}{\rho c_p T_0} \right)^{\frac{1}{3}} \right)$$

H_0 = surface heat flux

T_0 = air temperature at the surface

g = gravitational acceleration

ρ = density of air

c_p = specific heat of air at constant pressure

κ = von Kármán's constant

z = height above the surface

hs = surface layer height (= 0.1*mixh)

lmo = Monin-Obukov length scale

lmo_l = local lmo (= $lmo \cdot (1.0 - z/zii)^{1.25}$)

$mixh$ = height of the mixed layer

E3.3.6 The Three-Dimensional Wind Field

The construction of the surface (two-dimensional) wind field is described in *section E3.1*. In order to create a three-dimensional wind field, necessary for the three-dimensional grid model, vertical profiles of the horizontal wind field are calculated at every grid point. The profiles are calculated according to methods described in another section. The profiles are distributed through the boundary layer up to the height $mixh$, the mixed layer height. Above $mixh$ a free wind field, constant up to the top of the calculation domain, is assumed to prevail.

Having obtained horizontal wind fields (u, v) at each level in the numerical calculation grid, the vertical, cartesian, wind components are calculated with the use of a numerical formulation of the mass continuity equation,

$$\frac{\partial w}{\partial z} = \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}$$

or, if the horizontal wind fields are evaluated directly in the ζ -system:

$$\frac{\partial w^\zeta}{\partial \zeta} = \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}$$

where w^ζ = vertical velocity in the ζ -system.

E3.3.7 Source Initialisation

The Grid model only uses the EDB to obtain emission input data. Point sources are treated individually and all other sources are collected together onto an emission grid.

The sources are distributed in the three-dimensional grid according to type and size. The source strength for a road source passing through a grid square is transformed to an equivalent grid area source.

A point source from a stack is initially modelled by a series of puffs until the puff radius has grown to the size of two grid sizes. The puff is then released as a three-dimensional source

into the grid equation solver. Plume rise and downdraft is calculated according to E3.2.2 “Plume Rise Formulation”.

E3.3.8 Dry Deposition of Gases and Non-Gravitating Particles

The process of dry deposition of gases and very small non-interacting particles is determined by the turbulent conditions in the boundary layer. The transport through the air down to the ground is therefore incorporated in the turbulent diffusion term in the transport equation. The transport from the lowest part of the surface layer to the ground, the boundary condition in the diffusion term, is in principle modelled as:

$$\left(K_z \frac{\partial c}{\partial z} \right)_{surface} = v_g c_{surface}$$

v_g is called the dry deposition velocity. When dry deposition is calculated in the grid model, direct estimates of the dry deposition velocities for the different land use classes, i.e. sea, field, wood etc., are given by default in a resource file. Discussions about dry deposition can be found in Hanna et al (1985), McMahon and Denison (1979) and Schmel (1980).

It is also possible to calculate the dry deposition velocities to adapt to the actual local conditions.

For gases the deposition velocity is modelled as:

$$\frac{1}{v_g} = r_a + r_b + r_c$$

r_a is the atmospheric resistance for the surface layer (the aerodynamic resistance), r_b is resistance in the laminar boundary layer and r_c is the canopy resistance.

The aerodynamic resistance is a function of the surface layer conditions. During unstable conditions ($L < 0$) r_a is calculated as:

$$r_a(z_r) = \frac{0.74}{\kappa u_*} \left[\ln \left(\frac{x-1}{x+1} \right) - \ln \left(\frac{y-1}{y+1} \right) \right]$$

where

$$x = \sqrt{1 - 9 \frac{z_r}{L}} \quad \text{and} \quad y = \sqrt{1 - 9 \frac{z_0}{L}}$$

For stable stratification ($L > 0$) we have:

$$r_a(z_r) = \frac{1}{\kappa u_*} \left[0.74 \ln \frac{z_r}{z_0} + \frac{4.7}{L} (z_r - z_0) \right]$$

and for neutral conditions

$$r_a(z_r) = \frac{0.74}{u_*} \ln \frac{z_r}{z_0}$$

The resistance in the laminar boundary layer, r_b , depends also on the physical properties of the air and the gas:

$$r_b = \frac{2}{\kappa u_*} \left(\frac{\nu}{D} \right)^{\frac{2}{3}}$$

where

ν = kinematic viscosity of air

D = molecular diffusion coefficient of gas

The canopy resistance, r_c , is a function of the type of gas and vegetation, the vegetation density and the type of ground surface:

$$r_c = \left(\frac{1}{R_m} + \frac{LAI}{r_{st} + r_{mes}} + \frac{LAI}{r_{cut}} \right)$$

where;

R_m = ground surface resistance

$r_{st} + r_{mes}$ = foliage resistance, a stomatal and mesophyll part

r_{cut} = cuticle resistance

E3.3.9 Wet Deposition

The wet deposition depends on the concentration of the actual gas and on the precipitation. The most important processes for the small particles are the condensation of water on the particles, i.e. forming cloud water drops, and the impaction against falling water drops under the clouds. The uptake of gases in the cloud drops depends on the chemical processes in the drops. The interchange of gases between the drops and their surroundings is relatively fast and therefore in equilibrium.

The wet deposition is modelled as

$$-\lambda c$$

where λ is a washout coefficient defined as:

$$\int_0^h \lambda(z) c(z) dz = dep = W_r c_0 P$$

Both λ and c are functions of the height, λ is in addition a complicated function of the precipitation. On the right hand of the equation we have W_r , the washout ratio, P , the precipitation and c_0 the ground level concentration. These variables are better known than the complicated washout coefficient and the approximation:

$$\bar{\lambda} c_0 \text{mixh} \Rightarrow \bar{\lambda} = \frac{W_r P}{\text{mixh}}$$

$$\int_0^h \lambda(z) c(z) dz = \bar{\lambda} \bar{c} \text{mixh} =$$

which for the moment is applied in the grid model. mixh is the mixed layer height. Estimations of the washout ratio are for example found in Hanna et al (1982) and McMahon and Denison (1979).

E3.3.10 Particle Settling

Particles in a certain size range are affected by gravitational forces without being so big as to be ballistical. For the dispersion treatment of this class of particles, a settling or sedimentation velocity (w_s) coupled with the vertical concentration gradient, is used (see formula in E3.3.1 “Formulation of the Grid Model”).

Principles and estimates of the settling velocity can be found for example in Hanna et al (1982).

It is important to note that if the actual particle size distribution is wide, many dispersion calculations have to be done with each calculation representing a narrow size range. The reason is that the settling velocity is a very strong function of the particle diameter.

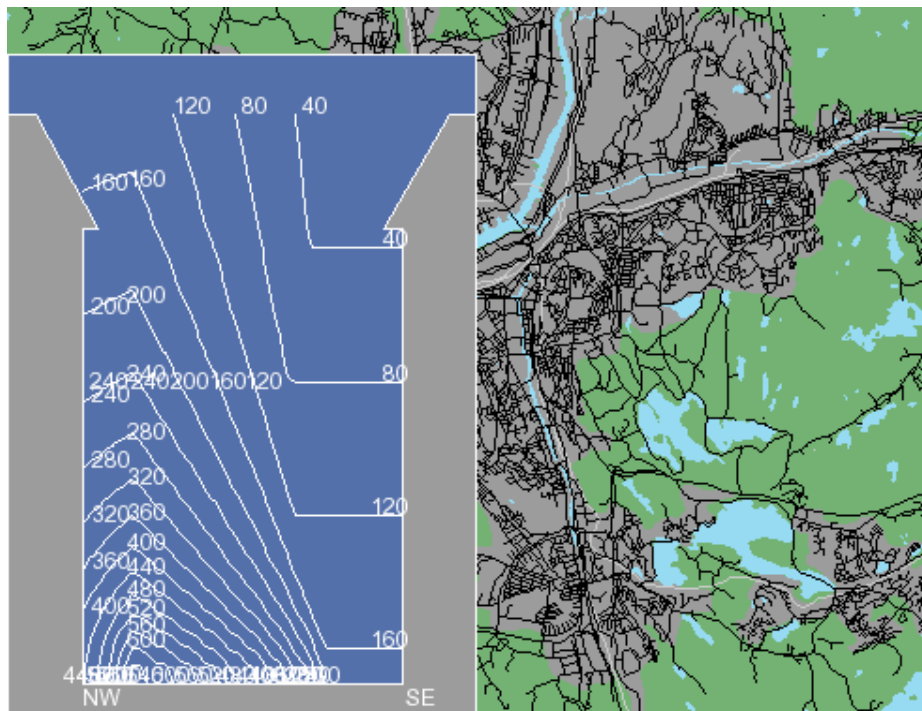
E3.4 The Street Canyon Model

Both the Gauss and the Grid model calculate roof level concentrations. The Street Canyon model is a small-scale model that allows you to simulate the street level concentrations on a single road that has a row of buildings on each side. The simulated concentrations are visualised on a vertical plane perpendicular to the street direction, the buildings creating the effect of looking down a canyon.

This model simulates the dispersion from traffic on a particular road. The user must be aware of the fact that traffic on other roads may very likely contribute to a substantial part of the pollution levels, especially if the simulated road has a low traffic intensity and is surrounded by larger streets. Will it then be possible to separately estimate the fractions of street pollution created by the local traffic and those created by emissions on other places?

A feasible way to do this within Airviro is to

- run the street canyon model with traffic emissions only from the particular road/road section of interest
- run a city-wide simulation with the Gauss or the Grid model, including all sources except for the traffic on the particular road/road section of interest. The concentration at roof level above the street of interest can then be considered as a result of non-local sources. Due to the eddy circulation mentioned earlier, the same contribution from non-local sources down in the street canyon itself can be expected. This concentration level can be considered as a background value to be added to the street canyon model results.



Example-Street Canyon Model result display

Necessary basic information for the Street Canyon model

Physiographic information

GIS information is used to create physiographic parameters like land use classification, surface roughness (z_0), topography, house heights or other map based information like “heat island areas” and “influence zones”. The map resolution (GIS) information should at least be 50 x 50 meter.

Meteorological pre-processed input data

Hourly data from meteorological station (-s). Basic measurements are wind speed and wind direction, ground temperature and vertical temperature difference, standard deviations of vertical wind speed and horizontal wind direction. In a built in meteorological pre-processor, boundary layer parameters representative for the station (-s) location are calculated.

Mesoscale analysis

The meteorological pre-processed input data and other available meteorological data are via profile methods transformed up to the level of free wind conditions and then interpolated/ extrapolated over the calculation area in order to get fields of free wind and temperature.

Wind modelling (2D)

Output from the meso-scale analysis, see above, and the ground surface conditions, are used as inputs to the wind model. The wind model generates a two-dimensional wind field representative for ten meters above ground.

Emission estimation

The emissions data are stored in an emissions database (EDB). When a dispersion calculation is started, an emissions modelling, appropriate for the simulation problem (substance, road), is made, i.e. a search in the EDB for the chosen emission scenario. The search result, a two dimensional emissions field and point emissions, is input data for the dispersion calculation.

E3.4.1 Model Description

The basis of the model originates from studies in San José, USA, where measurements indicated a vertical eddy circulation when the wind was blowing perpendicular to the street directions. The eddy circulation implies higher pollution concentrations on the upwind side of the road, because this air includes the traffic exhausts. The leeward side shows much lower concentrations, as the air originates from the roof level. The model is referred to as the “Stanford model”.

The “Stanford model” expressions have been tested and modified in a study in Scandinavia (SNV, 1977) and the expressions for the CL (concentration leeward side, i.e. on the upwind side of the street) and CW (concentration wind side) are used in the Airviro model. The original CL-equation is modified with a wind polynomial reported in Laurin and Omstedt (1987):

$$CL = \frac{K \cdot Q}{(u + 0.5) \cdot \left[(x^2 + y^2)^{\frac{1}{2}} + L_0 \right]} (0.27 \cdot u - 0.016 \cdot u^2 + 0.65)$$

$$CW = \frac{K \cdot Q \cdot (H - z)}{W \cdot (u + 0.5) \cdot H}$$

where

K is an empirical constant, set to 14

Q is the traffic emission in g/(m,s)

u is the wind component perpendicular to the street axis, in m/s

L₀ is a length scale of the individual cars, set to 2 m

W is width between the houses, H the typical house height in m

x, z are horizontal and vertical distances from the street emission segments

The vertical section between the houses is divided into a grid, on which the concentrations are evaluated. The road, i.e. the part of the street width (RW) where the emission takes place, is divided into a large number of road segments with equal emission rate.

The wind component is taken from the wind field calculation, evaluated at the street location. If the wind is blowing within 22.5 degrees from the principal street direction, the concentration will be found as an average of CL and CW, being symmetric.

For cases with a wind direction more perpendicular to the street direction, we will find an asymmetry with higher concentrations on the side of the road from where the roof wind blows (lee side) and lower values on opposite side (called wind side). The concentrations on the wind side of the emitting road are calculated according to CW. At the other grid points, a

summation of CL values takes place, implying a contribution from each emitting segment situated upwind the grid point itself (no impact from an emitting segment situated downwind).

E3.5 The Heavy Gas Model

The Heavy Gas Model is a model system for the description of the emission and dispersion of gases heavier or denser than the ambient air.

Dense gases are gases that are heavier than the ambient air because of the following reasons:

- they have a higher molecular weight than the air at the air temperature
- they are stored as condensed gases at a low temperature
- they are stored as condensed gases at a high pressure
- a mixture of the above mentioned reasons

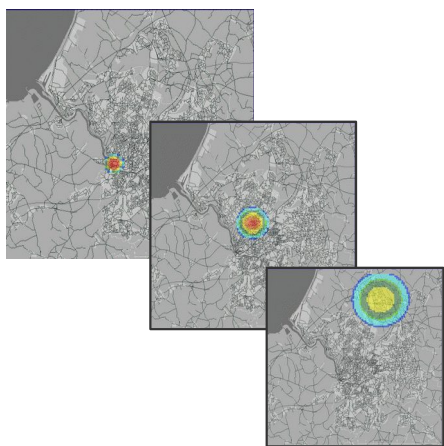
These types of gases are often toxic and in addition a condensed gas is very cold when it is released. It can therefore cause frostbite in people who come into contact with a released condensed gas cloud. The gas cloud can also have suffocating effects even if it is neither toxic nor very cold.

The model should be applied to industrial and transportation environments, where storage and transportation of this type of gas, for example chlorine, ammonia and propane, takes place.

The accidents or scenarios which can currently be simulated in the model are,

- The rupture of a storage container, resulting in a “large” hole in a pressurised container. The emission from this type of accident is assumed to be quite a violent boiling off of the condensed liquid. The release time is assumed to be short. This scenario is therefore classified as an instantaneous liquid phase release. A dense puff is eventually formed which is transported away with the wind while collapsing gravitationally. After some time the puff is diluted and it behaves as a neutral density puff.
- A “small” hole leakage, which could mean a leakage from a valve or a broken small pipe. The release time is assumed to be quite long. The release can originate from both the liquid and the gas phase of the pressurised storage vessel. This scenario type is called a continuous liquid or gas phase release. A heavy gas continuous plume or slab is formed. The slab stretches out in the wind direction and gets wider because of the gravitational spread perpendicular to the main slab direction. When the plume density is the same as the ambient air, the plume behaves as a neutral Gaussian plume.

It is clear that a simulation includes the application of several models. Emission models, models for initial cloud forming, gravitational phase models and models for the neutral plume phase. A description of appropriate models for each release scenario are given below.

	
Example-Tank burst development	Example-Continuous leak

Necessary basic information for the Heavy Gas model

Physiographic information

GIS information is used to create physiographic parameters like land use classification and surface roughness (z_0). The map resolution (GIS) information should at least be 50 x 50 meter, see also, Airviro Specification, D3, "Data Required for System Preparation for Dispersion Calculations".

Meteorological pre-processed input data

Hourly data from meteorological station(-s). Basic measurements are wind speed and wind direction, ground temperature and vertical temperature difference, standard deviations of vertical wind speed and horizontal wind direction. In a built in meteorological pre-processor, boundary layer parameters representative for the station (-s) location are calculated, see also, Airviro Specification, D3, "Data Required for System Preparation for Dispersion Calculations".

Emissions estimation

Emissions inputs are made by direct specifications when a dispersion calculation is made. The characteristics of the emitted substances are stored in a model specific resource file.

E3.5.1 Continuous Release or a Leakage From a Small Hole

The initial phase - Emission from the liquid phase

A choked two phase outflow is assumed (Winter et al (1984)). The emission or outflow is:

$$q_0 = A c_f G_0 \quad (\text{kg/s}) \quad (\text{eq E3.5.1})$$

A is the prescribed outflow area, c_f a frictional coefficient and G_0 is the maximum of the function:

$$G(p) = \sqrt{\frac{p_0 - p}{v(p)}} \quad (\text{kg/s,m}^2) \quad (\text{eq E3.5.2})$$

where p_0 is the pressure in the vessel, p is the pressure which maximises the function, normally higher than the atmospheric pressure. $v(p)$ is the specific volume of the binary substance at the outlet section. A two phase momentum jet forced by the momentum outflow and the difference between the pressure p and the atmospheric pressure p_a , is assumed to stagnate and form an continuous initial heavy (or neutral) gas cloud. The momentum of the jet is constant and equal to the initial momentum:

$$M = q_0 u_0 + A(p - p_a) \quad (N) \quad (\text{eq E3.5.3})$$

where u_0 is the outlet velocity.

$$u_0 = \frac{q_0}{Av(p)} \quad (\text{m/s}) \quad (\text{eq E3.5.4})$$

The jet formulae are (Winter et al. (1984)):

$$\text{- massflow} \quad q(x) = C_1 \sqrt{M \rho_a x} \quad (\text{kg/s}) \quad (\text{eq E3.5.5})$$

$$\text{- centre velocity} \quad u_c(x) = C_2 \sqrt{\frac{M}{\rho_a}} \frac{1}{x} \quad (\text{m/s}) \quad (\text{eq E3.5.6})$$

C_1 and C_2 are coefficients and ρ_a is the air density. The initial cloud is formed when the centre velocity is of the same order as the ambient wind velocity. The distance x to the cloud forming and the massflow at that distance are given by equations E3.5.6 and E3.5.5 respectively. The relation between $q(x)$ and q_0 gives the dilution. The size of the cloud, the average concentration and the average temperature are then easily calculated. The cloud is assumed to be rectangular, with the wind parallel side decided by the local trajectory length and the height is half the wind perpendicular side. The duration of the release is found by the assumption that the whole tank contents are released.

Emission from the gas phase

The gas outflow is tested for critical flow conditions. If the relation between the outlet pressure, the atmospheric pressure p_a , and the tank pressure p_0 :

$$\frac{p_a}{p_0} \leq \left(\frac{2}{\kappa + 1} \right)^{\frac{\kappa}{\kappa + 1}}, \kappa = \frac{c_p}{c_v} \quad (\text{eq E3.5.7})$$

is less than a certain gas specific value, the outflow is critical. c_p and c_v are the specific heat capacities at constant pressure and constant volume, respectively. Critical conditions give the velocity and mass flux at the outlet:

$$\text{- velocity} \quad u_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} p_0 v_0} \quad (\text{m/s}) \quad (\text{eq E3.5.8})$$

$$\text{- mass flux} \quad q_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} \left(\frac{2}{\kappa + 1} \right)^{\frac{2}{\kappa - 1}} \frac{p_0}{v_0}} \quad (\text{kg/s}) \quad (\text{eq E3.5.9})$$

otherwise, if condition E3.5.7 is not fulfilled,

$$\text{- velocity } u_0 = \sqrt{2 \frac{\kappa}{\kappa+1} \left[1 - \left(\frac{p_a}{p_0} \right)^{\frac{\kappa-1}{\kappa}} \right]} \quad (\text{m/s}) \quad (\text{eq E3.5.10})$$

$$\text{- mass flux } q_0 = \sqrt{2 \frac{\kappa}{\kappa-1} \left[\left(\frac{p_a}{p_0} \right)^{\frac{2}{\kappa}} - \left(\frac{p_a}{p_0} \right)^{\frac{\kappa+1}{\kappa}} \right] \frac{p_0}{v_0}} \quad (\text{kg/s}) \quad (\text{eq E3.5.11})$$

Using the jet equations E3.5.3 to E3.5.6, with the initial values given by equations E3.5.8 to E3.5.11, gives the necessary initial cloud characteristics, the height and length of the cloud are calculated as described earlier. The duration of the release is found by the assumption that the release is over when the tank liquid temperature has decreased to its boiling point.

The gravitational dispersion phase

If the initial cloud is denser than the ambient air, it will collapse because of the gravitational forces. When the cloud height decreases, the sides of it will travel outwards, forming a pancake-like cloud. Simultaneously the cloud will be advected by the wind in the wind direction. A ground based plume, stretching out in the wind direction and widening primarily by gravitational outflow, will be formed. Mixing and entrainment will take place at the top and the edges of the plume. The mixing processes used are the same as described in Eidsvik (1980). The gravitational widening velocity is:

$$u_g = C_3 \sqrt{gH \frac{\rho_p - \rho_a}{\rho_p}} \quad (\text{m/s}) \quad (\text{eq E3.5.12})$$

C_3 is a coefficient, here equal to 1.0. g is the gravitational acceleration, H is the cloud height and ρ_p is the plume density.

The neutral dispersion phase

When the plume is diluted so much that the plume density is close to the density of the ambient air, the gravitational effects are small and the plume behaves like a traditional non-buoyant ground surface plume. At this stage a Gaussian plume model, described on an other place in this documentation, takes over and proceeds with the dispersion calculations (see *Appendix E3.2*).

E3.5.2 Instantaneous release or a tank rupture - Emission only from the liquid phase

In this case a large hole is assumed to be formed. An accident could for example be caused by overfilling of the storage container. A slight temperature rise could cause a fracture in a weak section of the container. A violent boiling creating an intense two phase jet could be the result.

The hole area is assumed to be (Winter et al. (1984)):

$$A = C_4 V^{\frac{2}{3}} \quad [\text{m}^2] \quad (\text{eq E3.5.13})$$

where V is the tank volume and C_4 is a coefficient. The emission phase follows equations E3.5.1 to E3.5.6. The whole tank contents are assumed to boil off. The maximum distance between the source and place where the initial cloud is formed is (Winter et al. (1984)):

$$x = C_5 \left(\frac{u(x) T \tau}{\rho_a} \right)^{\frac{1}{4}} \quad [\text{m}] \quad (\text{eq E3.5.14})$$

C_5 is a coefficient, T is the mass contents in the tank, $u(x)$ is the jet velocity when the jet pressure has decreased to the atmospheric pressure and t is the release duration time. The volume of the initial cloud is:

$$\text{Vol} = C_6 \left(\frac{u(x) T \tau}{\rho_a} \right)^{\frac{3}{4}} \quad [\text{m}^3] \quad (\text{eq E3.5.15})$$

The initial cloud is assumed to be cylindrical with equal radius and height. The gravitational and the neutral dispersion phase are in principle the same as in the earlier description.

E3.5.3 Substances and Coefficients

Currently the model can handle the following substances:

Ammonium, chlorine, sulphur dioxide, propane, vinyl chloride and methane.

The coefficient values are (Winter et al. (1984):

$C_1 =$	0.284
$C_2 =$	7.21
$C_3 =$	1.0
$C_4 =$	0.05
$C_5 =$	2.9
$C_6 =$	1.7

E3.5.4 Comments

It should be noted that if the stored gas is condensed by refrigeration, the release phase is expected to be much less violent than if it is pressurised.

It is important to note that small-scale topography and big roughness elements, like houses, are not considered in the model. The influence of these disturbances has to be estimated by the user. Further, the emission phases in the model are constant in time while they in reality are very transient. A general treatment of Vapour Cloud Dispersion Models is given in Hanna & Drivas (1987) and is recommended.

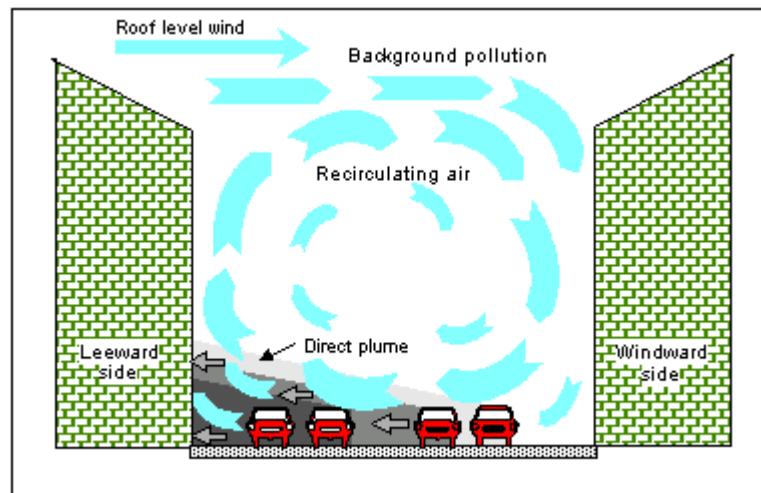
E.3.6 OSPM Street Canyon/SMHI Open Road Model

The Operational Street Pollution Model (OSPM) is an [atmospheric dispersion model](http://www.dmu.dk/en/air/models/ospm) for simulating the dispersion of air pollutants in so-called street canyons. It was developed by the [National Environmental Research Institute of Denmark](http://www.dmu.dk/en/air/models/ospm), Department of Atmospheric Environment. (<http://www.dmu.dk/en/air/models/ospm>)

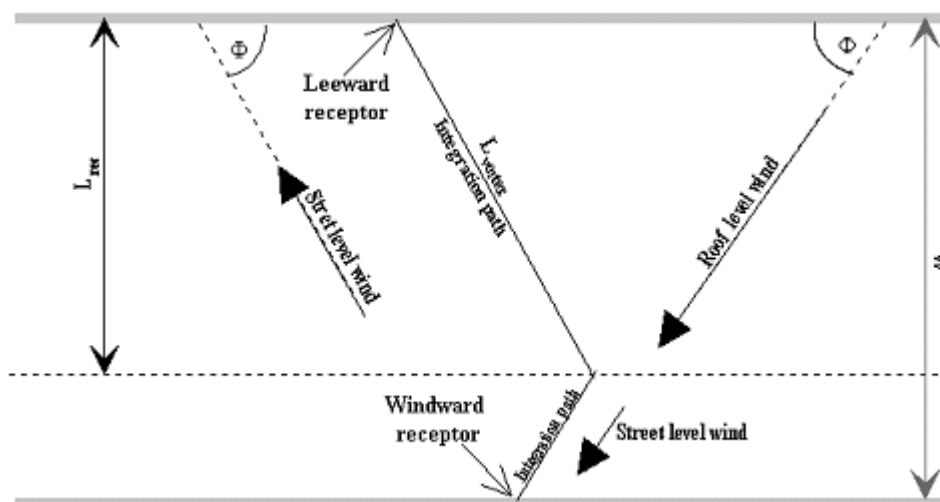
The basic principles are in as follows reference:

<http://www.dmu.dk/en/air/models/ospm/ospmdescription/>

Concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the re-circulating part of the pollutants in the street.

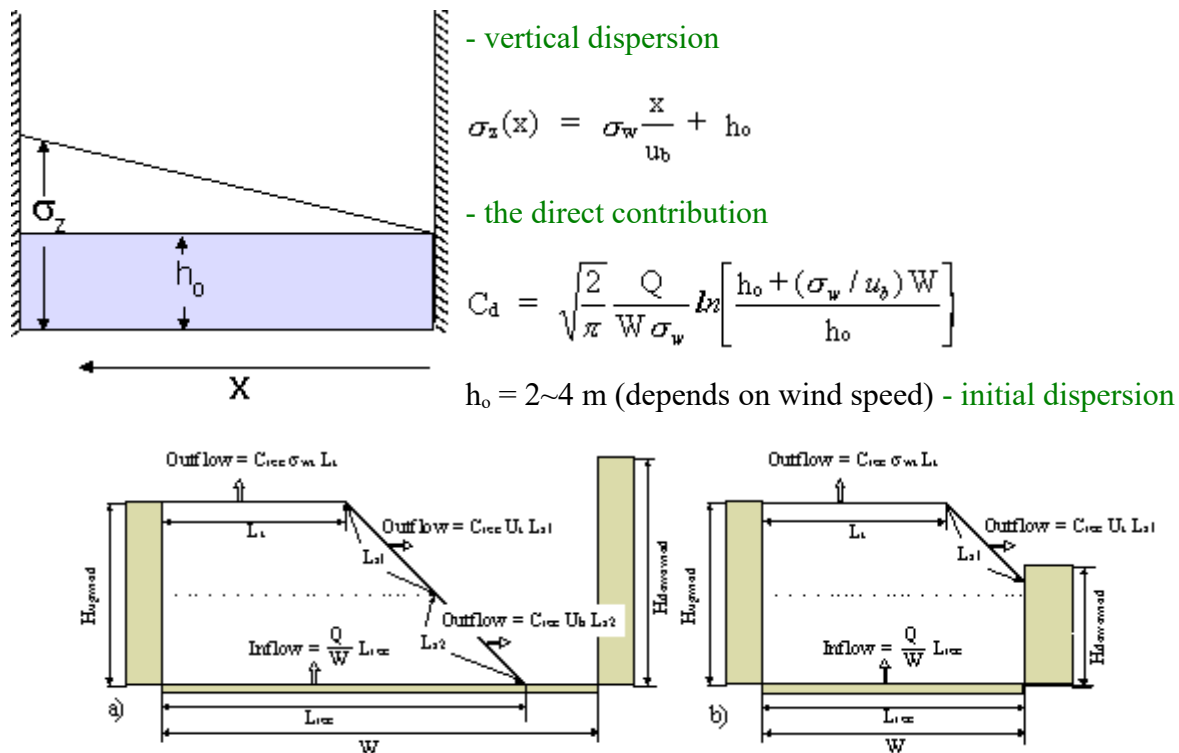


The direct contribution is calculated using a simple plume model. It is assumed that both the traffic and emissions are uniformly distributed across the canyon. The emission field is treated as a number of infinitesimal line sources aligned perpendicular to the wind direction at the street level. The cross wind diffusion is disregarded. The wind direction at the street level is assumed to be mirror reflected with respect to the roof level wind. The plume expression for a line source is integrated along the path defined by the street level wind. The length of the integration path depends on the extension of the recirculation zone.



- The length of the vortex, calculated along the wind direction, is 2 x the upwind building height. For roof-level wind speeds below 2 m/s, the length of the vortex decreases linearly with the wind speed. The buildings along the street may have different heights, affecting thereby the length of the vortex and subsequently the modelled concentrations.
- The upwind receptor (lee-side) receives contribution from the traffic emissions within the area occupied by the vortex (the recirculation zone), the recirculated pollution and a portion of the emissions from outside of the vortex area.
- The downwind receptor (wind-side) receives contributions from the recirculated pollution and the traffic emissions from outside of the recirculation zone only.

- As the wind speed approaches zero or is parallel with the street, concentrations on the both sides of the street became equal.
- The vertical dispersion is modelled assuming a linear growth of the plume with the distance from the source.



The contribution from the recirculation part is calculated using a simple box model. It is assumed that the canyon vortex has the shape of a trapeze, with the maximum length of the upper edge being half of the vortex length. The ventilation of the recirculation zone takes place through the edges of the trapeze but the ventilation can be limited by the presence of a downwind building if the building intercepts one of the edges. The concentration in the recirculation zone is calculated assuming that the inflow rate of the pollutants into the recirculation zone is equal to the outflow rate and that the pollutants are well mixed inside the zone.

Traffic Created Turbulence

The turbulence within the canyon is calculated taking into account the traffic created turbulence. The traffic induced turbulence plays a crucial role in determination of pollution levels in street canyons. During windless conditions the ambient turbulence vanishes and the only dispersion mechanism is due to the turbulence created by traffic. Thereby, the traffic created turbulence becomes the critical factor determining the highest pollution levels in a street canyon.

Street geometry

The model can be used for streets with irregular buildings or even buildings on one side only but it is best suited for regular street-canyon configurations. The model should not be used for crossings or for locations far away from the traffic lanes.

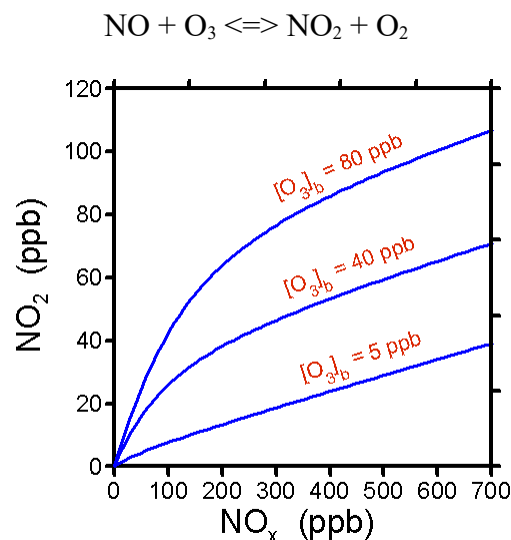
Wind meandering

Concentration distribution of pollutants in the street is calculated taking into account wind direction fluctuations. For each calculation hour, the resulting concentrations are averaged over a wind direction sector centered around the hourly mean wind direction. The width of the averaging wind sector depends on the roof level wind speed and increases with the decreasing wind speed. For calm conditions the averaging sector approaches 360°, which results in uniform concentration distribution across the street.

NO₂ chemistry

The NO₂ concentrations are calculated taking into account NO-NO₂-O₃ chemistry and the residence time of pollutants in the street.

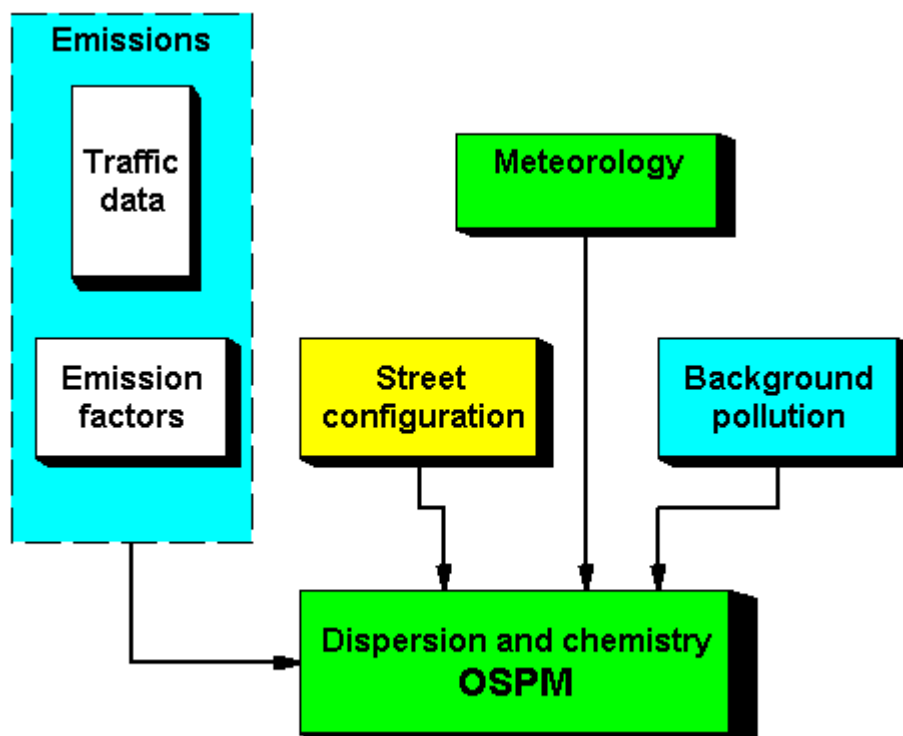
The presence of NO₂ in ambient air is mainly due to the chemical oxidation of the emitted NO by background ozone. Under sunlight conditions, photodissociation of NO₂ leads to partial reproduction of NO and O₃.



The relationship between NO₂ and NO_x concentrations in the ambient air is non-linear and depends on the concentrations of ozone. The time scales characterising these reactions are of the order of tens of seconds, thus comparable with residence time of pollutants in a street canyon. Consequently, the chemical transformations and exchange of street canyon air with the ambient air are of importance for NO₂ formation.

Model structure

The model is designed to work with input and output in the form of one-hour averages.



The required input data are hourly values of wind speed, wind direction, temperature and global radiation. The two last parameters are used for calculation of chemical transformation of NO-NO₂-O₃. The model requires also hourly values of urban background concentrations of the modelled pollutants. Beside the hourly input parameters, the model requires also the data on the street geometry and the traffic in the street.

The SMHI Open Road model is applied in open streets without buildings.

E.3.7 US/EPA AERMOD Model

A steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.

(http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#aermod)

The basic principles are in as follows reference *EPA-454/R-03-004.September2004. Aermod: Description of model formulation.*

E.3.8 US/EPA CALPUFF/CALMET

CALPUFF is a multi-layer, gridded non-steady-state puff dispersion model that can simulate the effects of temporally and spatially varying meteorological conditions on pollutant transport, remove pollutants through dry and wet deposition processes, and transform pollutant species through chemical reaction.

(http://www.epa.gov/ttn/scram/dispersion_prefrec.htm#calpuff)

CALPUFF can be applied for long-range transport and for complex terrain. This complexity requires a significant effort in creating the meteorological data file for CALPUFF. CALMET is a diagnostic 3-dimensional [meteorological](#) model. (*EPA-454/B-95-002. A user's guide for the Calmet meteorological model*)

The basic principles are in as follows reference *Part III Environmental Protection Agency. 40 CFR Part 51. Appendix W. Revision to the Guideline on air quality. Models: adoption of a preferred general purpose. Dispersion model and other revisions final rule.*

E3.9 Airviro application of Austal2000

Austal2000 is a German developed dispersion model that has been incorporated into the Airviro Dispersion by an interface, which in principal extract data from the Airviro databases in a similar way as for the Gaussian model, executes Austal2000 and stores the results. No changes in the original source code have been done.

Appendix 3 of the German regulation TA Luft (Technical Instruction on Air Quality Control) demands for dispersion calculations a Lagrangian particle model in compliance with the German guideline VDI 3945 Part 3. The computer program AUSTAL2000 is a reference implementation of the specifications given in this Appendix. AUSTAL2000 has been developed on behalf of the German Federal Environmental Agency. See also www.austal2000.de.

E3.10 The Airviro MATCH Model application

Since 1990 the Swedish Meteorological and Hydrological Institute, SMHI, has developed a model system for regional dispersion of atmospheric pollutants which is called **MATCH** (Multi-scale Atmospheric Transport and Chemistry model). The MATCH-model can today be applied on a range of different scales and atmospheric dispersion problems.

A MATCH model covering the whole of Sweden and surrounding water areas is since 1994 used operationally. This operational application - called MATCH-Sweden – which runs on a 11 km grid, facilitate support to environmental authorities through annual mapping of deposition of sulphur and nitrogen compounds as well as base cautions.

MATCH has also been applied for more detailed deposition assessments with higher horizontal resolution (5x5 km) in smaller regions of Sweden. In these cases a coupling has been made with the operational work on the national scale. The coupled system can then provide information on contributions from long-range transport, national (Swedish) emissions and regional emissions to the total observed deposition within a region.

For studies of urban air pollution horizontal resolutions below 1 km has been tested successfully in the Stockholm area.

Different versions of the MATCH model are presented in a number of reports. Examples of regional studies for the Swedish West Coast, for Stockholm, and for two regions south and west of Stockholm have been done. MATCH is also used on the European scale in an operational application for emergency response in case of nuclear accidents as well as for studies of tropospheric chemistry and ground level ozone.

Output from Match calculations are different types of maps, iso-lines or coloured grid, or as 3d three dimensional binary grid files.

Necessary basic information for the Match model

General

MATCH is a three-dimensional, Eulerian, off-line, regional chemistry and transport model developed at SMHI. It is a flexible tool used for simulating the emission, dispersion, chemical and physical transformation, and deposition of selected chemical species in the atmosphere.

The meteorological data needed to drive MATCH can originate from a weather forecast model, an analysis system or from a climate model. MATCH is routinely used together with meteorology generated by SMHI's in-house weather forecast model HIRLAM (High Resolution Limited Area Model), or weather data from ECMWF's (European Center for Medium range Weather Forecasting) global analysis and forecast system. MATCH has also been configured to operate together with other meteorological drivers.

The horizontal resolution of MATCH is determined by the input meteorology and emission data. We have successfully applied MATCH on scales from 500 m to 100 km grid resolutions. The model atmosphere is typically divided into 10-20 vertical layers extending from the surface to at least 5 km above ground. The boundary layer should be divided into at least 5 model layers.

Physiographic information

Physiography and land use data are required for application of MATCH. This information is used to derive surface roughness, which is used for calculations of near surface turbulence. Land use information is also needed for modelling of dry deposition of pollutants. In the standard set-up four land use classes are used: open land, forest, water and urban but this can be extended by additional classes if necessary.

Meteorological data

In order to apply the MATCH model a substantial amount of meteorological input data is required for each simulation period. This includes horizontal wind, temperature, humidity and cloud cover at different levels as well as precipitation and fluxes of humidity and heat at the surface. Depending on application these data are prepared through the use of a combination of observations and numerical weather prediction (NWP) models. The meteorological data is read into the model, usually on a three hourly basis. Data for each grid point and vertical level is then interpolated to hourly values. The overall time step in the transport part of the model is 5-10 minutes depending on horizontal resolution. For certain parts of the calculations, e.g. in the chemistry code, a shorter time step is applied.

Emission estimation

Emission of trace species in the model can be specified both as area and point sources and with a high resolution in time. The variation of the emissions with time on annual, daily, and hourly basis can either be specified as scaling functions in MATCH, or alternatively, hourly emissions can be read directly from an emission database e.g. SMHI- Airviro. Emissions from near surface sources are introduced directly into the lowest layer of the model while elevated emissions from point sources are divided between different layers depending on stack height, flue gas flux and temperature as well as aerodynamic effects of buildings and stacks.

Chemistry

Several different chemistry modules have been implemented in MATCH ranging from simple linear sulphur chemistry to advanced photochemistry. Deposition assessment studies have mainly utilised a compact scheme for sulphur, oxidised and reduced nitrogen, used extensively in the EMEP programme (EMEP is a European co-operation on studies of long-range transport of air pollutants). The following chemical components are included in this scheme: Sulphur dioxide (SO_2), ammonium sulphate ($(\text{NH}_4)_2\text{SO}_4$ and NH_4HSO_4), other sulphates (SO_4^{2-}), nitrogen oxide (NO), nitrogen dioxide (NO_2), ammonium nitrate (NH_4NO_3), other nitrates (NO_3^-), nitric acid (HNO_3) and ammonia (NH_3). A local photochemical adjustment of the ozone (O_3) concentration in the model domain is done in this scheme using observed O_3 concentrations at background locations. This is especially important for the NO_2 concentrations in urban areas. The acid deposition scheme is one of the available chemical modules that can be applied together with MATCH in the SMHI- Airviro framework. The other currently available options are a linear sulphur scheme with two chemical components (SO_2 and sulphate) and single components with or without deposition processes.

Deposition

Wet deposition is calculated by assuming proportionality between the wet deposition flux and the product of the precipitation intensity and a species-specific scavenging coefficient. The calculation of wet deposition is critically dependent on the quality of the precipitation data calculated by the meteorological pre-processor. Depending on application and availability of data the precipitation intensity could be derived directly from numerical weather prediction models or as a combination of observations and NWP data. Dry deposition is modelled as proportional to the concentration at the lowest model level and a species specific dry deposition velocity. Since the lowest model layer usually has a thickness of about 50 m, a transformation of the flux calculation is done from the surface to the centre of the first model layer using standard similarity theory for the atmospheric surface layer.

The MATCH user can specify the parameter values used to describe the sink processes (dry- and wet deposition). Default values have been taken from recent literature. Since the model includes information about the physiography of the land surface and a description of the variation of the sink processes over the year and over the diurnal cycle as well as for different weather conditions, a strong variation in the deposition velocity and wet scavenging is obtained for each species studied. For e.g. NO_2 the dry deposition can vary from 0 (over a water surface) to $1.0 \text{ cm}\cdot\text{s}^{-1}$ (over a forest in case of strong turbulence on a summer day). Similar variations occur for other chemical species.

Long-range transport of air pollution

For deposition studies over Sweden a method for deriving long-range transport contributions to air concentrations and deposition of air pollutants has been developed. The method is based on a combination of model calculations and observations at background locations. A similar or simplified methodology can be applied for regions outside Scandinavia. An alternative option is to derive long-range transport contributions from a European scale application of MATCH.

MATCH model versions currently available in Airviro:

MATCH model (M1)	1	Inert tracer	Arbitrary inert tracer without deposition to the surface.
MATCH model (M2)	2	Inert tracer with deposition.	As M1 but with species dependent dry and wet deposition.
MATCH model (M3)	3	Sulphur chemistry	Linear sulphur chemistry based on the concept of EMEP. Including deposition.
MATCH model (M4)	4	Acid deposition chemistry	Chemical scheme including sulphur and reduced and oxidised nitrogen. Including deposition.

E3.11 The meteorological pre-processor, MPP

Below is a description of the meteorological pre-processing process used in the Airviro system in order to create proper meteorological input data, from synoptic data, for dispersion calculation.

Necessary (as a minimum) meteorological input data for Airviro dispersion models are,

- Temperature at 2 m level
- Temperature difference between 8 and 2 m (normally from mast measurements)
- Wind speed and wind direction at 10 m

Routinely collected meteorological data does however not cover the required temperature difference. The meteorological pre-processor is therefore used in order to produce the temperature difference with the following necessary input data,

- Temperature at 2 m
- Wind speed at 10 m
- Cloudiness
- Geographical data
- Physiographical data
- Date and time

The calculation process is as following:

1. Calculate solar angle
2. Calculate ustar and tstar and Monin Obukov length scale iteratively by estimating the energy balance at the surface
3. Calculate the temperature difference by using the similarity profile for temperature for two different heights.

$$(T(Z2)-T(Z1))/tstar = 1/k(\ln(Z2/Z1)-\Psi(Z2/L)+\Psi(Z1/L))$$

E3.12 Scenario Calculations

E3.12.1 General principles

The Airviro dispersion models, except the Heavy Gas Model, simulate hourly concentration values. To make it possible to simulate the long-term impacts of emissions, without running through a very long time series, a certain technique is applied, which we call scenario calculations. The procedure involves a statistical approach. By extracting a representative sample of the joint variation of weather and emissions, expected mean values and extreme values of air quality can be simulated based on a limited number of representative hours.

The basic principles are as follows: When you select weather conditions in the main menu of the dispersion module you will activate the Weather sub-window. Choose Scenario.... A list box will appear and you can select one of a number of headings. In the REF database you will find the alternatives WINTER and SUMMER.

Scenarios are defined in special configuration files. The Airviro configuration files are described in detail in the on line manual (man) pages. A statistical sample of a winter and a summer period in Göteborg is specified within these files. The statistical sample is given as specific dates and hours, (representing different weather and emission events) and a figure describing the frequency of occurrence.

When a dispersion calculation is performed based on the WINTER scenario, the weather information given in the time series database is extracted, using the dates/hours defined in a configuration file as the selection criteria, and the frequencies of the various weather classes will be used to estimate mean values and extremes (95-99 percentile).

E3.12.2 A standard Method to Generate a Statistical Sample: klmstat

Airviro includes a utility program to prepare statistical samples based on long term measurements of weather. A description of the program (klmstat) can be found in the man-pages.

In order to achieve a climatology that reflects the local variation of weather conditions, more than one, preferably five years of monitoring data of the horizontal wind vector, the air temperature and the vertical temperature gradient from a meteorological mast is necessary. However, additional measurements of the standard deviation of the horizontal wind direction and of the vertical wind velocity, the solar radiation and the precipitation, are recommended.

Provided that the monitoring data (described above) is available in the time series database, the klmstat program will extract a representative sample using the following technique:

The data is classified according to the wind directions. The user can decide how many classes to use. As default, it is recommended to use 60, i.e. each class representing a sector of 6°. All events falling into a specific sector will be classified according to the atmospheric stability conditions (as default discriminated by 6 intervals of Monin-Obukhov lengths). When all data have been sorted, frequencies of all classes will be estimated and the median values (of the Monin-Obukhov lengths) of each class (in this case 360 classes) are identified, including the specific date/hour when each class example occurred.

The number of classes required depends on the characteristics of the area. In several countries, regulations concerning the number of classes exist. The number of classes should

be chosen as a balance between the required quality of the calculation results and the computing time. An objective method to decide the number of cases is as follows:

1. Start with 60 wind direction classes. When the representative dates/hours have been determined, plot the diurnal distribution of hours extracted in the sample (do not forget to weight the hours together with the estimated frequencies). Examine the distribution, and be sure that the distribution is fairly uniform. If not, extend change the number of classes. This test is important in order to find a representative joint distribution of weather and emissions.
2. Use the dates/hours determined as selection criteria for extracting the sample mean and 95/99 percentile for the concentration of one or several gases (measured at one or several ambient air monitoring stations). Compare these figures with the mean and 95/99 percentile (from the identical ambient air quality stations) determined from the entire period. If the estimated figures based on the sample deviates from the figures based on the entire period you need to change (probably increase) the number of classes.

Experiences from Stockholm and Göteborg indicate that 60 wind direction classes and 6 stability classes are sufficient.

E3.12.3 General Applications using the Scenario Feature

The Scenario concept can be used in a variety of ways. In fact any set of data can be used as long as the date, hour, and frequency of occurrence are defined in the configuration files, and the weather information is available in the time series database. Some examples of how the Scenario feature could be used:

- **Episodes of SO₂.** Examine the last 5 years measurements of SO₂ and determine the 100 worst cases. Note the corresponding dates/hours and assume frequencies to be equal. Include this information in the configuration files in order to define an episode scenario. The Scenario calculation can then be used to illustrate what cost effective measures could be taken to improve the situation at these worst cases.
- **Validation of an intensive measurement period.** In order to validate the EDB/dispersion model the user could use a large amount of passive samplers during a given period, such as a month. By defining the period as a Scenario, it would be possible to run validation calculations in a simple way.
- **Special events.** If there are certain events, such as: Olympic games, world cup arrangements, national conference week, international exhibition, train strike etc. it would be possible to define the period of the event as a Scenario and combine it with a modified EDB, in which the emission consequences of the event are described, in order to simulate the environmental impact.

E3.13 Aircast – Forecast of air pollution

Aircast is a system that uses Airviro modules to produce air pollution forecasts. With Aircast, the following tasks can be automatically performed:

- Collect a weather forecast from a service provider.
- Make a deterministic forecast with Dispersion for one or more substances prepared in the EDB.

- Estimate the forecast error for one or more substances at monitoring site.
- Adjust the deterministic air pollution forecast with statistical correction in the map area.
- Evaluate the concentration level according to a health risk index for certain substances.
- Produce hourly thematic maps with colour coded risk levels in the map area.
- Distribute the forecasted results to a web server.

With these components, Aircast is an integrated system for environmental monitoring, forecasting and warning within the map area. Pollution levels may be forecast and broadcast days in advance, in order to influence decisions and plans in the local community.

Aircast is a Bourne shell program that starts at regular intervals, e.g. once per day. Aircast waits for a weather forecast, covering 1-3 days ahead in the area of interest. The weather forecast, which should include hourly values for wind, temperature and certain pre-processed meteorological data for dispersion modelling, is entered into the Airviro system by using Aircast to collect the forecast from a service providers web site.

Aircast sets up dispersion calculations for up to five substances, typically including SO₂, NO₂, O₃, CO and PM₁₀. The calculations are performed with either of the models that Airviro is configured for, e.g. Grid or Gauss. These deterministic forecasts yield time series of forecast fields, one field for each hour ahead and each substance.

A receptor time series (DFC) is extracted from the deterministic forecast for each substance and each monitoring station that is involved in the Aircast process. Values are stored in the time series database.

A statistical forecast (SFC) is generated for each monitoring station and substance, based on the quality of earlier deterministic forecasts, as compared with measured data during previous forecast periods. Values are stored in the time series database.

The difference between statistical and deterministic forecast is calculated at each monitoring station and is further used to enhance the entire deterministic forecast field. The process generates an adjusted forecast field for each substance.

The mass concentration fields are evaluated according to an air quality index for health effects in 7 severity classes. Hourly maps of forecasted air pollution indexes are produced as picture files, which are automatically distributed to a web server.

Dispersion and Indico may be used to look at intermediate results, such as deterministic and statistical forecast fields or time series.

E4 Calculation Formulae

Calculation formulae can be applied to data corresponding to selected time series or to a group of dispersion results. The formulae can be defined by the operator and can include the following functions:

E4.1 Arithmetic Functions

-	Negation	
+, -, *, /,	Standard	operators
^, **	Power	
?:	Conditional, e.g. (x1>0?x1:0)	“If x1>0 then use the value x1 else use the value 0”

E4.2 Relational Functions

EQ (==)	Equal	to
NE (!=) (<>)	Not equal	to
GT (>)	Greater	than
GE (>=)	Greater	than or equal to
LT (<)	Less	than
LE (<=)	Less	than or equal to
exist(x)	unary function that is true if x exists, false otherwise	

E4.3 Logical Functions

AND (&)	And
OR ()	Or
NOT (!)	Not

E4.4 Mathematical Functions

Algebraic functions:	ln(x), log(x), exp(x), int(x), abs(x), sqrt(x)
Trigonometric functions:	sin(x), cos(x), tan(x), cot(x)
Inverse trigonometric functions:	arcsin(x), arccos(x), arctan(x), arccot(x)
Hyperbolic functions:	sinh(x), cosh(x), tanh(x), coth(x)
Fill functions:	interpol(x,n) fills in missing values for x by interpolation of the nearest surrounding values. Requires that at least one value before and at least one value after the current time is within n time steps. sustain(x,n) fills in missing values for x by copying the nearest previous value. Requires that at least one value before the current time is within n time steps. interps(x,n) is the same as interpol(), but also makes a constant extrapolation if only one of the surrounding values around the current time is within n time steps.
Miscellaneous functions:	reep(x,a) (=0 if x<a else =1) aver(x1,x2,...) Mean value of x1,x2... (aver(x1:x5) Mean value of x1 - x5) min(x1,x2,...) Minimum value of x1, x2, ... max(x1,x2,...) Maximum value of x1, x2, ... eaver, emin and emax also exist and are the same as aver, min and max, except for the case when one or several arguments are missing, where eaver, emin and emax still return a figure if possible, while aver, min and max do not.

E4.5 Time Shift Functions

The expression $x3[-1]$ refers to the time series selected as $x3$, shifted by -1 time unit. As an example, if $x3$ is plotted together with $x3[-12]$ using the hourly database, then the values for $x3[-12]$ will be the same as those for $x3$ but will be displayed 12 hours later.

The general syntax is:

$xn[d]$

where n is the number of the time series and d is the time shift required (d can be positive or negative).

E4.6 Special Variables

Th	Contains the number of the hour [1..24] for the current value
Td	Contains the number of the day [1..31] for the current value.
Tm	Contains the number of the month [1..12] for the current value.
Ty	Contains the year [YYYY] for the current value.
NTh	Contains the number of the current hour [1..24].
NTd	Contains the number of the current day [1..31].
NTm	Contains the number of the current month [1..12].
NTy	Contains the current year [YYYY].

E4.7 The Air Pollution Index

Functions are additionally available that can be used to calculate an Air Pollution Index in the Indico Presentation module.

The API (Air Pollution Index) is a mathematical function that transforms a concentration of a particular substance to an index value using the following function:

$$API(x) = I_j + \frac{I_{j+1} - I_j}{c_{j+1} - c_j} \cdot (x - c_j) \quad \text{for } c_j \leq x \leq c_{j+1}$$

where x is the concentration of a substance (rounded to an integer), and the c_j and I_j are the break points on the stepwise linear function which defines the relation between the concentration and index values.

The following function is available:

$API(x, c_1, i_1, c_2, i_2, \dots, c_n, i_n)$

where x is the database parameter, and the pairs c_i, i_i are the break points which specify the stepwise linear function which defines the API-function. An arbitrary number of break points can be defined, but the origin is not specified ((0,0) is by default used for the first break point). A minimum of one break point (c, i) must be defined.

The definition of API is in compliance with the United States PSI (Pollution Standard Index).

A composite index can be formed which is defined as a maximum of all the sub-APIs.

E5 Model Descriptions for the Receptor model

E5.1 The Source Location Model

The method assumes time series of

- hourly meteorological data: wind speed and direction at one or two levels, temperature difference in the surface layer and standard deviations of wind direction and vertical wind speed
- hourly concentration values of a pollutant from one or - preferably - several monitor stations (point or open path measurements)

A grid consisting of 24 x 20 cells is created over the calculation domain. A fictitious source is located in each cell centre (i.e. 24 x 20 sources). All sources emit according to

$$q_h = a_h \cdot q_0 \quad (h=1,...,24)$$

where a_h is the emission amplitude as specified by a normalised EDB formula and q_0 is a constant emission rate (the absolute value is not of interest, only variations).

We start with the first fictitious source ($i=1$) and simulate the effect on concentration levels at the monitoring locations. The initial diffusion - in the Gaussian plume model named σ_{yinit} and σ_{zinit} - depends on the horizontal dimensions of the calculation grid (dxy):

$$\sigma_{yinit} = 0.5dxy \text{ and } \sigma_{zinit} = 0.22dxy^{0.78}$$

The simulation uses the Gaussian plume model, using the mast data for the estimation of stability, mixing height and plume growth coefficients σ_y and σ_z (see E3.1.4 “Stability and Turbulence Estimation - Preprocessing of Meteorological Data”). The evaluation of the wind at plume height uses the following assumptions:

- Plume height: Specified by user.
- Trajectory: Since a homogeneous wind field is used, the plume axis will be a straight line.
- Vertical wind profile: The free wind speed (V_g) is estimated by the extrapolation at 25m with the help of the power law. The wind direction is twisted according to empirical data (Holtslag).

The estimation of the wind at plume height will thus relate to the measured wind at measurement level (z_u) and the free wind (V_g) at the height of the mixed layer ($mixh$). With wind measurement at only one level, we get:

-Plume height $< z_u$: adiabatic wind profile (logarithmic)

-Plume height $> z_u$: power law between z_u and $mixh$, based on measured wind and V_g . If plume height is within surface layer ($0.1h$), no turning of wind direction from measured level to plume height is assumed. With plume height

above surface layer, the wind direction will turn linearly between measured wind vector and V_g .

With wind data from two levels, the power law is used for estimating wind speed at plume heights in between the two measurement levels. For plume heights above the upper wind measurement level, the power law is used in the same way as described for the one-level measurement.

The concentrations are evaluated at the locations of the monitoring stations. If an open path instrument is used, the simulated concentration level is calculated at 10 points along the path. The mean value is found after averaging the concentration values.

Time series data are given for $j=1,...,m$ hourly values, and the measured concentrations are given at $k=1,...,l$ number of monitoring stations. The simulated concentration at monitoring station k is written as a result of the i th source and the j th hour of meteorological data (S_{ijk}).

For each fictitious source i , the correlation between simulated and measured time series is calculated as

$$\text{corr}_i = \text{corr}(S_i, C)$$

where each of the two series - the simulated (S_i) and the measured (C) - include data from $j=1,...,m$ hours and $k=1,...,l$ stations.

The calculations are repeated for all fictitious sources. The horizontal distribution of the correlation coefficients is displayed as isolines multiplied by 100.

E5.2 The Emission Estimation Model for Dominant Sources

The method assumes the same kind of data as for the localisation of sources:

- hourly meteorological data: wind speed and direction at one or two levels, temperature difference in the surface layer and standard deviations of wind direction and vertical wind speed
- hourly concentration values of a pollutant from one or - preferably - various monitoring stations (point or open path measurements)

The user assumes the presence of one or various area sources, specified with either a constant or a time variation in its emissions. The user also has to specify the plume height together with the location and geometry of each source. Normally the background concentration, i.e. the part of the registered levels that are not explained by the specified sources, is assumed to be constant in time. There is, however, an option that permits a time varying background concentration.

As a starting point, each specified area source will be divided into 9 subareas and the emission represented by 9 point sources. The initial diffusion is as described in E5.1 "The Source Location Model" (but dx will now be the dimensions of the 9 subareas). All sources are assumed to emit with a normalised, default emission rate, as an average over the specified period. During the period, each area source may have a unique variation specified by a normalised EDB formula. For the chosen time period, the model will evaluate simulated concentration time series at all receptor points/open paths. The simulation uses exactly the same wind evaluation and Gaussian plume model concept as described in Section E5.1 "The Source Location Model".

For each specified source, we will then have a simulation time series S_i consisting of data from $j=1, \dots, m$ hours and $k=1, \dots, l$ stations, assuming a normalised emission rate from every source. The emission estimation method consists of a multiple regression analysis of the simulated source contributions (predictors) with the actual, measured data C (as predictand). The regression method - stepwise regression with a forward selection principle - is described in E1.1 “The Stepwise Regression Scheme”.

The multiple regression analysis will optimise the expression:

$$C = b_0 + b_i S_i + \varepsilon$$

where b_0 is interpreted as the average background value, b_i gives the amplitude of source i and ε is the (minimised) estimation error.

E5.2.1 Monitor Option for a Time Varying Background Concentration

When the user suspects that there are some remote sources that contribute considerably to the monitored pollution levels, the monitor option may be used as a complement to the normal assumption of a constant background level. This calculation will be able to pick out the part of the contamination levels that are spatially uniform over the calculation domain, i.e. one should think of a remote source that gives a time varying but equally distributed impact on the all the pollution monitors included in the model. The method uses only a minor part of the time series, which is why this method should be thought of as only complementary.

With the monitor option activated, only hourly values where:

- at least one monitor is influenced by the local sources defined by the user
- at least one monitor is not influenced by any of the local sources defined by the user will be used. The average value of the monitored data with no influence is assumed to be the background value of that particular hour, and this value will be subtracted from all monitored data values before the data is used as input to the regression analysis.

The model output will then consist of:

- two numbers of hourly values, one showing the number of hours where data exists and the other showing the number of hourly values where the restrictions above are fulfilled.
- two background values, one being the average of the monitor time series, and the other being the output from the regression analysis.