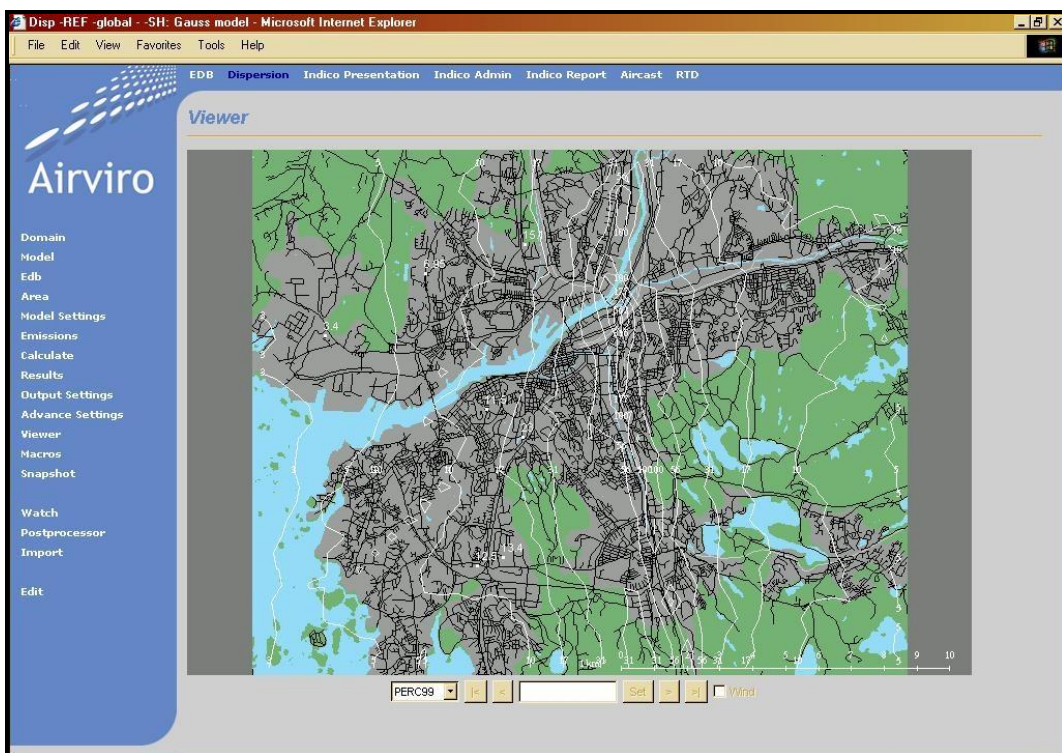


## Working with the Dispersion Module



**How to simulate the dispersion of pollutants**

## Working with the Dispersion Module

# How to simulate the dispersion of pollutants

### Amendments

Version	Date changed	Cause of change	Signature
3.11	Ago2007	Upgrade	GS
3.12	January2009	Upgrade	GS
3.13	January2009	Upgrade	GS
3.20	May 2010	Upgrade	GS

# Contents

<b>2.1</b>	<b>Introduction.....</b>	<b>7</b>
2.1.1	Why You Need to Use Dispersion Models .....	7
2.1.1.1	What's the Use of Dispersion Simulations.....	7
2.1.1.2	How Can Airviro Help?.....	7
2.1.2	Model Assumptions .....	7
2.1.3	Brief description of the available models.....	8
2.1.4	How does Dispersion Module client work? .....	13
2.1.5	Guidance for the beginner: .....	13
2.1.6	Overview of the Dispersion Module Main Window .....	15
2.1.6.1	Changing Weather Conditions – Model settings.....	15
2.1.6.2	Specifying Emissions .....	16
2.1.6.3	Submitting a Dispersion for Calculation .....	16
2.1.6.4	Viewing Existing Dispersion Calculations .....	16
2.1.6.5	Finding Local Values.....	17
2.1.6.6	Using Receptor Points .....	17
2.1.6.7	Map Functions.....	17
2.1.6.8	Sub menus on the left-hand side in the Dispersion main windows .....	17
2.1.6.9.	What is the grid resolution of the simulation? .....	20
<b>2.2</b>	<b>The Gauss Model.....</b>	<b>23</b>
2.2.1	Examples Based on the Case Weather Condition .....	23
2.2.2	Ordering a Calculation.....	24
2.2.3	Examples Based on Emission for a Specific Hour .....	29
2.2.4	Using Scenario Weather Conditions .....	31
2.2.5	Using the Advanced Result Options .....	34
<b>2.3</b>	<b>The Street Canyon Model.....</b>	<b>37</b>
2.3.1	Street Canyon Overview.....	37
<b>2.4</b>	<b>The Grid Model .....</b>	<b>40</b>
2.4.1	Looking at Dispersions for a Specific Time Period .....	40
2.4.2	Looking at Dispersions for a Season .....	43
<b>2.5</b>	<b>The Heavy Gas Model.....</b>	<b>44</b>
2.5.1	Simulation of a Continuous Liquid Leak .....	44
2.5.2	Simulation of a Tank Burst .....	46
<b>2.6</b>	<b>Introduction to the Receptor Model .....</b>	<b>49</b>
2.6.1	Where is this pollution coming from? .....	49
2.6.2	For proper use of the Receptor module: .....	49
2.6.4	Overview of the Receptor Model Settings Window .....	51
2.6.5.	Source Location .....	54
2.6.6	Emission Estimation .....	56

<b>2.7</b>	<b>Aermod Model</b> .....	<b>59</b>
<b>2.8</b>	<b>OSPM Model</b> .....	<b>62</b>
<b>2.9</b>	<b>MATCH Model</b> .....	<b>66</b>
	<b>Appendix 2A:The Wind Model - Calculation of the Wind Fields</b> .....	<b>68</b>
2A.1	Principles of Wind Field Calculations .....	68
2A.1.1	Wind Model Equations .....	68
2A.1.2	Initialisation .....	69
2A.1.3	Stability and Turbulence Estimation - Preprocessing of Meteorological Data .....	69
2A.1.4	Mesoscale Interpolation .....	72
2A.1.5	Procedures for Solving the Wind Model Equations .....	73
2A.1.6	Numerical Methods .....	73
2A.1.7	Reference Literature .....	73
	<b>Appendix 2B:Results from Verification Studies</b> .....	<b>74</b>
	<b>Appendix 2C: The Gauss Dispersion Model</b> .....	<b>77</b>
2C.1	Introduction .....	77
2C.2	When to Use the Gauss Plume Model .....	77
2C.2.1	Source Type Definitions.....	78
2C.3	Plume Rise Formulation .....	78
2C.4	Building Downwash .....	81
2C.5	The Gaussian Plume Model .....	82
	<b>Appendix 2D:The Eulerian Advection-Diffusion Grid Model</b> .....	<b>84</b>
2D.1	Introduction .....	84
2D.2	Formulation of the Grid Model .....	84
2D.2.1	Numerical Methods .....	85
2D.2.2	The Numerical Grid, Coordinate Transformations.....	86
2D.2.3	The Turbulent Exchange Coefficient .....	86
2D.2.4	The Three-Dimensional Wind Field .....	89
2D.2.5	Source Initialisation.....	89
2D.3	Particle Deposition .....	89
2D.3.1	Dry Deposition of Gases and Non-Gravitating Particles .....	89
2D.3.2	Wet Deposition .....	91
2D.3.3	Particle Settling.....	91
	<b>Appendix 2E:Street Canyon Model</b> .....	<b>92</b>
2E.1	Model Description.....	92
	<b>Appendix 2F:The Heavy Gas Model</b> .....	<b>94</b>
2F.1	Continuous Release or a Leakage From a "Small" Hole .....	94
2F.2	Instantaneous Release or a Tank Rupture - Emission Only from the Liquid Phase.....	96
2F.3	Substances and Coefficients.....	97
2F.3.1	Comments.....	97
	<b>Appendix 2G:Scenario Calculations</b> .....	<b>99</b>
2G.1	General Principles.....	99

---

2G.2 A Standard Method to Generate a Statistical Sample: klmstat.....	99
2G.3 General Applications Using the Scenario Feature .....	100
<b>Appendix 2H: A Method to Locate Dominating Sources .....</b>	<b>101</b>
<b>Appendix 2I: A Method to Estimate Emissions from Dominating Sources.....</b>	<b>103</b>
2.I.1 Monitor Option for a Time Varying Background Concentration.....	104
<b>Appendix 2J: The OSPM Model.....</b>	<b>105</b>
<b>Appendix 2K : References .....</b>	<b>110</b>



## 2.1 Introduction

### 2.1.1 Why You Need to Use Dispersion Models

#### 2.1.1.1 What's the Use of Dispersion Simulations...

Measured data provides a strong argument: This is the situation at a specific place, and non-experts easily understand the results if they are well presented. The weaknesses of measured data are mainly that:

- They only represent single locations (even if the results from various measurement stations sometimes may be generalised to larger areas)
- They describe present and perhaps historical conditions, but say nothing about future air quality.

#### 2.1.1.2 How Can Airviro Help?

Measuring everywhere continually would certainly make it possible to gain full knowledge of the ambient air quality (except for future conditions). But even minor steps in this direction would lead to exorbitant costs. Simulation models offer a cheaper way of describing air quality conditions over large areas, as well as permitting statements about the future. Moreover, the important planning aspect can be treated: "What happens if...".

The Airviro system is an integrated system, a tool for both data analysis and dispersion modelling. For an investigation of air quality conditions, a combination of measured and simulated contamination levels using the Airviro Indico Presentation Module Client and the set of dispersion models is suitable. The simulations give the overall description, while the data should be used to confirm the validity of the model results. Although the dispersion models are tested in many ways, we recommend that the results be verified at a few key spots, for every application area. Validation of simulation results from measurements gives confidence in forecast simulations.

The Airviro Receptor model illustrates the advantage of an integrated system, where measured and simulated values are statistically evaluated over a given period. Simulation models are of great value in the interpretation of measured data.

### 2.1.2 Model Assumptions

The following sections describe the Airviro dispersion models. We must first state the major assumptions that motivate the particular methods chosen. In order to describe the existing or future pollution levels of an urban area, the following is necessary:

- Emission data must be close to reality, both in magnitude and in time/space variation. Sophisticated dispersion models will give poor results if emissions are erroneously specified. This motivates the complexity and versatility of the Airviro emission database (see Users Reference Volume 3: Working with Emission Database (EDB)).

- Realistic descriptions of the local wind fields and other meteorological conditions are of utmost importance. The meteorological parameters used in the simulations should refer to locally determined conditions as much as possible, preferably through profile measurements in masts. The wind model must be able to realistically cope with calm situations with weak vertical mixing (stable stratification), i.e. when critical pollution levels are likely to occur.
- For the scale considered in small scale urban applications (that is, a few tenths of a kilometre), the use of the Gauss plume model has many advantages: it is simple and fast to run, it is well tested and the empirical coefficients have been documented, compared and discussed in books and papers for many years.
- For other large-scale applications, such as simulations over a large city or a regional area, simulations in a complex topography, or event simulations where pollutants are accumulated over a period of time, the advection/diffusion grid model should be used instead of the Gauss model. The grid model also gives an easy way to simulate deposition and sedimentation of particles.
- Model results should be presented in a form that can be directly compared with national standards. This means that the simulations should cover not only specific weather conditions (present, historical or forecast), but also longer periods (e.g. seasons or years). The seasonal calculations include mean as well as extreme concentrations.
- If you don't know where pollution is coming from, then you can use Receptor Model / Source Location. The Receptor Module will calculate a probability field that will pin point any dominating sources, based on the concentrations of monitored time series.

If you know where pollution is coming from, then you can use Receptor Model / Emission Estimation. The Receptor Module will calculate the estimated emission for one or various sources, based on the concentrations of monitored time series. However the quality demand on the input data for carrying out the emission estimation is even higher than that required for locating the dominating sources.

### 2.1.3 Brief description of the available models

The available models in this version are:

- Airviro Gauss.

This model is used to simulate ground concentrations distribution of pollutants over urban or industrial areas, with a typical scale of one or a few tenths of kilometres. The lower limit of the application area size is limited by the fact that the Gauss model coefficients are not valid near to the source (distances below approximately 25 metres). The upper limit is given by the fact that more or less stationary conditions should prevail during 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 can be more or less constant during such a period (daily averages would not be sufficient). For 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 over too large areas, producing unrealistically long plumes, the plume length in the Airviro Gauss model is limited. The maximum plume length is defined



in a resource file and depends on 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 are entered into the model through local roughness values and, as a consequence, through the wind field. Buildings create a rougher surface; more friction means a lower wind speed, which influences the dispersion, and so on.

The default height for calculations is 2 m, but the user may specify any other value. The height at which the simulated concentration values are valid will match 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. Thus, the default setting will give concentrations at roof height, not the concentration at street level. The blocking effects of buildings surrounding a street, resulting in raised concentration levels, can be studied separately.

Note that the Gaussian dispersion model simulates steady states of pollution concentrations. Accumulation of polluted air over a period of several days cannot 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) mentions, among other things, the following points:

- It produces results that match 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 horizontally homogenous wind fields, 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 be used in the dispersion calculation.

- Aermod.

Use Aermod when you consider 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.

- Grid.

The Eulerian Advection-Diffusion grid dispersion model built into Airviro is specially designed to meet the requirements given by areas with complex topography, e.g. valleys. This model has some additional advantages when 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 are entered into the model through local roughness values and, as a consequence, through the wind field. Buildings create a rougher surface; more friction means a lower wind speed, which influences the dispersion, and so on.

The default calculation height is 2 m, but the user may specify a different value. The height at which the simulated concentration values are valid will match 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. Thus, the default setting will give concentrations at roof height, not the concentration at street level. The blocking effects of buildings surrounding a street, resulting in raised concentration levels, can be studied separately.

The Grid model should be used on larger areas. It is not suitable for calculations on small scale and therefore a minimum of 25 m has been set for the size of the sides of the grid boxes used for calculations.

- Street Canyon.

The Street Canyon model is a small-scale model that allows you to simulate concentrations at street level on a single road flanked by buildings on each side. The simulated concentrations are visualized on a vertical plane perpendicular to the street direction, creating the illusion of looking down the 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 to contribute to a substantial part of the pollution levels, especially if the traffic in the simulated road has a low intensity and larger streets surround it. Is it possible to separately estimate the fractions of street pollution created by the local traffic and those created by emissions in other places?

A feasible way to do this with Airviro is:

- Run the street canyon model with traffic emissions only for the road segment in study
- Run a citywide simulation with Gauss or Grid model, including all sources except those for the traffic on the road segment in study. The concentration at roof level above road segment in study can then be considered as a result of non-local sources. Due to the eddy circulation already mentioned, 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.

- Heavy Gas.

Heavy Gas model describe the emission and dispersion of gases heavier or denser than the air.

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

- They have a molecular weight higher than the air
- They are stored as condensed gases at low temperatures
- They are stored as condensed gases at high pressures
- A mixture of the above mentioned reasons

These gasses are often toxic, in addition, a condensed gas is very cold when released to the atmosphere. Therefore, it may cause frostbite to people who come into contact with a cloud of released gas. The gas cloud can also have suffocating effects even if it is not toxic or very cold.

This model should be applied to industrial and transportation environments, where storage and transportation of this type of gasses; like chlorine, ammonia and propane, takes place. Accidents, or scenarios, that can be currently simulated by this model, are:

- The rupture of a storage container, causing 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 and carried away by the wind while collapsing gravitationally. After a while, the puff is diluted and it behaves as a neutral density puff.
- A small hole leakage, which could be a leakage from a valve or a broken small pipe. The release time is assumed to be quite long. The release can be originated from both the liquid and the gas phase of the pressurised storage vessel. This scenario 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 due to the gravitational spread perpendicular to the main slab direction. When the plume density match the density of 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.

- MATCH (Mesoscale Atmospheric Transport and Chemistry Model)

The MATCH model is used for air pollution assessment studies on different geographical scales. MATCH is an Eulerian atmospheric dispersion model, which includes physical and chemical processes governing sources, atmospheric transport and sinks of oxidized sulphur and oxidized and reduced nitrogen. Using a combination of air and precipitation measurements and

the MATCH model, the national and long-range transport contributions to air pollution and deposition can be quantified in the model region.

- Receptor

The receptor model actually consists of two different models:

- The source location model that is used to find the most likely position for a dominant source.
- The emission estimation module that is used to estimate the emission from dominating sources.

### **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)
- 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).

Concentrations are evaluated where monitoring stations are located. 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  $j=1, \dots, m$  hourly values, and the measured concentrations are given at  $k=1, \dots, l$  number of monitoring stations. The simulated concentration at the 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,  $\text{corri} = \text{corr}(S_i, C)$ , where each of the two series - the simulated ( $S_i$ ) and the measured ( $C$ ) - include data from  $j=1, \dots, m$  hours and  $k=1, \dots, l$  stations.

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

### **The Emission Estimation Model**

The method assumes the same kind of data as for the localization 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, specifying its emissions either with a constant or a time variation. The user also has to specify the plume height along 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 lets you use a variable background concentration.

As a starting point, each specified area source will be divided into 9 sub areas and the emission represented by 9-point sources. All sources are assumed to emit with a normalized, default emission rate, as an average over the specified period. During this period, each area source may have a unique variation specified by a normalized EDB formula. For the chosen time period, the model will evaluate simulated concentration time series for all receptor points/open paths.

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 normalized emission rate from each 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).

- Austal 2000

Austal 2000 from the Environment German Federal Agency is an air dispersion model that uses Lagrangian particle tracking and contains its own diagnostic wind field model. It also considers the influence of topography on the wind field.

- US/EPA Calmet/Calpuff

#### Calmet

It is a diagnostic meteorological model in 3D that also can accept pre-processed wind fields.

#### Calpuff

Provides a complete spatial variation of wind and stability, hour by hour. It is applicable at distances under 300 km

## 2.1.4 How does Dispersion Module client work?

Airviro has is a web based user interface. Airviro can be used from a PC or any other device running Internet Explorer 6 or later and Firefox.

After logging in on Airviro the DISPERSION module can be selected. All data processing is made on the Airviro server and the results are transferred to the web browser.

Please note that JAVA JRE (run time plugin) must be installed and enabled in the web browser.

## 2.1.5 Guidance for the beginner:

The dispersion chapter consists of two major parts:

- An introduction - section 2.1-2.4 - on how to operate the menus and subwindows in the different dispersion modules, and how to run some simple examples.
- A reference part collected in the appendices where some of the models are described and references are available.

It is recommended that the beginner looks through the first, instructive part and does one or more of the illustrated examples before penetrating the reference part.

The following sections provide an introduction to the dispersion simulation facilities and how to use the menus and subwindows in the Dispersion module client. You will find that the subwindows where you specify and present your different dispersion calculations are almost identical for different models, although the actual dispersion calculations that take place as batch jobs differ strongly in complexity and computer time demand (the Canyon model calculation being the fastest, the Grid model the most time consuming).

The examples refer to the Reference database, delivered as a training environment with all Airviro installations. The Reference area is Göteborg on the Swedish west coast, and the data are real (although the emission database is certainly not the latest and the most complete one).

## 2.1.6 Overview of the Dispersion Module Main Window



The menu main window is mainly taken up by the different options of the models.

On the left side are various buttons which you click on with the mouse, whose functions are:

- You can select the Project and a model
- You can the type source and the emission
- You can select hypothetical or observed weather conditions.
- You can postprocessor the results.
- You can save macros with the results.
- You can import the results
- You can display result for the specific receptors

The functions of the different buttons are explained below, but more detailed explanations of how to use them are given through worked examples in following sections.

### 2.1.6.1 Changing Weather Conditions – Model settings

The weather plays a crucial role in dispersion calculations, and you can select weather conditions by clicking on **Model Settings**. This takes you to the **Settings** subwindow where you can select hypothetical or observed weather conditions as a basis for dispersion calculations. Different weather options are available, depending on the model that has been chosen.

The screenshot shows the 'Settings' dialog box for the Gauss model. It includes a 'Type' dropdown menu with options: Time period, Scenario, Specific hour, Case, and Case with Edb. Below this is a 'Form' dropdown menu with options: Point, Area, and Road. The 'From' and 'To' date fields are set to 900101 14 and 900101 16 respectively. There are navigation buttons for Year, Month, Week, Day, and Hour. The 'Emission model' section has radio buttons for 'Normal' (selected) and 'Resuspension'. An 'Apply' button is located at the bottom of the dialog.

Figure 2.1.6.1 Example of the type for Gauss model

---

**HINT:** in version 3.20 the user can select Case with Edb. This selection allows you to run case using an emission database.

---

### 2.1.6.2 Specifying Emissions

The **Emissions** page changes depending on the model selected. Most models use emissions from an EDB and the user can select the sources using the EDB search criteria page. Some exceptions exist: For Gauss and case the user can specify point, area or road sources. For heavy gas the user specifies the type of leakage. For Airviro Street Canyon the traffic in the street canyon is described. For OSPM a number of roads can be picked from an EDB and an OSPM simulation is made for each of them.

The **Apply** button under **Emissions** saves settings of the source specifications entered.

### 2.1.6.3 Submitting a Dispersion for Calculation

When you have defined the source emissions, select **Calculate**, which takes you to a subwindow where you specify the calculation height and give a name to your dispersion calculation before ordering the calculation.

When you have ordered a calculation, an information window automatically appears once it has finished.

### 2.1.6.4 Viewing Existing Dispersion Calculations

**Results** allow you to access all completed calculations, both those stored under separate projects and those that were executed by other users. Here you can also delete unwanted result files (but only if you own them).



### 2.1.6.5 Finding Local Values

Use left mouse button to find out the concentrations at specific points on the map. You can click on different parts of the map to find the pollution levels at specific points.

### 2.1.6.6 Using Receptor Points

**Receptors**, under **Snapshot**, allows the extraction of values at pre defined locations. Simulated concentration levels are shown in a new text window. The receptor points must have been previously defined in **Edit, Receptors**. All point definitions start with **#POINT** and all station references start with **#STN**. A typical receptor definition could be:

```
#POINT 1264626 6401932
#STN GO1
#STN GO2
#STN GM5
```

This definition contains the x and y coordinates for one point definition and the station keys for three stations in the station database.

Note that for DOAS-measurements, the concentration value is integrated over the entire length of the measurement path.

### 2.1.6.7 Map Functions

Under **Area** you find the usual map functions. You can switch between different maps if more than one map is installed on your system, **Zoom** into a subarea (this operation can be repeated), **Clear** the map and unzoom with **Whole**. If you have zoomed in your map and would like to display the other area map with the same scale, then click on **Pan** in the map dialogue area and move the map toward this area.

Note that the wind model resolution can be different for different maps.

### 2.1.6.8 Sub menus on the left-hand side in the Dispersion main windows

More menus are found for each button.

<b>Domain</b>	This is the same as the option in the EDB module, where you can choose another Domain to work with.
<b>Model</b>	Here you can choose between a set of different models.
<b>Edb</b>	This is the same as the option in the EDB module, where you can choose another EDB to work with. The default is the global EDB.
<b>Area</b>	Here you can choose between a set of different options the maps and area of the map. These configurations are used in the dispersion calculation.
<b>Model Settings</b>	Here you can select type of the calculations. It's depending the meteorological data, period, height and re-suspension of the particles.
<b>Emission</b>	Here you can select of the source data and your emission for the simulation calculation.

- Calculate** Here you can calculate the simulation.
- Results** Here you can select the different results.
- Output Settings** This page is used to control how the result is shown on the map.
- **Grid rectangles**  
This displays the grid rectangles that show the resolution of the dispersion calculations.
  - **Grid points**  
This is the same as **Grid rectangles** but instead the middle point of each rectangle is displayed.
  - **Calculation area**  
This shows the boundary around the area that you have chosen to zoom into. Note if you have zoomed into the map then the calculation area is not usually the whole map area that you can see on the screen (since when you zoom you do not usually choose an area that has exactly the same aspect ratio as the window in which you are working).
  - **Description**  
This shows a description of the current result at the top of the map. Information such as the weather conditions and your calculation description is presented.
  - **Colour legend**  
This can be used when the output configuration format has been set to grid or isocolour, and shows the grid colours and levels used down the left hand side of the map.
  - **Field output configuration**  
Here you can specify how the result field is presented. There are four different presentation types: Isolines, Grid, Isocolour and Class enumeration. The isoline frequency is adjustable and the levels and colours for coloured grid and Isocolour is configurable. The colour palette can be changed. There are 31 levels available.
  - **Output window**  
It is possible to configure the window size here for **Snapshot GIF**.

### Advance Settings

A mathematical or logical formula can be applied on the result field. The name of the variable is x1. The syntax is the same as for the formulas used in Indico Presentation except for the time lag which can't be used. To smooth out transients in the result the **Smoothing** option can be used. Running averages can be calculated when viewing a time series result. The calculated average is shown for the last time stamp in the averaging period. Finally a constant background level can be added to the field.

**View** Here you can view your simulation result selected with **Result**.

### Macros

- **Load:** You may load plot instructions, such as plot type, isoline intervals as a template for the chosen model, if they were saved before. A macro may also contain advanced settings, such as result proportioning or regression models for other chemical compounds.
- **Save:** In order to save your settings for a Dispersion macro, choose **Save macro** to define a **dsp-file** for the actual model type, project and user.
- **Delete:** Here you may delete saved Dispersion macros for the actual model type and project.

### Snapshot

If you select **Snapshot** then whatever is currently displayed on the map will be copied to another window (select **PDF** or **GIF**). This new window is completely independent of the Dispersion module that you are running and can be moved to another part of the screen where you can use it for reference or comparison. The snapshot window size for a **GIF** is specified in **Output settings**, and after it has been created it cannot be resized.

Text or EXCEL opens a window with a textual representation of the result: Coordinates of the calculation area, Description of the calculation, and concentration values for the result.

Receptors calculates the concentration value at specified points on the map. The output is shown in a text window.

Shape is used to export the result to a zip archive containing shape files.

### Watch

This brings up a subwindow showing the progress of dispersion calculations. Calculations can be cancelled here.

### Postprocessor

This option uses at least the selected dispersion result as input. The main functionality is based on the processing of results from time period calculations, but there are also some functions that may operate on other types. The result of the operations is a new dispersion result.

Available processing types:

- Spatial evaluation. Used for calculating statistics from time series fields such as averages, percentiles etc.
- Time series export. A time series representing the location of a station can be exported to Indico for comparison with monitoring data.
- Model adjustment. An Indico macro is used to adjust the chosen result. The macro may contain more than one station. The result is

adjusted in such a way that the location of the station in the result will have the same value as the Indico time series. An interpolation is made for the values between the stations.

- Split model result. A time series result can be split into smaller parts. Each part is a new result.
- Merge model result. A number of time series results is concatenated into one single result.
- Combine model result: One or more model results are combined with an arithmetical expression. This works on time series fields as well as single field results.

**Import** External results that have been calculated by other models outside the Airviro system can be imported from file if they are in one of the accepted formats. External results are stored under the simulation type **Extern** in the **Results** subwindow.

#### **Edit**

##### **Project**

It is possible to have up to 26 projects on a system and these can be created here. Once a project has been created it can only be deleted by the user that created it.

##### **Receptor**

Here you can edit receptors. The receptor points are defined with the X and Y coordinates. A comment can be added typing a # symbol after the x and y coordinates.

### 2.1.6.9. What is the grid resolution of the simulation?

There are three spatial resolution scales in the horizontal: the wind field, the emissions and the grid where the concentrations are evaluated.

- The wind field has one unique resolution that depends upon the input of topographic and physiographic information, normally given of a 500 \* 500 or 250 \* 250 m grid. The wind model calculations will always yield an output wind field with this resolution. If you zoom up over a smaller area, a final grid net will be generated. However, the wind field will be linearly interpolated from the original grid.
- The point sources will always be introduced into the dispersion calculation with their actual positions. The area and line sources are collected on an emission grid before they enter the dispersion model, and the grid size will be adjusted to fit the simulation domain. This means that a smaller simulation (map) area will yield a higher resolution for emissions. The resolution of the emission grid is twice as high as that of the concentration grid.
- The concentrations are evaluated on a grid, which adjusts to the size of the map. This means that the more you zoom up on a particular area, the better the resolution (in metres) you will get out of the dispersion results. The best available resolution is 25 \* 25 m for all models except the grid model, for which the best resolution is 100 \* 100 m.

**Is it possible to zoom up on an already existing simulation result?**

No. The result can only be presented on the map area chosen before executing the dispersion calculation.

**Can the results be influenced by sources outside the calculation domain?**

No. What you see on the map is all that you get out of the simulation. All impact from sources outside the area must be considered as a background influence.

**What is the precision of the simulated concentrations?**

The precision of simulated results depends upon the quality of a chain of input data: emission data, description of the surface and meteorological data. There are also uncertainties built into the model assumptions. It is impossible to give a quantitative answer that is valid for every application of the Airviro models. A general rule of thumb says that a model result should be within a factor of two from measured (good quality) values. Various Airviro applications have shown a much better precision after a careful inspection of the input data. The user is therefore recommended to verify the model results with a few monitored values, both as long-term averages and for special events.

**Getting Started**

The best way to get acquainted with using the Dispersion module is by carrying out lots of examples. We have devised a set of examples based on the Göteborg reference database, which are designed to lead you through the main features of the different dispersion models. The first example is very detailed but for the rest of the examples a lot of the more trivial details have been left out.

In the following sections, you will find guidance on how to perform simple (but realistic) simulations. All beginners are advised to work through these examples. The first example is explained in a lot of detail, describing fully how to use the different subwindows, but after that the examples are much more concise. Keep in mind that it is always possible to refer to the appendices to find out details on how the calculations are performed, model assumptions, etc.

Click on the **Dispersion** to start the Dispersion Module. Before you start trying to repeat the examples yourself you have to choose the reference database. Select **REF** under **Domain**.

Once the Dispersion module has started you will have to select a model to use, under **Model**. The following models can be included in an Airviro system but your particular system may not have all of them:

- SMHI Gauss (SH)
- SMHI Grid (EU)
- SMHI Street Canyon (CN)
- SMHI Heavy Gas (HG)
- SMHI MATCH (MA)
- SMHI Receptor (RD)
- OSPM Street Canyon / SMHI Open Road(OS)

- US/EPA AERMOD (AM)
- US/EPA Calmet/Calpuff (CP)
- Austal2000 model (AU)

Click on the model name that you are going to use and then click on **Apply**.

Then, select a personal edb. The procedure is the same as in the EDB Module.

Click on the **Area** to select the area for the calculation. This shows the boundary around the area that you chosen to zoom into.

## 2.2 The Gauss Model

### 2.2.1 Examples Based on the Case Weather Condition

The simplest type of weather condition that can be set up is called **Case**. This uses only homogeneous wind fields and does not take the topography and physiography into consideration. The wind speed and wind direction can be selected together with one of six stability options.

The first example deals with the impact of three stacks with different fundamental characteristics, all of them emitting NO<sub>x</sub>.



Figure 2.2.1.1. Case weather condition

The ground level concentrations caused by these emissions will be calculated for a particular weather event. A fairly stable event will be used with the wind coming from SW and wind speed 2.5 m/s.

Start by defining the weather conditions - click on the **Model Settings** on the frame. In the **Settings** subwindow use the option text box menu **Type** to choose **Case**. This enables you to enter the case conditions lower down in the subwindow. First select the **Stability** condition to use - for this example we will simulate stable conditions so choose **MOD.UNSTABLE**. Then enter a wind speed and direction. The wind speed has to be given in degrees so for SW enter 225. Give a wind speed of 2.5 m/s (referring to conditions 10m above ground level).

The calculation **height**, which by default is 2 m, is the level above ground where the model evaluates the concentration values.

Click on **Apply**, which will save the weather settings (**settings saved**).

You will study the impact of three point sources with the following different characteristics:

	source 1	source 2	source 3
<b>Substance:</b>	NOx	NOx	NOx
<b>Chimney height: (m)</b>	50	20	150
<b>Outer diameter: (m)</b>	7	7	7
<b>Inner diameter: (m)</b>	6	6	6
<b>Exhaust gas temperature: (°C)</b>	175	10	175
<b>Exhaust gas velocity: (m/s)</b>	20	5	20
<b>House width: (m)</b>	0	0	0
<b>House height: (m)</b>	0	0	0
<b>Absolute emission: (g/s)</b>	25	25	25

Store the point sources using the EDB module. Click on Emissions and check Point to include the emission from point sources only.

The screenshot shows the 'Emission' subwindow. It has a title bar 'Emission'. Below the title bar is a section 'Name Information' with three text input fields labeled 'Name', 'Info', and 'Info2'. Below that is a 'Substance' dropdown menu with 'NOx' selected. There are two main columns of settings: 'Sources' and 'Correction'. The 'Sources' column has four checkboxes: 'Point' (checked), 'Area', 'Road', and 'Grid'. The 'Correction' column has three input fields: 'Point' (value 1), 'Area & Grid' (value 1), and 'Road' (value 1). To the right of these is a 'Restrictions' section with a dropdown menu 'Point, Area & Grid' and four buttons: 'Road', 'Searchkey', 'Sub area', and 'Alob'. Further right is a 'Variation' section with a 'Time & Temp' dropdown and a 'Scenario' dropdown set to '2007'. At the bottom left are 'Clear all' and 'Apply' buttons. At the bottom right, the text 'Settings saved' is displayed in green.

Figure 2.2.1.2 .1 Emission subwindows

## 2.2.2 Ordering a Calculation

Now that you have specified weather and emission data, its time to click on the **Calculate** to submit the batch calculation job. You will see your user name, the project under which your result files will be saved and the job number. As a user, you are allowed to store your results under whatever project from the list (you share the project list with your colleagues working in the Airviro system).

The screenshot shows the 'Calculate' subwindow. It has a title bar 'Calculate'. Below the title bar is a 'Project' dropdown menu with 'A: Proj 1' selected. Below that is a 'Description' section with a text area containing 'My first simulation'. Below the text area is a 'Host' dropdown menu with '[any]' selected. Below the host dropdown are two columns of buttons: 'Nesting...', 'Parallelization...', and 'Apply' on the left; and 'Clear' and 'Clear' on the right.

Figure 2.2.2.1. Calculate

You can change the project that you are working in or create a new project name by choosing the **Project** option under the **Edit** on the frame.

The text string below **Description** should be carefully edited, since this text will be your key to remember the way you performed the simulation.

You can select the host on which you want the dispersion to be executed.



**Nesting**

Nesting admits a calculation in a smaller area (local) to use the background concentrations from a larger area (urban) without double calculating the emissions in the smaller (local) area. An overview of the nesting operation can be found in *Figure 2.2.2.1*.

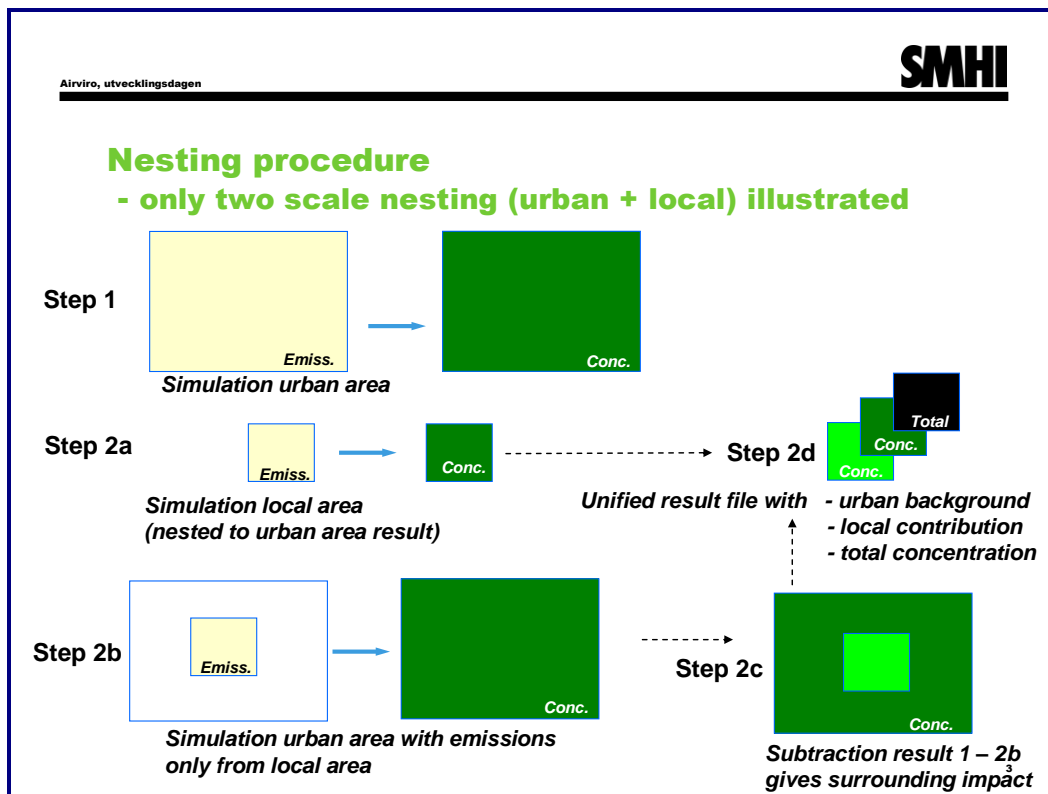
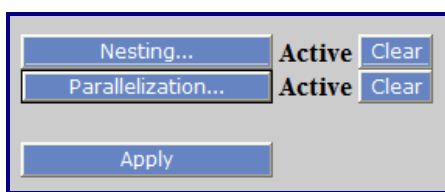


Figure 2.2.2.2. Nesting operation.

The final result from the nesting operation contains the total concentration as well as the local contribution and the urban contribution.

Typically nesting is used when we want a result with very high resolution, for example 20x20 meters in the local area, but we also want the concentrations from a simulation with a resolution that is a lot lower, for example 500x500 meters. To make this using nesting saves a lot of calculation time compared to running a simulation of 20x20 meters over the whole area.

In the **Calculate** menu from Dispersion module, there are two buttons located in the left lower corner of that window: **Nesting** and **Parallelization**.



The **Clear** buttons allows the user to clean the selection made in both **Nesting** and **Parallelization** menus.

The **Nesting** button opens a window that lets you select an existing dispersion result to do the nesting with. See Figure 2.2.2.3.

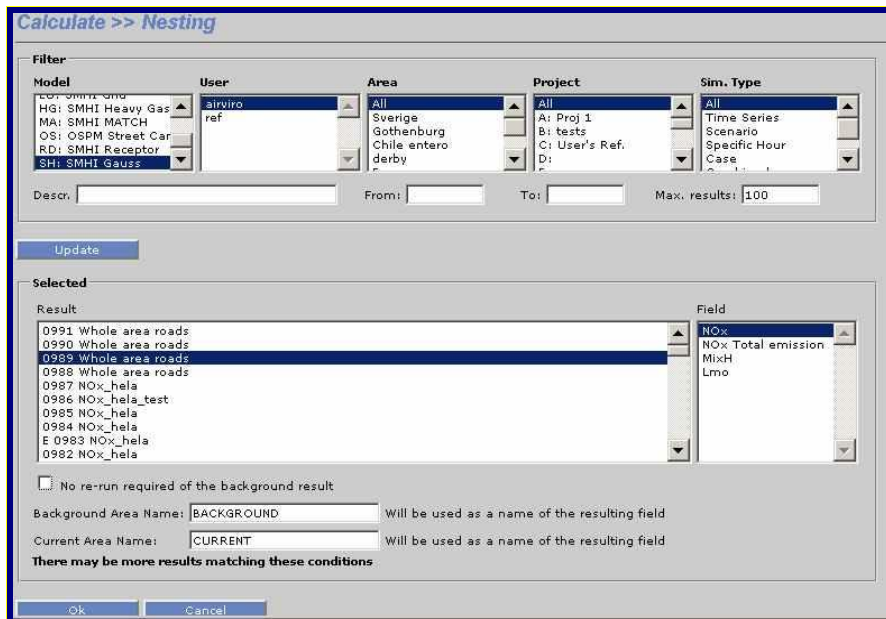


Figure 2.2.2.3. Calculate. Nesting

The result of the nesting is shown in Figure 2.2.2.4. Observe that we have three concentration fields: Total, CURRENT and BACKGROUND. The name of the BACKGROUND and CURRENT field was chosen in the nesting menu.

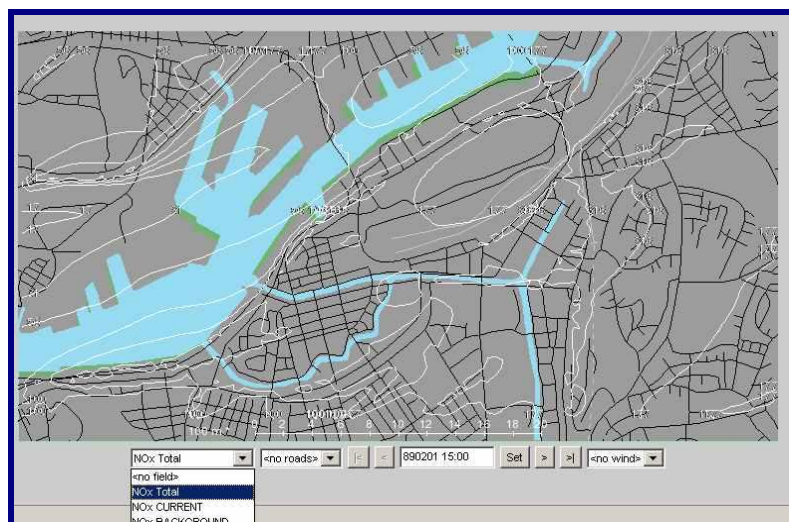


Figure 2.2.2.4. Nesting. Result.

The nesting operation can be done in any number of steps, in which case the last result will contain contribution from each step as well as the total.

**Parallelization**

The time series simulation will be split up into several parts that can run in parallel and the result will be joined together and give the same result as if the run was not split.

If the model has a memory (accumulating between time steps), an optional overlap can be specified to give the model a chance to accumulate. This startup period will then be skipped when joining the result.

The user must manually specify the number of parts and number of overlapping time steps (hours).

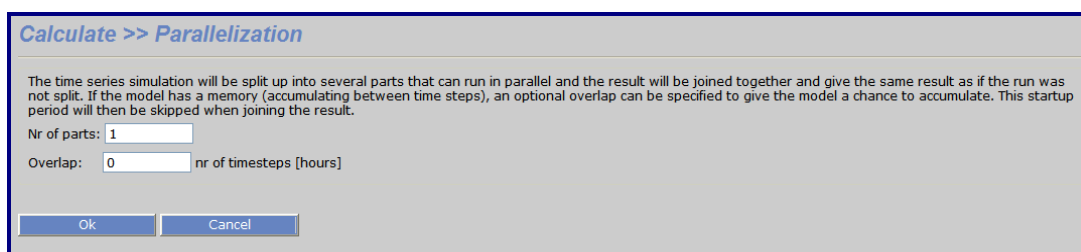


Figure 2.2.2.4 Parallelization

An overview of the parallelization operation can be found below:

- Time series simulation
- At start time it is possible to specify: Number of parts, Overlap (hour)

**Example:** A Grid model run over 4 weeks is split into 4 with a 24 hour overlap to minimize loss of accumulated concentrations.

!Error!

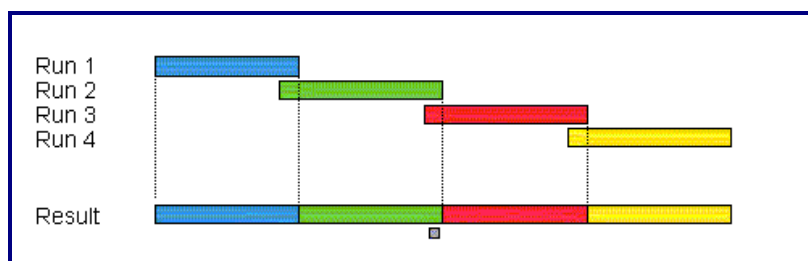


Figure 2.2.2.5 Example Parallelization

### 2.2.2.1 Displaying Results

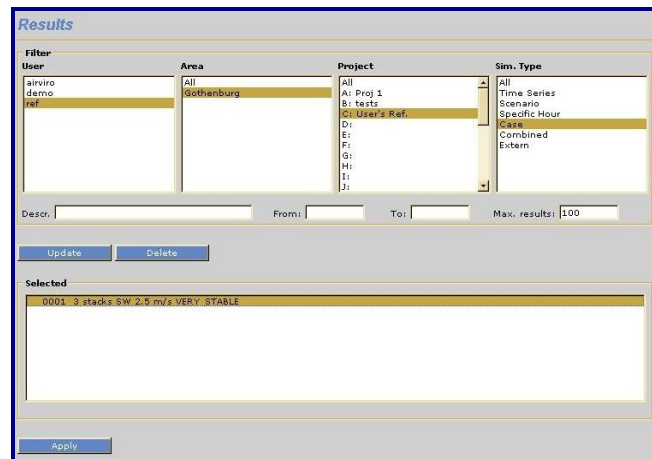


Figure 2.2.2.6. Results.

Now the order process behind a simulation calculation has been gone through carefully. Once the calculation is complete an information message will appear on the screen informing you of this, and you can then display the finished result. Click on the **Results** to find all Gauss result files that have been performed in the Airviro system, grouped under four identification lists: **User**, **Area**, **Project** and **Simulation type**. This gives you the facility to display results created by other users, under different map areas and in other projects. Under **Update** is a list of all results that have been chosen to view. This list can be cleared by clicking on the **Delete**.

---

**HINT:** All examples discussed in this section are stored under the username **ref** and under project C: Users Ref. You change Project by choosing the **Project** option under **Edit** on the frame.

---

In order to display the results of a recent calculation, first click on the relevant user name, map area, project and simulation type, and then click on the corresponding text string description for the calculation that you want to view. The concentration isolines will be displayed when you click on **Viewer**.

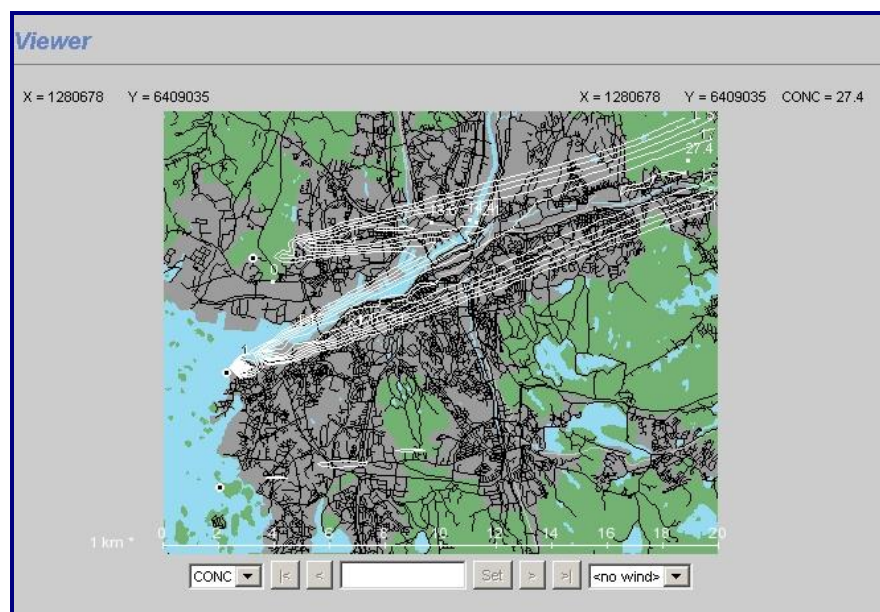


Figure 2.2.2.7 Three stacks with a 2.5 m/s SW wind

In the **Viewer**, if the calculation had more than one result field, these fields can be shown. If a wind field was produced by the calculation it can be shown.

---

**HINT:** By using the **Output configuration** option under **Output Settings** on the frame, you are able to choose between three ways of spacing the isolines: either with a logarithmic spacing (which is default), a linear spacing or just one single line.

---



---

**HINT:** You can use the **Description** choice under **Output Settings** on the frame, to toggle between whether or not you want the job description to appear on the screen or printer output.

---

The three plumes created by our three sources are displayed in *Figure 2.2.2.7*. If you have repeated the example on your own Airviro system, you can click on the left mouse button, which you can use to click on different parts of the calculation, to see the NO<sub>x</sub> concentrations displayed as number on the screen. (The unit is always µg/m<sup>3</sup>). The **Receptors** under **Snapshot**, can be used to display the simulated concentrations at certain locations defined in a file outside the system. There you can for example define the locations of up to 10 monitoring stations (or open path instruments), which allows you to obtain the simulated values evaluated at the measurement stations by a simple click on the **Receptor**. For information on configuring receptor points see *2.1.2.6 Specifying Source Types*.

## 2.2.3 Examples Based on Emission for a Specific Hour

This time a summertime event will be simulated for a specific hour in the summer. You will study the impact of two emission sources of volatile hydrocarbons (VOC), the first from storage of gasoline and the second from a petrochemical industry. These can be treated as area sources.

An area source covers a large area horizontally, e.g. it might consist of a number of vents at the top of an industrial building or an area where petrol evaporates from leaking tanks. It is not possible to calculate the plume rise for the emission from an area source, so the dispersion will be that of a neutral pollutant which is just exposed to advective transport and diffusion.

Specify two area sources as follows in EDB module client:

	source 1	source 2
<b>Substance:</b>	VOC	VOC
<b>Plume height: (m)</b>	5	20
<b>Absolute emission: (g/s)</b>	25	25

Start by select Domain, Gauss Model and EDB personal in Dispersion Module Client.

Click on the **Area** button; locate the hair cross at one corner of the area source and press down the left mouse button. Move the mouse while still pressing down the left mouse button, until you cover the source area (the area source in the Northwest in *Figure 2.2.3.1*. is source 1).

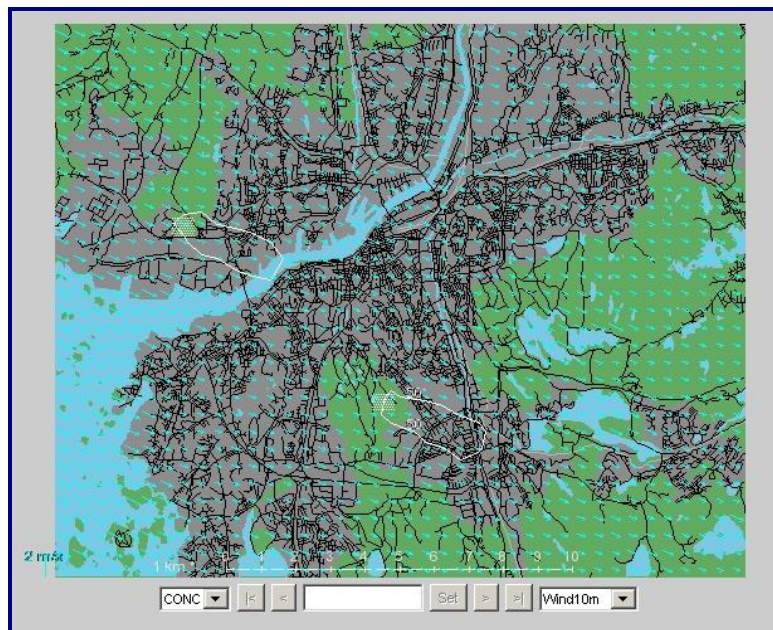
Now, you set the model (defining the weather conditions). Select Type: **Specific hour** and select the time period 900727 07 to 900727 08 (note that you are only allowed to alter the **To:** time, the **From:** time is automatically one hour less).

This time, select **Area** from the **Emission** subwindows.

- Choose the relevant **Substance (VOC)**
- Click on **Apply**

The calculation is submitted in the **Calculate** subwindow, after editing the description text. When you display the result (*Figure 2.2.3.1*), you notice a much stronger impact close to the area sources as compared to the point sources in *2.2.1 Examples Based on the Case Weather Condition*, although all examples have used the same emission rate (25 g/s). The low emission height together with the absence of a plume rise explains the high concentrations found close to the area source.

The number of grid points in which the concentrations are evaluated will normally be the same, no matter if you have zoomed or not (see *2.1.3 Comments on Resolution and Precision in the Dispersion Module*). This means that by zooming into a small, fairly square area, you will increase the spatial resolution of the dispersion calculation, which may be very valuable when you look on the conditions close to for example a road. The resolution in the description of the emission source location is high. But remember that the wind field will always have a rather low spatial resolution, typically calculated on a 250 or 500 m grid.



*Figure 2.2.3.1 Two area sources together with the wind field*

*Figure 2.2.3.1.* shows only the  $50 \mu\text{g}/\text{m}^3$  isoline, which clearly shows the directions of the plumes. This is done by choosing **Single 50**, under **Output configuration** in the **Output settings** on the frame.

---

**HINT:** If you want to get a better feeling for the grid resolution, use the **Output settings** on the frame. There you can toggle the grid rectangles and/or the grid points to be displayed above your map area.

---

## Result View Control

In addition the wind field is shown over the map, showing how the wind changes direction over the map area. This can be shown by selecting the **Wind10m** in the Viewer. The Result View Controller automatically appears. Other fields that can be examined using the Result View Controller are the Monin-Obukhov length (LMO) and the mixing height (MIXH).

## 2.2.4 Using Scenario Weather Conditions

The E6 is a very busy motorway that passes through Göteborg in the north-south direction. This road has been entered into the reference database as several different segments where each section reflects the traffic flow between two junctions. You can look at these road segments using the EDB module if you want. All these E6 segments have names containing E6.

By extracting this information from the global reference EDB we can find out the impact of this single road on the winter seasonal mean levels of NO<sub>x</sub> in the central parts of the city.

First select **EDB personal** under **EDB** (the EDB option is the only option available) and select **Area** source in the **Emission** subwindows.

Now select the weather conditions to use in the **Settings** subwindow (select **Model settings** on the frame). Chose Type: **Scenario** and select the scenario called **WINTER**.

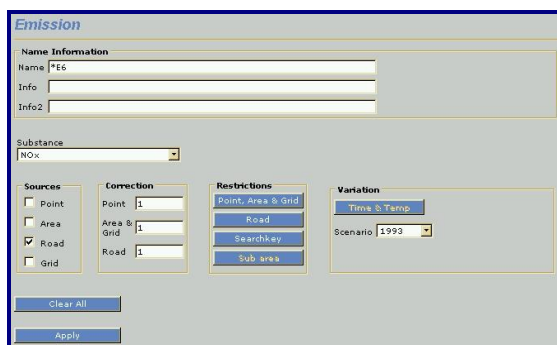


Figure 2.2.2.1. Emission

Enter the search conditions to find all road sources containing the string E6. Use the settings shown in the subwindow above. It is advantageous to use EDB search macros for complicated queries. See *Saving your search criteria* in *User's Reference Volume 1: Working with the Emission Database (EDB)*.

Now you can start the calculation. Don't forget to enter a precise description of the calculation in the **Start calculation** subwindow. Include information about which EDB sources are included and what weather conditions were specified. Once it has started you can keep an eye on the progress of the calculation by starting the **Watch** watchdog, which is found on the frame. Season scenario calculations are based on the classification of each season into a number of scenario classes (usually 180). For a description of the calculation principles, refer to *Appendix 2G: Scenario Calculations*.

---

**HINT:** You might be interested to see how your dispersion calculations are progressing, particularly if you have submitted more than one calculation. Alternatively you may want to kill a submitted batch job, because you have discovered that something was incorrectly specified. This can be done in the **Watch simulations** subwindow under the **Watch** on the frame.

---

When the calculation is ready you will see that you have actually obtained several calculation results for both the mean conditions and also some of the percentile conditions. Select the **MEAN** result field.

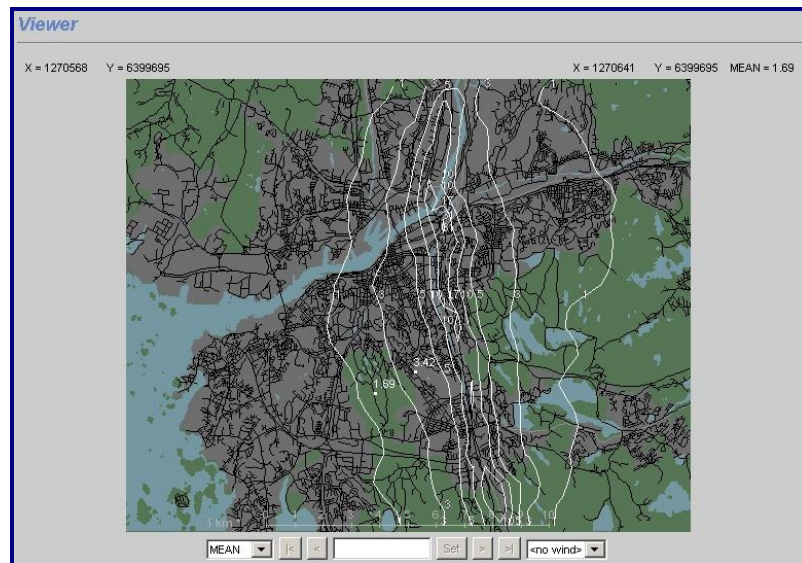


Figure 2.2.2.2. The E6 through Göteborg with winter mean weather conditions

The result in *Figure 2.2.2.2.* illustrates the effect of the inhomogeneous wind fields for the rather hilly Göteborg. You will find higher concentration in the valleys running east/west (such as the river valley), and lower values up on the hills. Note also that the winter mean calculation yields nearly symmetric concentrations west of the road, although the majority of time the winds tend to go from west to east. The relatively large importance of the sparse occurring east winds can be explained by a low degree of mixing during this weather situation. Thus the east wind situation is connected to stable and low wind speed situations while the frequently occurring southwest winds show higher wind speeds and more vertical mixing.

For a different way of presenting this dispersion result, you can display it in the form of a coloured grid. All calculations are actually performed over a grid. The grid size is displayed in the bottom right corner of the main window and you can show the grid rectangles on the map by selecting **Grid rectangles** under the **Output settings** on the frame. The size of the grid rectangles is determined by how much you have zoomed in on the map, since the number of grid rectangles is approximately the same for all calculations (unless you have zoomed up on an extremely small subarea).

Select **Output configuration** under the **Output Settings** subwindow.



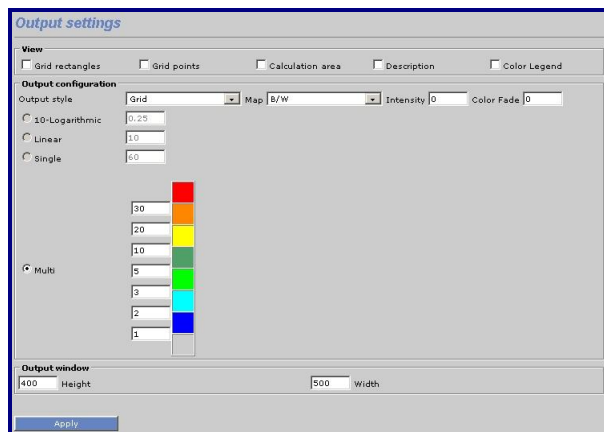


Figure 2.2.2.3. Output settings

Next to **Output style** select **Grid** (if you select **Class enumeration** then a class number is printed instead of a colour). It is best if you also select **B/W** (Black and White) next to **Map**, as the grid doesn't show up so well on a coloured map.

The values for **Intensity** goes from -100 (black) to +100 (white), keeping the colour but changing the intensity of the map. You can use **Colour Fade** to reduce the colours in scale of grey of the map. The values for colour fade goes from -100 (complete grey scale) to +100 (more bright colours).

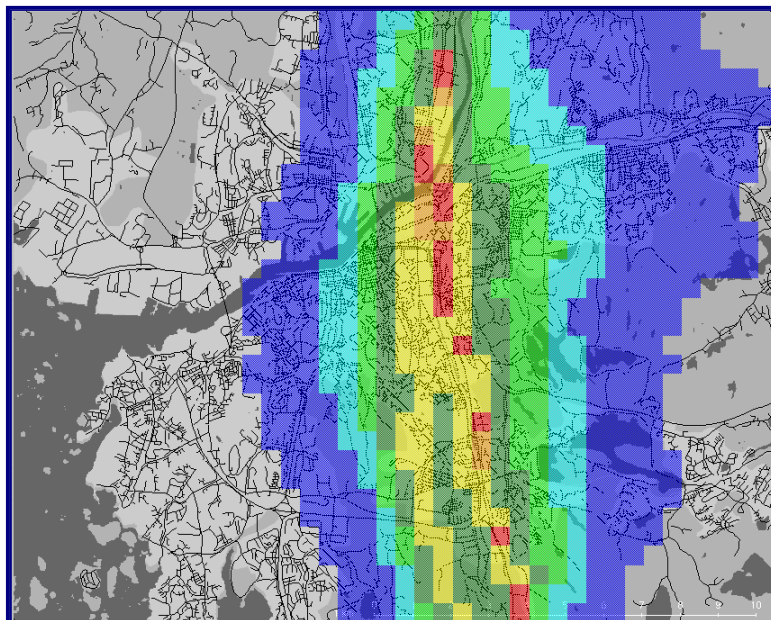


Figure 2.2.2.4 . E6 through Göteborg with winter mean weather conditions, shown as a grid.

You can alter the colours used as well as the class limits by clicking on **Multi**, a row of limits that you can change, and a row of colours. To change a colour, just click on it and a colour palette appears where you can select a different colour to use.

Now when you click on **Apply** the map and the dispersion pattern will be redrawn. If you would like to see the colour legend for the grid displayed beside the map, then select **Colour legend** under the **View Colour legend** menu in the **Output setting** subwindows.

## 2.2.5 Using the Advanced Result Options

This function allows you to perform some very useful operations with your dispersion result files created in the earlier examples. The function is activated in the **Advance settings** on the frame, and does not alter the stored result files in any way.

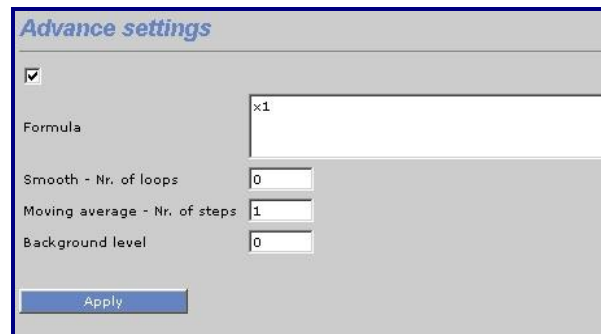


Figure 2.2.5.1. Advance settings.

### 2.2.5.1 Example Formula 1: conversion of NO<sub>x</sub> to NO<sub>2</sub>

The photochemical reactions that regulate the fractions of NO and NO<sub>2</sub> (together constituting the NO<sub>x</sub> amount) are fast and complicated, which means that a realistic simulation including these reactions is a rather advanced task. However there is an empirical way of estimating the NO<sub>2</sub> content from the total NO<sub>x</sub> levels. This is important, since NO<sub>2</sub> is the more harmful of the two oxides.

The prerequisites that allow you to use this conversion are:

- Historical NO<sub>x</sub> and NO<sub>2</sub> measurements should be available for a station that is located in a representative place (i.e. a station that is situated at a height - e.g. above roof level - equal to where the simulated NO<sub>x</sub> values are evaluated) and from a time period that is similar to the one simulated
- The simulation should be a long term value, e.g. winter or summer season (the conversion is not valid for individual hourly NO<sub>x</sub> concentrations).
- You have used the multiple regression formulas to find long term correlations between NO<sub>2</sub> and NO<sub>x</sub> levels (see Appendix 1 - Model Describing the Conversion of NO<sub>x</sub> to NO<sub>2</sub> in Users Reference Volume 2).
- The conversion is performed when you first select a NO<sub>x</sub> result file and specify a conversion formula. In the example here, a regression relation is used that was found from monitored data (station Femman at roof level) in Göteborg. Convert the NO<sub>x</sub> field simulated in 2.2.3 *Using Scenario Weather Conditions*, i.e. the effect of the European highway passing Göteborg:
- On the **Formula**, insert the NO<sub>x</sub>→NO<sub>2</sub> formula and enter the following algorithm:

$$0.73*x1*\exp(-0.00452*x1+0.003014*0.0001*x1*x1)$$

- Click on the **Apply** button

The displayed isolines will now be considerably lower than those from the NO<sub>x</sub> result file itself. The formula is based on the existence of a statistical relation between the NO<sub>2</sub>/NO<sub>x</sub> ratio to the absolute NO<sub>x</sub> level, in that the ratio normally is higher for low NO<sub>x</sub> concentration values.

### 2.2.5.2 Example Formula 2: Adding Various Result Files Together

This function allows you to build up your own combination of various different concentration fields. These results do not need to have been created over the same sub area, as long as they share the same map. A prerequisite is of course that the same weather conditions should prevail for the results that are summed together.

The function is particularly useful in the calculation of Air Pollution Indices, which are built up by different pollutant concentrations summed together, but with different weight functions. Another interesting use of this function is the calculation of the difference between two result files, e.g. to answer questions like "How much better will the situation be if I take this action....?"

Initially, you have to select the files from the **Results** subwindows, by clicking on first one result and then clicking **Update**. A list of chosen files is built up in the box under **Select**. Now click on **Advanced settings** to access the advanced result viewer.

The default operation when more than one file is selected is pure addition, which serves our purpose. The result presented on the screen is hence the way to combine effects of different sources (which can not be done directly in one simulation). The functions available in the Combination formula box are the same as those available in the Indico package (see *Exploiting the Mathematical Functions for Calculation Parameters in User's Reference Volume 3: Working with Indico Presentation*).

As an exercise, assume that the VOC emissions of the area sources in 2.2.3. *Examples Based on Emission for a Specific Hour* contained a toluene fraction of 11%. Plot the toluene concentration levels for the simulated summer mean values.

---

**Hint:** Also you can use the **Postprocessor** subwindow, select **Combined result model** as working tool. Remember: select one result first and then press **Update**, followed by another result and Update again. A list of chosen files is built up in the box under **Selected**. To replace a selected result, first highlight the result to be replaced by clicking on it in the Selected results box, then choose the result to replace it with from the list under **Description** and click on **Replace**. Instead, if you click on **Remove** the result will be taken away from the Selected results list. The **Remove All** button clears all the results in the Selected box.

---

### 2.2.5.3 Smoothing of Concentration Isolines

The need might arise for you to smooth your isoline pattern, without actually changing the levels (although this should be used with care). The smoothing function consists of a Laplacian filter, whose effect increases as more iteration are asked for. Test the output by a stepwise increase in the number of iterations.

#### **4.2.5.4 Moving average**

Many air quality standards use moving averages. If you do not want to apply a moving average, make sure that the size of the filter is 1 time step, otherwise it might be applied by mistake.

#### **2.2.5.5 Adding a Background Value ( $\mu\text{g}/\text{m}^3$ )**

When you know that your calculated concentration values only contribute to a part of the measured levels, you may add a constant background value. The background concentrations refer to sources not included in the simulation, within, or more commonly outside the calculation domain.

The background level will simply be added to your simulated concentrations. The isoline pattern remains exactly the same.

## 2.3 The Street Canyon Model

### 2.3.1 Street Canyon Overview

The street canyon model allows you to perform small scale simulations of the situation at a particular street segment surrounded by buildings. The model output is presented as concentration isolines on a vertical plane perpendicular to the street (for more details, see *Appendix 2E: Street Canyon Model*).

First select **Canyon model (CN)** under **Model** on the frame. Now you can define your street canyon. The definition of the weather conditions is identical to that of the Gauss model (2.2 *The Gauss Model*). Other model specifications are given in the **Emission** subwindow.

The screenshot shows the 'Emission' subwindow with the following details:

- Substances List:** Methanol, Mn, N2O, NH3, NO, NO2, **NOx**, Naphthalene, Ni, Nitrate, O3, PAC, PAH, PAN, PCB, PCDD, PCDF, Pb, PetroleumSpirit, Phenanthrene, Phenol, Propane, Propanol, Propene, Propeneglycol, SO2, SO3, SolventCl total, SolventHC total, Soot, Styrene, Sulphate, TCDD, TDI, Terpenes, Tetrachloroethe.
- House information:** Distance between houses [m] = 20; Height of houses [m] = 30.
- Street information:** Street width [m] = 14; Street direction [degrees] = 45; Position of street = 1275083 9608125.
- Emission:**  Fixed;  Roadtype; Emission [microg/m,s] = 100.

Figure 2.3.1.1. Emission of the Canyon model.

Start by choosing a substance from the list under Substances. Then work down the right side of the subwindow, filling in the correct information.

The **Distance between houses** and the **Street width** are not the same - **Distance between houses** has to include pavements and verges while **Street width** is just the part of the canyon base where the substances are emitted, e.g. the width of the part of the road that the vehicles actually drive on.

The **Height of houses** is the height of the buildings on each side of the canyon. The model assumes that the buildings on both sides of the canyon are approximately the same height.

The **Street direction** is the angle of the street in degrees measured clockwise from north.

Now click on the **Position of street** button and define the position of the canyon on the map. This is necessary in order to estimate the local wind at roof level for the dispersion calculation.

When you come to specifying the emission from the street you have two choices. Either you can specify a constant emission value (in microg/m,s) or you can link the emission to the road types defined in the EDB. Select the option that you want.

If you have chosen **Emission** then just enter the emission figure in the text box. Otherwise click on the **Emission from road types** button to get options.

Figure 2.3.1.2. Emission from road types

First choose the road type from the list under **Road types**, and enter the average number of vehicles per day, road type, and scenario. Finally select the average speed of the vehicles in the canyon with the option menu next to **Speed** and click on **Apply** to save settings.

### Example: Use of the EDB emission model in a Street Canyon simulation

This example studies midday VOC levels on Linnégatan, one of the principal inner city streets in Göteborg. The pollution levels along the pavements are of special interest, as many outdoor restaurants and cafes can be found in the vicinity. The traffic volume is about 21 000 vehicles per day, with a heavy traffic percentage of about 5%. The case will be studied with a typical north westerly wind of around 1-3 m/s during the summer season.

Choose the following weather settings:

**Type (Model Settings):** Time period  
**Period:** 9908021-99080220

If you want to find out the wind speed and direction for the chosen hours then you can use the Indico Presentation module Client to look at the wind speed and direction at Lejonet. You will see that at 5 pm, at a height of 8 m the wind speed is around 2.8 m/s with a direction of 325° (315° would be true northwest). At 8 pm, the wind has calmed to about 0.6 m/s

In the **Emission** subwindow, specify the following input data:

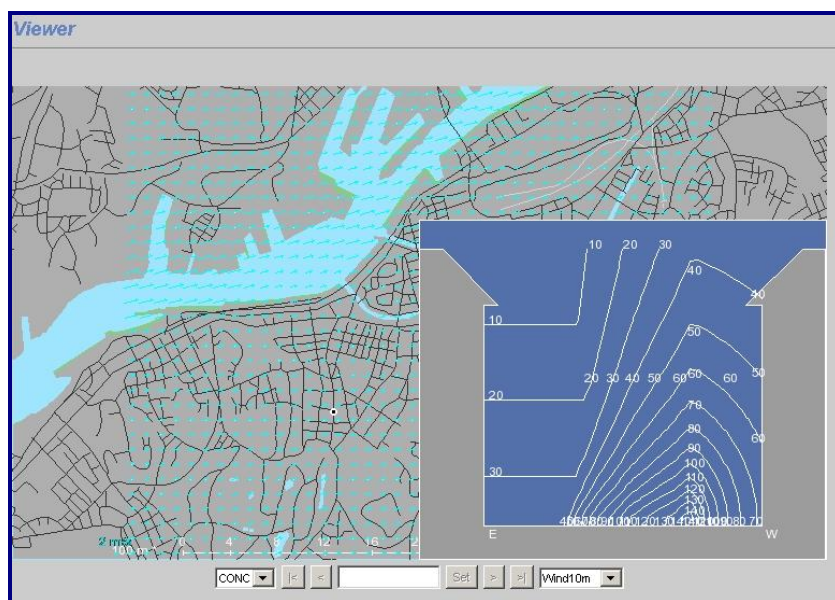
Substance:	VOC
Distance between houses (m):	30
Height of houses (m):	25
Street width (m):	15
Street direction (Degrees):	0
Road types	City centre 5% 5 s
Vehicles per day	21000
Speed	40 km/h
Scenario	1999

The position of the Linnégatan model section is shown as a white rectangle on the map to the left of the result shown in *Figure 2.3.1.3*. Use the hair cross to locate the position where you want your simulation to be performed.

Street Canyon calculations are submitted for batch execution in exactly the same way as for the Gauss model. Don't forget to give a proper calculation description.

The finished dispersion result consists of several fields, one for each hour chosen. When you select the result, a Result View Controller automatically appears where you can use the arrows under **Time** to step through the hours. If you activate **Wind**, you will also be able to see how the wind field changes from hour to hour.

The result file will be presented as in *Figure 2.3.1.3*. Note the higher pollution levels along the western side of the street, i.e. on the side to which the vertical eddy circulation will bring the traffic exhausts. Use the left button mouse to find VOC levels along the pavement (about 5 m from edge of the buildings, 1-2 from ground). Percentile values for season calculations can be viewed using the sub-menu shown below.



*Figure 2.3.1.3. Canyon model of a typical summer west wind across Linnégatan*

## 2.4 The Grid Model

Although the examples for the Gauss model have shown that different kinds of sources may be entered manually for each individual simulation, you will probably use the emission database for the majority of our dispersion calculations. There are various advantages with the EDB choice:

- all source characteristics are already stored in the Airviro and ready for use in dispersion models
- the EDB allows time and temperature dependence of the emission rate
- the EDB includes an emission model for road traffic, which means that you use traffic intensity as input instead of absolute emissions (the former being considerably easier to conceive)

When using the Grid model, you can only use input from an EDB. If you want to make a simulation from a single source, then you first have to create the source in an EDB and then specify search conditions that will find only that source.

Start by selecting the **Grid model** under the **Model** subwindow. Then you must make sure that you are working with the correct EDB. This is done in the **Select EDB** subwindow found under **Edb**. For this example you should use the global EDB for the REF database (the global EDB is usually the default EDB in Dispersion module).

### 2.4.1 Looking at Dispersions for a Specific Time Period

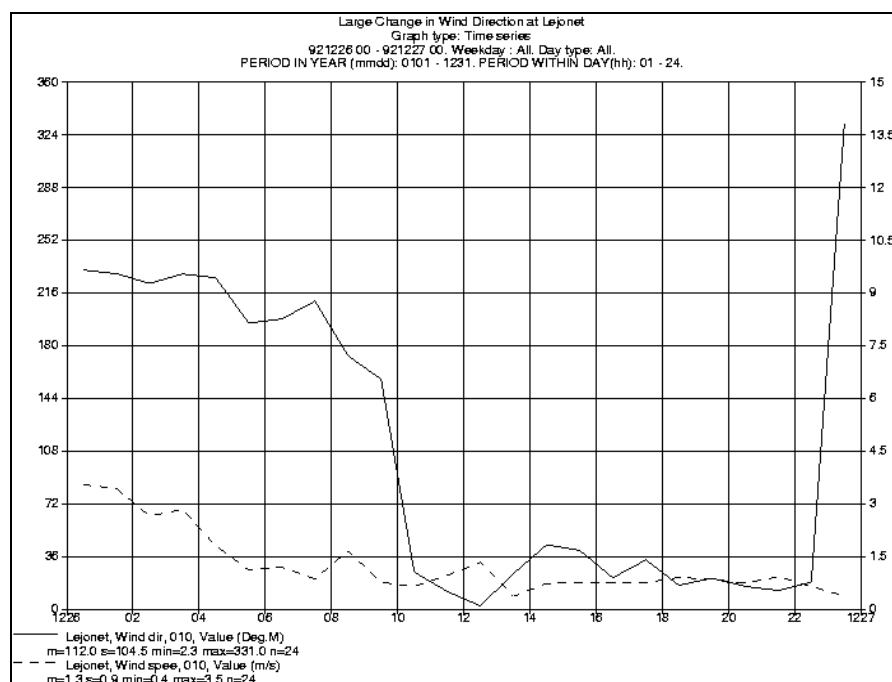


Figure 2.4.1 Wind speed and direction at Lejonet 921226



This example examines the way the dispersion pattern changes from hour to hour for the case when a dramatic change in wind direction occurs. The wind data to be used can first be examined using the Indico Presentation module client.

Choose the station Lejonet and the parameters wind direction and wind speed. Select the time period 921226 00 to 921227 00 and execute the graph. You will see that at 10 o'clock the wind was from the southeast but at 11 o'clock it had backed to a northerly wind. During the entire period the wind speed is very low.

Now some EDB sources are needed as input to a dispersion calculation with these weather conditions. Ideally it is best to use a large point source in order to be able to clearly see the effects of the changing wind direction. Start the EDB module client and examine the global EDB. Search for all point sources that have Large NO<sub>x</sub> as search key 1. This should show one large source in the north eastern part of the map, which is an incinerator, and a cluster of smaller sources in the western part of the map, which are part of the Shell oil refineries. The total emission is 1144 tons per year emitted at a constant rate throughout the whole year. Such high emission levels produce illustrative plumes in the dispersion models. Note however that the two largest NO<sub>x</sub> sources found by the search have a stack height of over 100m. This means that under certain weather conditions all or part of the emission plume breaks through the inversion layer and can be transported outside the map area.

Now return to the Grid model and set up the parameters for the dispersion calculation. Under **Model Settings** choose Time period and enter the period 921226 07 to 921226 15.

Under **Emissions** only EDB is available; select it, then select Large NO<sub>x</sub> as search key 1.

You are now ready to submit the calculation. Click on **Calculate** and enter a proper description including the date and times for the time period chosen. Start the calculation.

The final dispersion result consists of several fields, one for each hour chosen. When you select the **Results** option and click on **Viewer**, the Viewer page is shown and you can use the arrows under **Time** to move through the calculations. If you **select Wind10m** then you will also be able to see how the wind field changes from hour to hour. Looking more carefully at the wind field, you will see how it is affected by both topography and ground type.

For a clear overall picture of the areas of highest concentration and the way the plume moves around use the **Grid** rectangles output option (under Output Settings).

The following pictures show some of the resulting fields. If you have not run the simulation yourself then you can find it under the user **ref** for the project Users Ref. so that you will be able to look at the whole time series of simulations.

The first dispersion output in *Figure 2.4.2* shows the dispersion pattern at the start of the period. Emissions reach above 30 µg/m<sup>3</sup> for left plume and above 20 µg/m<sup>3</sup> for the right plume. The south-south-westerly wind is stronger over the sea and rotates to the right over land. Variations in the wind field over land can be seen between built up areas and open fields.

The second picture in *Figure 2.4.2* shows the dispersion pattern at midday. The wind has completely changed and is now coming from the north. The wind is a bit stronger and there has been no build up of emissions yet so the emission levels are lower (the highest value is just above 10 µg/m<sup>3</sup>). Small variations in the wind field can be detected.

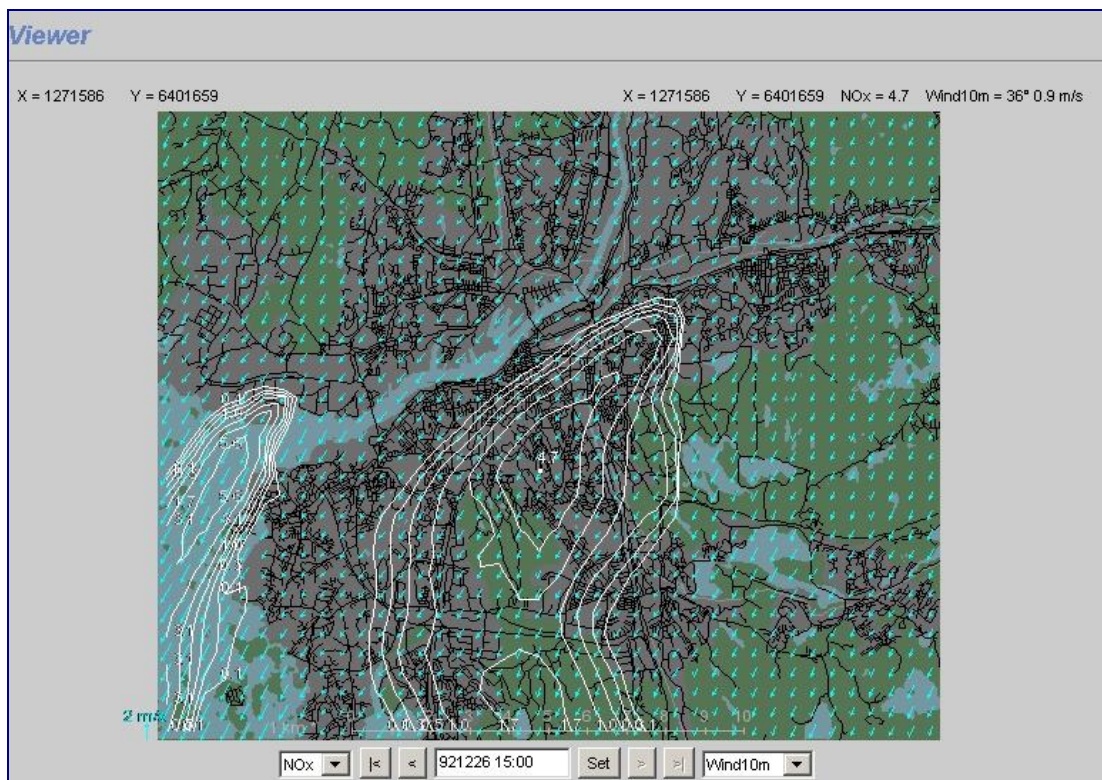
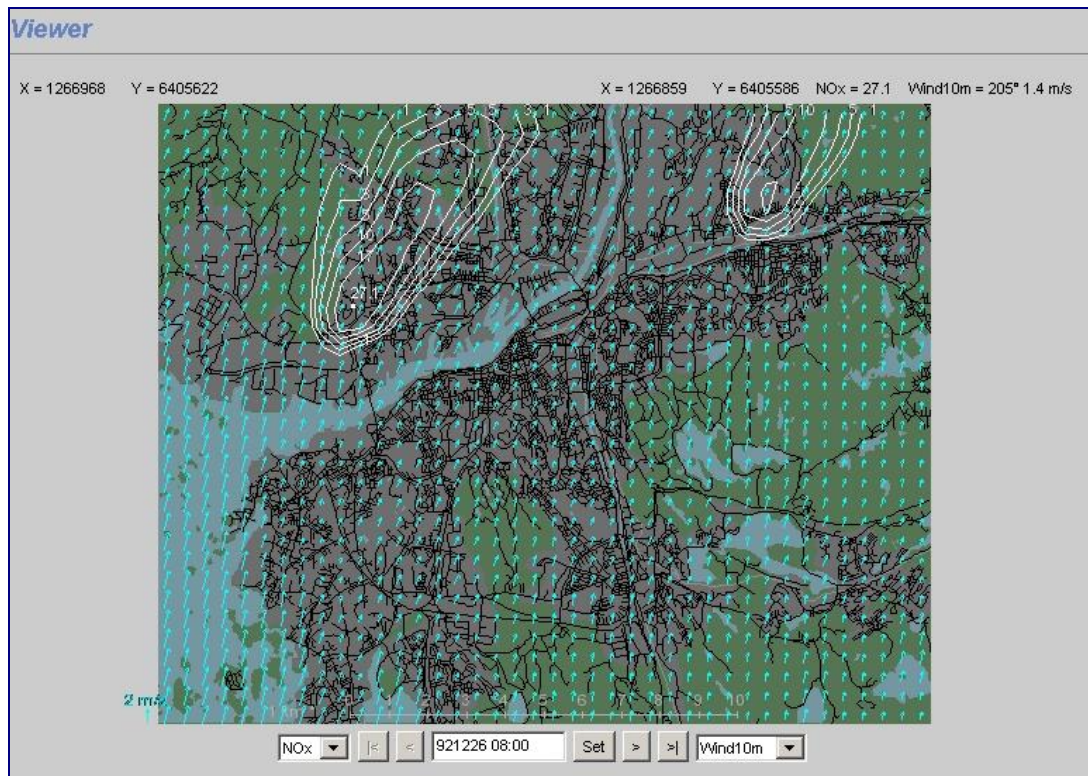


Figure 2.4.2 The two NO<sub>x</sub> plumes and the wind field at 921226 08 and 921226 12

## 2.4.2 Looking at Dispersions for a Season

Seasonal calculations for the Grid model are very complicated and only accept input from the EDB. Therefore these calculations can take a very long time, at least several hours and even longer if you have many EDB point sources as input.

The output from the Grid model can be compared with that of the Gauss model. In 2.2.3 *Using Scenario Weather Conditions* a simulation of the emissions from the E6 motorway was carried out for a winter scenario. The same simulation can be run with the grid model and the mean wind field is shown in *Figure 2.4.3*.

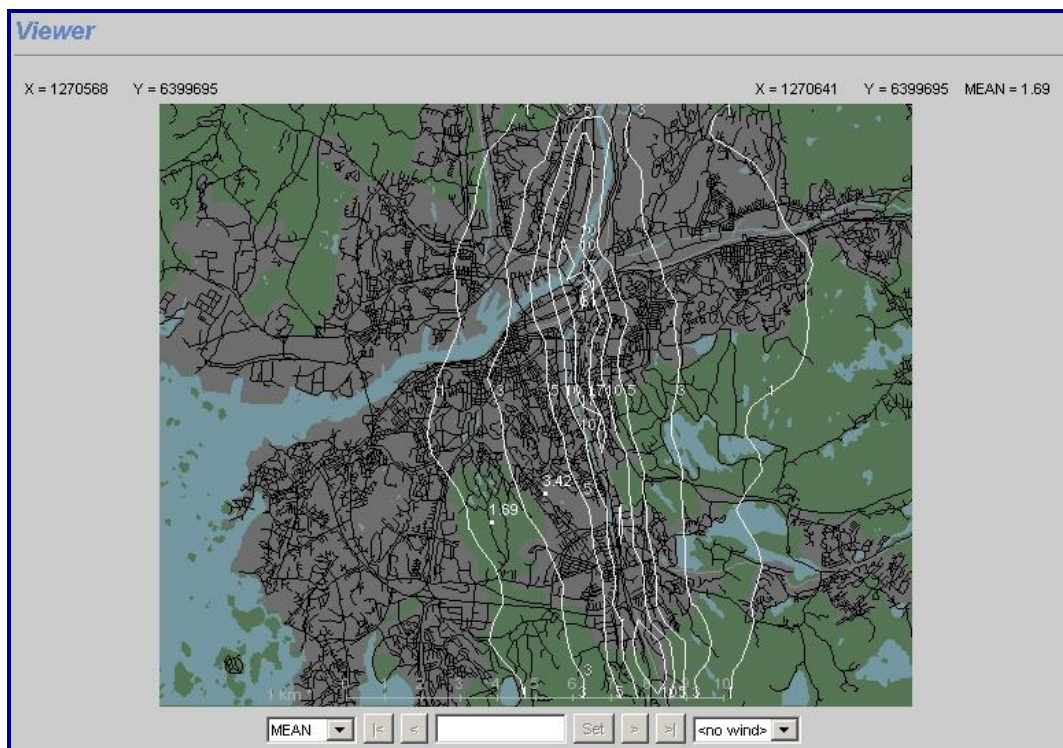


Figure 2.4.3 Winter mean scenario from the E6 highway

## 2.5 The Heavy Gas Model

The Heavy Gas model is unlike any of the other models. As its name implies, it cannot use the ordinary substances used as input to the other models, but has its own predefined substance list where properties such as molecular mass and specific heat capacities are taken into account.

The Heavy Gas model has been developed primarily for estimating the emission of pressure-condensed gases from accidents such as a leaking pipe or a fractured tank. The emission can be specified in one of three ways:

- As a tank burst (where all the gas is emitted instantaneously)
- As a continuous liquid leak (where the leaking liquid evaporates to a gas)
- As a continuous gas leak
- As a continuous pipeline leak

The weather input to the model is either a hypothetical case or a specific hour extracted from the time series database. A wind field is then calculated and this together with some information about the amount of gas and size of the leakage are used as initial conditions to the model. The output produced is however a time series and the result can be presented for up to 20 predefined time steps.

The initial wind field is used for the entire calculation period (usually less than one hour). A major difference compared to the case alternative when using a specific hour is that the topography and surface roughness are taken into account in the calculation.

The Heavy Gas model should be used to give an indication of where the concentrations would be worst and how high this concentration level might be. It should be used for small areas (ideally a couple of square kilometres only). The initial dispersion process (the heavy gas phase) should be studied by zooming in as close to the source as possible.

Change to the Heavy Gas model by choosing **Heavy Gas** under the **Model** subwindow on the frame.

### 2.5.1 Simulation of a Continuous Liquid Leak

The following simulation describes a tank accident at midday in the town centre. Chlorine leaks out of the tank over a period of about half an hour. An hour after the leakage began; the chlorine has been carried away by the wind.

Figure 2.5.1 Emission-Heavy Gas.

First, set up the weather conditions in **Model Settings**. Choose **Specific hour** and specify the date and time 920524 12-13.

Zoom into an area of approximately 2\*2 km in the middle of the map. Click on **Pos. of source** and use the scale shown at the bottom of the map to get an idea of the size of the area you have selected.

Now click on **Emissions**, which is the only source option available for this model. Here you can enter the criteria for the heavy gas emission. Enter the following information:

<b>Events:</b>	Continuous Liquid Leak
<b>Substances:</b>	Chlorine
<b>Tank data</b>	
<b>Pipe length:</b>	0.1 m
<b>Pipe diameter:</b>	0.025 m
<b>Tank contents:</b>	10000 kg

Click on **Pos. of source** and locate the source somewhere towards the top right corner of the map.

The other options in the **Heavy Gas** subwindow are not available to you, so save your settings and close the subwindow by clicking on **Apply**.

Now choose **Calculate** and order the calculation. The calculation will be ready very quickly.

Figure 2.5.2 shows the concentration levels (in mg/m<sup>3</sup>) 10 minutes after the leakage began. The dispersion has now reached a steady state and the plume stops growing. However, 45 minutes after the accident, all of the chlorine has leaked out and the plume starts drifting away.

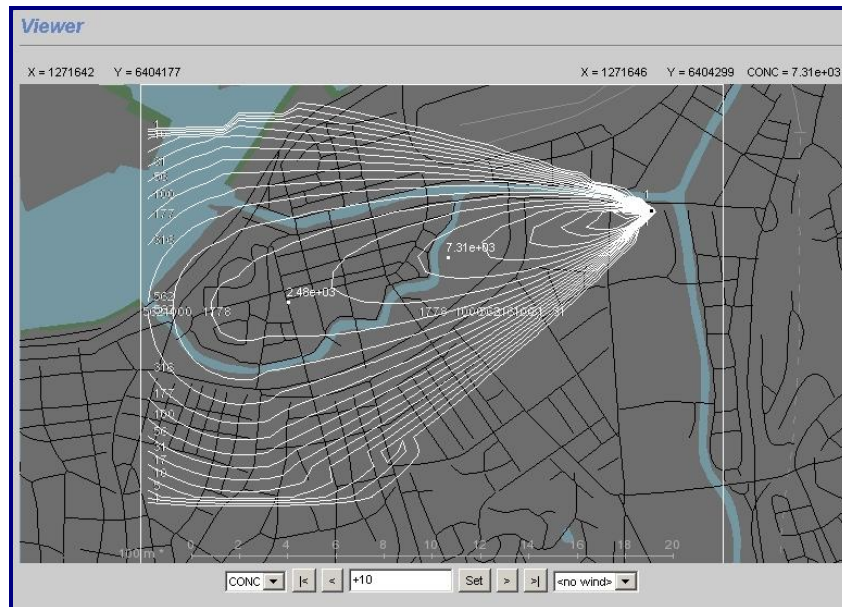


Figure 2.5.2. Simulation of Chlorine levels from 920524 12, 10 minutes after a leak began

## 2.5.2 Simulation of a Tank Burst

With a tank burst, all of the emission takes place instantaneously and the highest concentration levels immediately begin to drift away from the source location. The tank burst concentration is rather idealised and is always shown as concentric circles. For this simulation example a Case weather condition will be used.

Under **Weather...** choose **Case** and choose the **NEUTRAL\_POS** stability condition. Give a wind direction of 225 degrees and a wind speed of 3 m/s. Keep the same map area as for the continuous liquid leakage.

In the **Heavy Gas** subwindow specify the following settings:

<b>Events:</b>	Tank burst
<b>Substances:</b>	Ammonia
<b>Tank Data:</b>	
<b>Pipe length:</b>	5 m
<b>Pipe Diameter:</b>	0.025 m
<b>Tank contents:</b>	10000 kg

Click on **Apply** to save your settings and return to the main window.

Now order your calculation. It should be ready almost immediately.

Figure 2.5.3 shows how much the centre of the plume has moved just 10 minutes after the burst. An hour after the burst the plume has completely left the area.

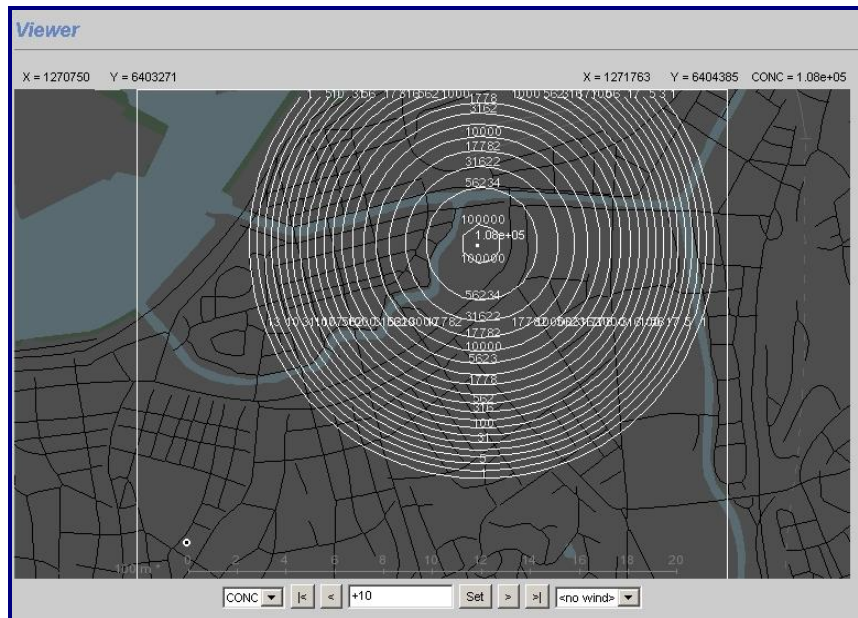


Figure 2.5.3 Ammonia leakage from a tank burst, 10 minutes after the burst.





## 2.6 Introduction to the Receptor Model

Suppose you have at your disposal:

- A number of high quality time series measurements of a particular pollutant
- Simultaneous time series measurements from a meteorological mast situated in the same area

Using the Indico Presentation Module Client, you have looked at the concentration time series, and have noticed occasional events where the pollution levels rise in a way that clearly demonstrates an impact of some source or sources. It is likely that your immediate question is:

### 2.6.1 Where is this pollution coming from?

Although you have your suspicions, you need more objective proof to support your ideas.

A first indication can be found in the Indico Presentation Module Client by performing one or various Breuer plot diagrams, which will inform you about the wind direction correlating to high pollution levels at a certain monitoring station (see section *Using the Polar Diagrams* in *User Reference Volume 3: Working with Indico Presentation.*). These diagrams will however only tell you directions to a potential source, not distance. You will be able to get a more detailed analysis of the measured data through the use of the Receptor module described in this volume. The Receptor Model implies the combined use of measured concentration values at certain locations (receptor points/open paths) and simulated concentrations evaluated at the same locations. This manual assumes that you are already familiar with using Indico Presentation Module Client.

The requirements for working with this module are that at least a few months of hourly concentration measurements and simultaneous data series from a meteorological mast measurement station are available. The need for high quality data is stressed repeatedly, since in the end it might be difficult for the user to discover erroneous results that depend on non-representative input data. This is the reason for accepting only meteorological mast data.

Although the Receptor model may in principle be used on any scale, we recommend that it be only applied to small areas, typically not more than a few square kilometers. This is partly because of the fact that the model assumes a homogeneous wind field, i.e. the dynamic wind model is not used. The Receptor model is easier to use for ground level sources than for stack emissions due to the fact that the height of the source is specified before execution. The height is vital in order to estimate the location.

### 2.6.2 For proper use of the Receptor module:

Use only high quality data, checked and controlled in the Indico Presentation Module Client

Small scale applications are recommended

It is better to use the model for ground level sources (sources where the emission height is lower than the height of the wind sensors on the meteorological mast)

You may also consider the case where you have a rather clear picture of the location/locations of the dominating pollution sources.

The next important question is:

**What are the emission rates from these dominating sources?**

The Receptor Model will calculate the estimated emission for one or various sources, based on the monitored time series concentrations.

Note however that the quality demand on the input data for carrying out the emission estimation is even higher than that required for the task of locating the dominating sources.

The use of the Receptor model will be explained through the discussion of some examples built on synthetic data, since the real Reference database lacks relevant data. More detailed descriptions of the calculation methods are given in *Appendix 4A: A Method to Locate Dominating Sources* and *Appendix 4B: A Method to Estimate Emissions from Dominating Sources*.

## 2.6.4 Overview of the Receptor Model Settings Window

In this model all the windows are equal to the explained and showed for other models, an exception of Model Settings windows. All the functionalities are the same that for other models, several the model settings.

First select **Receptor model (RD)** under Model on the frame. The definition of the weather conditions or model settings is different that the Gauss model. Now you can select your type settings. Other model specifications are given in the Emission subwindow. You will use the emission database of our dispersion calculations.

Click on **Model settings** and under **Period** you specify the start and stop dates for looking for data in the database.



Figure 2.6.3.1. Settings subwindow

Clicking on **Criteria** you can enter the criteria to set restrictions and conditions for the variables.

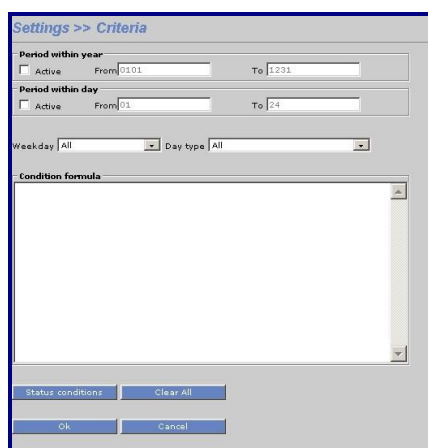


Figure 2.6.3.2. Criteria subwindow

The first thing to do is to select the meteorological data to use as a basis for your calculations. If you click on **Database** under the **Meteorology** heading then the familiar **Time Series** subwindow will appear. Choose one meteorological mast and select the parameters wind speed, wind direction, temperature, standard deviation of vertical wind direction and vertical wind speed, and temperature difference. It is possible to also include wind speed and direction from a second level if this data is available.

In this subwindow the data resolution is fixed on hourly values and you also cannot use the **Contents** button. Instead, when a calculation is started you are informed as to how many data values have been found. Note that for any given hour data is only used if it is present for **all** chosen parameters.

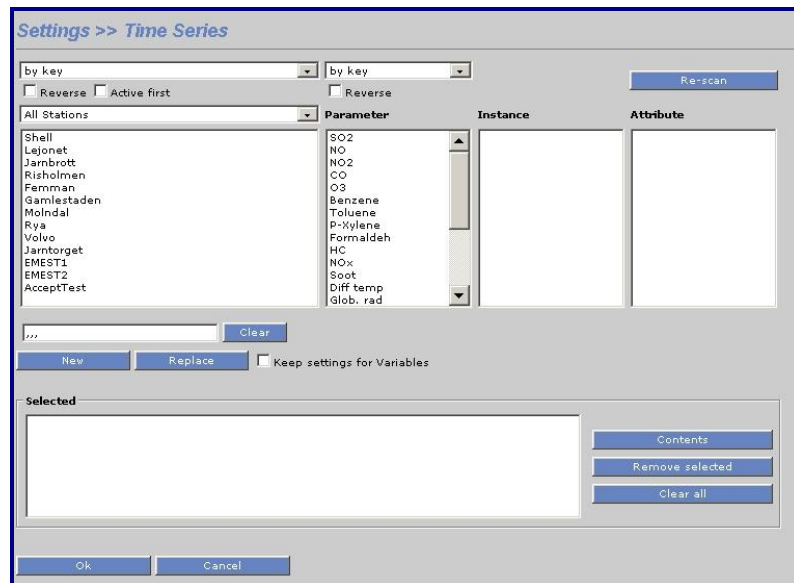


Figure 2.6.3.3. Time Series subwindow

The next button, **Variables**, can be used to apply mathematical transformations or criteria to the meteorological data.

Now move down to the **Concentrations** heading and in the same way select the time series data to use in the calculation. Again, you can apply mathematical transformations or criteria to the data under the **Variables...** subwindow.

---

**Note:** Use the on-line help if you have difficulty specifying the meteorological data.

---

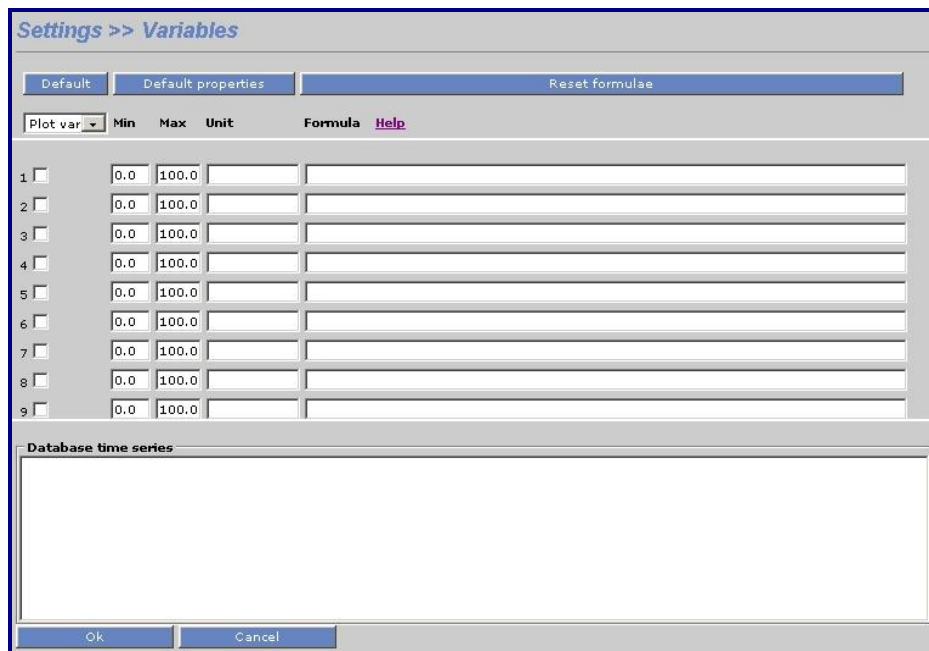


Figure 2.6.3.2. Variables subwindow

When the whole calculation has been defined, click on **Calculate on the frame...** Here you submit your calculation in the same way as in the Dispersion Module. Finished calculations can be viewed by selecting them under **Results**.

Under **Emission** you will get a different subwindow, depending on whether you are carrying out a **source location** or **source estimation**. This is where you must specify some characteristics of the sources that you are searching for.

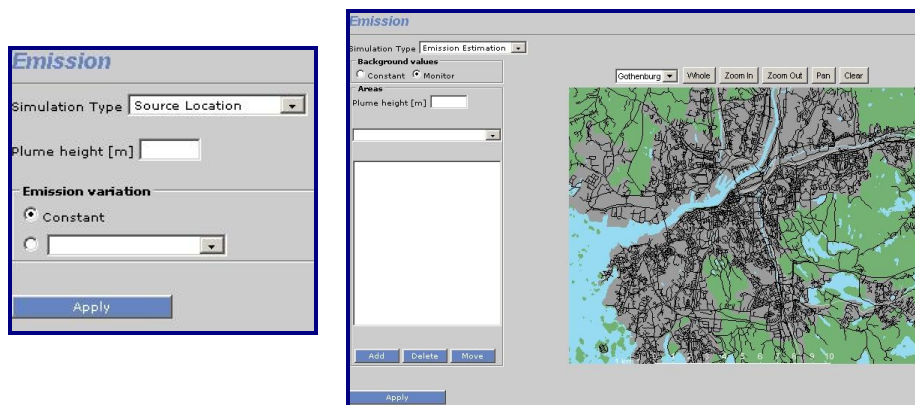


Figure 2.6.3.5. Emission subwindows

Under **Output Settings** you can choose to show extra information about the results displayed - you can have a description of the result at the top of the working area, a colour legend down the left side (for use with the grid output) or a box showing the actual calculation area. These are all toggle options - select them once to activate them, and select them once more to deactivate them.

## 2.6.5. Source Location

### An Example on How to Locate Dominating Sources

As has been stressed previously, high demands are put on data quality for this application. The example that will be worked through, first locating the sources and then carrying out the actual emission estimation is partly built on synthetic data. The reason for this is the lack of a good, high quality data set within the Reference database.

### The Data to be Used

The basis for the calculation consists of a three month long meteorological mast data series from station *Lejonet* in Göteborg, for the period 890201 to 890501. We have taken the Gaussian dispersion model and calculated the impact of two area sources on two DOAS stations, each of which is measuring along two paths (see Fig. 2.6.2.1.). In order to achieve more realistic time series, we have further introduced:

- an instrument noise randomly distributed within the interval  $\pm 2 \mu\text{g}/\text{m}^3$
- a randomly distributed background level in the interval 0 to  $20 \mu\text{g}/\text{m}^3$ , equal for all 4 DOAS paths, and with a long term average of  $10 \mu\text{g}/\text{m}^3$ .

The concentration data time series have been stored as measured toluene data in the Reference database. The stations are named EMEST1 and EMEST2. The area sources emit with a constant rate 10 and 5 g/s, respectively. Both emissions have plume heights of 10 m.

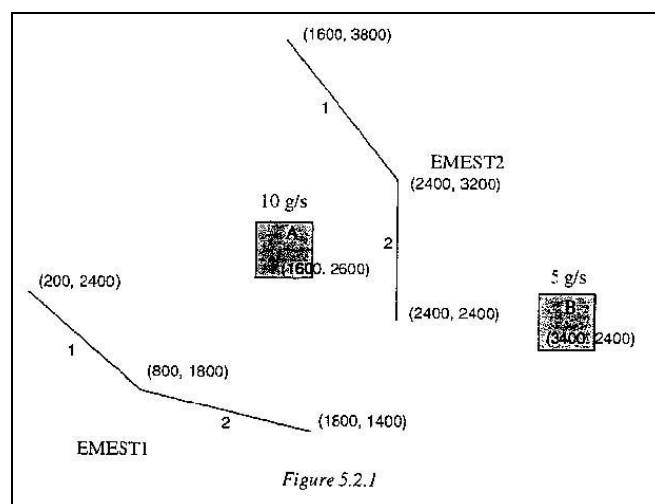


Figure 2.6.2.1. DOAS stations

### Carrying Out the Example

A piece of general advice is to study the concentration data in the Indico Presentation Module Client before using the Receptor Model. You may see the variation around the background level of  $10 \mu\text{g}/\text{m}^3$  plus some peaks where it is obvious that some dominating sources affect the DOAS stations.

Make the following settings in the Receptor Model:

---

**Meteorology:**

Database Lejonet, Wind speed, 010, Value

Lejonet, Wind dir, 010, Value

Lejonet, Temp, 002, Value

Lejonet, Std vert, 010, Value

Lejonet, Std vdir, 010, Value

Lejonet, Diff temp, 008, Value

Database: EMEST1, Toluene, 001, Value EMEST1, Toluene, 002, Value EMEST2,  
Toluene, 001, Value EMEST2, Toluene, 002, Value

Period From: 890201 To: 890501

When it comes to specifying the emission, there are several ways to do it. First you must guess the height at which the largest concentration is found (plume height). Then you can specify an emission variation, which you can assume either to be constant or to be based on a formula that has been previously defined in the EDB (monthly or daily variation).

For this application though, specify a plume height of 10m with a constant emission variation.

Now select **Calculate** and submit the calculation. Remember to give a meaningful description. A dialogue box will appear after a few seconds indicating how many values were found (there should be over 2000) and asking if you want to start the calculation. Answer **NO**. This is because you should now zoom into the area in the upper left corner of the map, where the opsis paths should now be shown. After you have zoomed up to a relevant subarea around the two DOAS stations, submit the calculation again and this time answer **YES**.

This calculation can take quite a long time, depending on the speed of your computer. You can watch its progress by choosing **Watch**. When it has finished, click on **Results**, choose the finished calculation and click on **Apply**.

The result should look like Fig. 2.6.2.2. as long as the subarea that you chose is similar to the one in the figure. With the left button (Local value) you will easily find the two area sources, although their physical size is not so easily deduced. If these area sources were real industries, it should be possible for you to combine your knowledge of the area with the isoline pattern to actually be able to guess the dimensions of the two dominating sources.



Figure 2.6.2.2. Result

## 2.6.6 Emission Estimation

When you have found one or various dominating sources, you can proceed to try to estimate the respective emission rates. We will use the same data set as in section 2.6.4 for this exercise. In order to specify the input data, use the result of the source location calculation as a good background on which you can base your estimate. Keep the same period and time series data as you used when locating the dominating sources.

You might find it easier to change to a grid output to help you to guess the size and location of the sources - this can be done under **Output configuration**. Select **Grid** next to **Output style**, change the map to **B/W** and select the **Multi** option. Experiment with configuration levels until you get a satisfactory grid output on the map.

Now change to the **Emission estimation** model.

Next you have to define the location and the size of the dominant sources, and estimate their individual emission characteristics. This is done in the Emission subwindow.

First you can select the type of source you are trying to locate. Currently you can only locate area sources. You can then use the result of a source location calculation to guess the rough location of the source(s) that you are looking for and in this way you can locate one or several sources on the map. Each emission source can be linked with an emission variation described by an EDB time variation formula that has previously been defined in the EDB module. It is also necessary to give each source an estimated plume height.

For this example use the isoline or grid pattern given by the source location calculation to locate two area sources, using a constant emission rate and 10 m plume height for both sources. You can link the sources to any of the formulae in your EDB, but for now use the **STANDARD** formula (which gives a constant emission that does not have any time or temperature variations).

You should also give some assumptions of the background concentration. The normal option is to assume it to be constant, but for cases where you expect the pollution monitors to be influenced by a remote source you may try the **monitor** option. The latter method will only use the hourly values when there are at least one monitor that is assumed to be influenced and at



least one that is not influenced by the local sources you have defined. The influence/not influence question is determined from the simulated concentrations. The average value of the non-influence monitor stations is used to create a background time series that will be subtracted from all monitor time series before they are used as input to the regression analysis.

The execution of the job is identical to that you learned in section 2.6.4, except that you must also give values for the statistical parameters **F-in** and **F-out**, which are used by the regression model. See section *Exploiting the Regression Models in User's Reference Volume 3 Working with the Indico Presentation* for more information about the station database. default values of **Fin** = 0.05 and **Fout** = 0.10 are recommended for use with the regression model.

The emission estimate will be presented on the map, showing the specified area sources with their respective emission rate (g/s) followed by the standard error (the standard deviation of the estimated error). If you have chosen to show the description, the background value will also be given.

**Hint:** Repeat the emission estimation while varying source location/sizes, emission variation and/or the emission height. A higher multiple correlation coefficient will indicate that your assumptions improve. For the same number of sources, the individual standard error may also be used as a sign of improvement of your assumptions for each individual source.

If you activate the **Description** option under **Output Settings** you will see information about the result clearly presented.

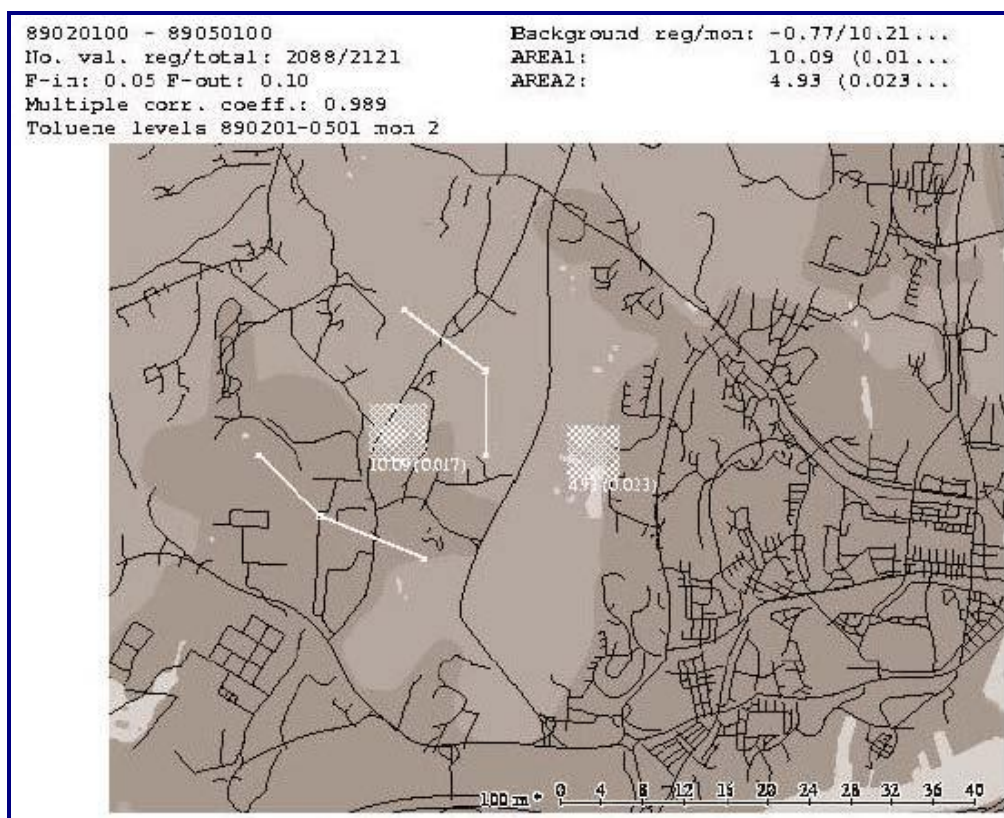


Figure 2.6.5.1. Result

With the monitor option for the background values, you will have both the average of the monitored time series as well as the background value that comes out of the regression.

Repeat the estimation but now using **Monitor** option instead of **Constant** in the subwindow where you specify the characteristics of the background levels. You should be able to pick out the background level mentioned in previous section.

If you have activated the **Description** option then you will get a lot more information:

The monitor option does not accept all time series data. The number of data values used out of the total available is given next to No. val. reg/total.

Beside Background reg/mon are two background values. The first is the background value detected by the regression analysis and the second is the average of the monitored time series.

The dates, statistical parameters, correlation coefficient and name of the calculation are also shown along with the estimated emission and standard error for each of the area sources.

See *Appendix 4B: A Method to Estimate Emissions from Dominating Sources* for more detailed information on the monitor option.

## 2.7 Aermod Model

The Aermod model is 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.

The topographical correction of the plume concentration is described in the document, **AERMOD: DESCRIPTION OF MODEL FORMULATION .EPA-454/R-03-004 September 2004**, 91 pgs . The formulas used for the plume rise are given in pp 51 – 53 in that EPA document. The segments, the model use to describe the influence of surrounding building for point sources are also described in the mentioned EPA documentation.

The Aermod model can only use data from EDBs. If you want to make a simulation for a single source, then you have to create the source in an EDB. The **Aermod** sub page allows the specification of buildings surrounding for point sources. One specifies the number of circle segments around the source and for each of the segments the width, height, length, distance from farthest wall and centre are specified.

In this Manual contains an example that you can follow step by step. Start by selecting the **Aermod model** under the **Model** subwindow. Make sure that you are working with the correct EDB. This is done in the **Select EDB** sub page found under **Edb**. For this example you should use the global EDB for the REF domain (the global EDB is usually the default EDB in Dispersion module).

In the **Settings** sub page select Time period. See *Figure 2.7.1*. Select the time period 900812 01 to 900812 03 (note that you are only allowed to alter the **To:** time, the **From:** time is automatically one hour less).

The calculation **height**, which by default is 2 m, is the level above ground where the model evaluates the concentration values.

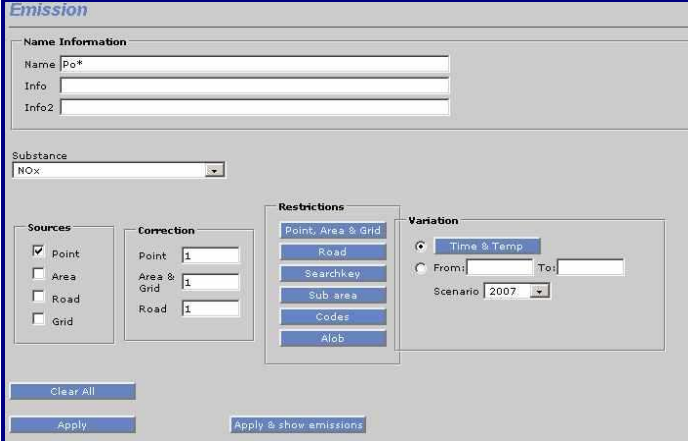
Click on **Apply**, which will save the weather settings (**settings saved**).



Figure 2.7.1. Aermod. Model Settings

Under **Emissions** only the **EDB** option is available.

You can use the **Apply&show emissions** button on the **Emission** window to check the availability of emissions for the calculation. See *Figure 2.7.2. Emission.*



*Figure 2.7.2. Aermod. Emissions.*

Now you are ready to submit the calculation. Click on **Calculate** and enter a proper description including date and times for the time period selected. Start the calculation.

The final dispersion result consists of several fields, one for each hour in the simulation period. When you select **Results** and click on **Viewer**, the Result View Controller automatically appears and you can use the arrows under **Time** to move through the calculations. See *Figure 2.7.3. Viewer.* This calculation used the source Point\_1\_ExampleAermod.

For a clear overall picture, under **Output Settings** select Isocolor in *Output style* and B/W (black and white) in *Map* and *Intensity 50*. See *Figure 2.7.4 Output Settings.*

The following picture show one of the result fields. If you have not run the simulation yourself then you can find it under the user **ref** for the project Users Ref.

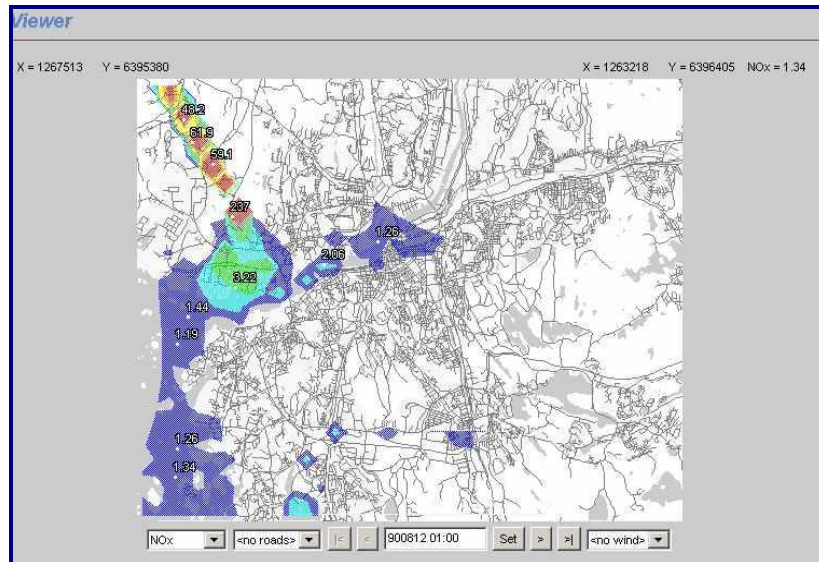


Figure 2.7.3. Viewer

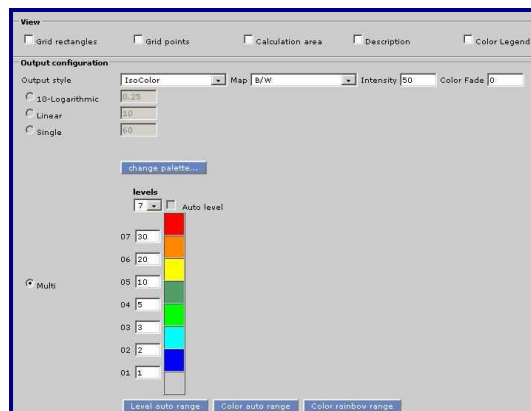


Figure 2.7.4. Output Settings

## 2.8 OSPM Model

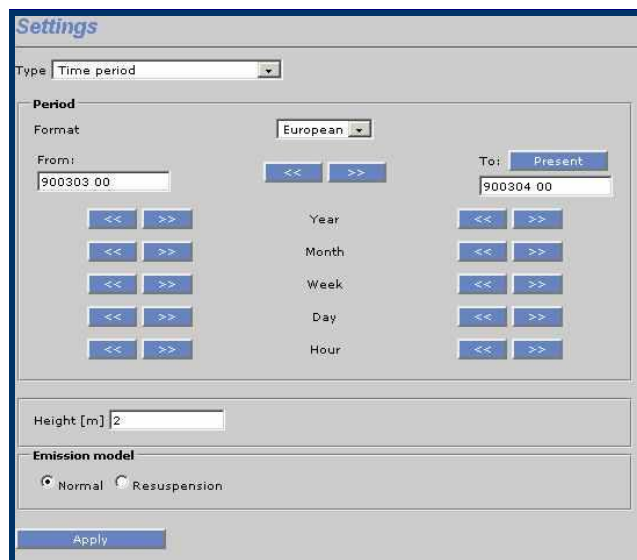
The OSPM street canyon model allows you to perform small scale simulations of the situation at a particular street segment surrounded by buildings. The model description summary is presented *Appendix 2J: OSPM Street Canyon Model*.

However, the SMHI Open Road model is applied in open streets without buildings. The heights of buildings are defined in EDB module as properties of the road (**Roads - Height**)

First select OSPM Street Canyon / SMHI Open Road (OS) under **Model** in the left frame. Now you can setup your model run.

In the **Model Settings** page, select Time period in the text box **Type**. See *Figure 2.8.1*. Select the time period 900812 01 to 900812 03.

The calculation **height**, which by default is 2 m, is not used by this model. Instead the characteristics are specified per road. Click on **Apply**, which will save the weather settings (**settings saved**).



The screenshot shows the 'Settings' dialog box for the OSPM model. It has a 'Type' dropdown menu set to 'Time period'. Below this is a 'Period' section with a 'Format' dropdown set to 'European'. The 'From' field contains '900303 00' and the 'To' field contains 'Present'. There are navigation buttons (left and right arrows) for 'Year', 'Month', 'Week', 'Day', and 'Hour'. Below the 'Period' section is a 'Height [m]' field with the value '2'. The 'Emission model' section has two radio buttons: 'Normal' (selected) and 'Resuspension'. An 'Apply' button is located at the bottom of the dialog.

*Figure 2.8.1. OSMP. Model Settings*

Now, you must specify the calculation area. Click on Area to open the area page and select the area for the calculation or input manually the grid and area. For this model, the grid is only used by the Danard Wind model to give the wind data for each street. *Figure 2.8.2*.

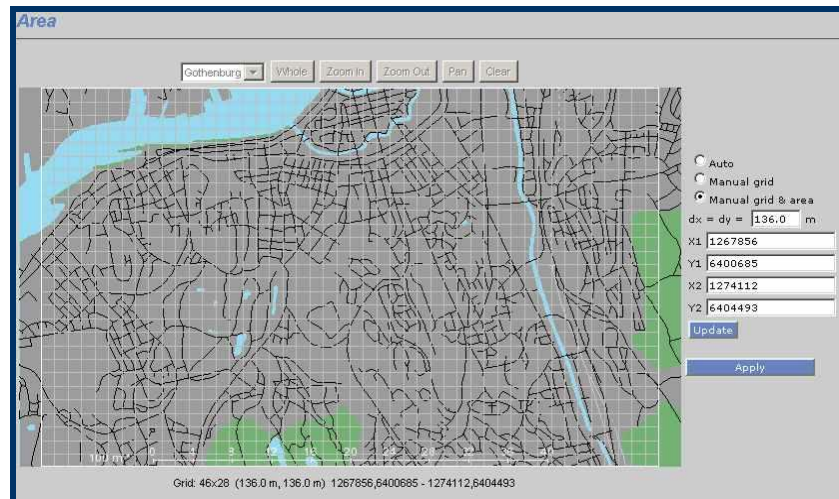


Figure 2.8.2. Area

Under **Emissions** a number of roads from the EDB can be picked and an OS simulation is made for each of them (see Figure 2.8.2).

The user must enter the following characteristics that apply to all roads in the model run:

- **Receptor Height:** The model requires the receptor height in meter. Example: 2 meters.
- **Distance from (open) road:** In case the road is an open road (no surrounding buildings) the model requires the distance from the road to the receptor. Example: 3 meters from road. This distance is not used if the road is a street canyon.
- **Substance:** select the substance for the calculation. Example:  $\text{NO}_x$

Click on the map to select emission sources for the calculation. If you click on a source a window appears to include or exclude that source from the calculation. The selected source is identified with its name. Roads included in the model run are shown in bold black.

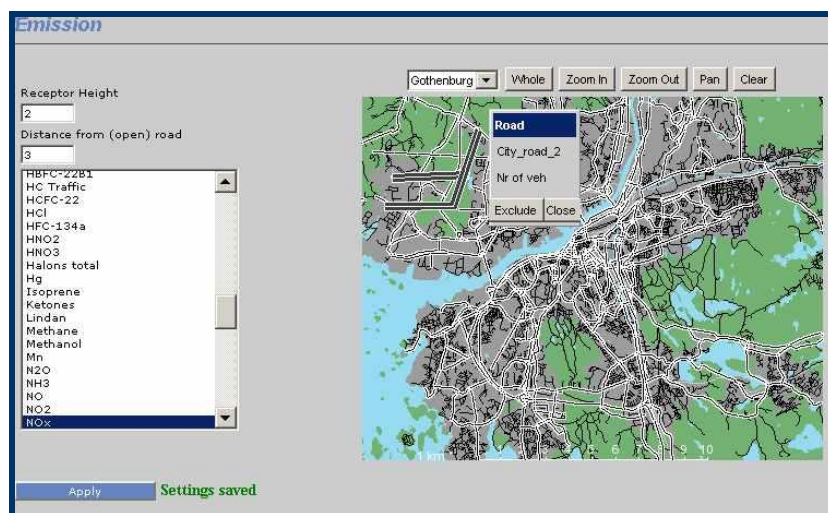
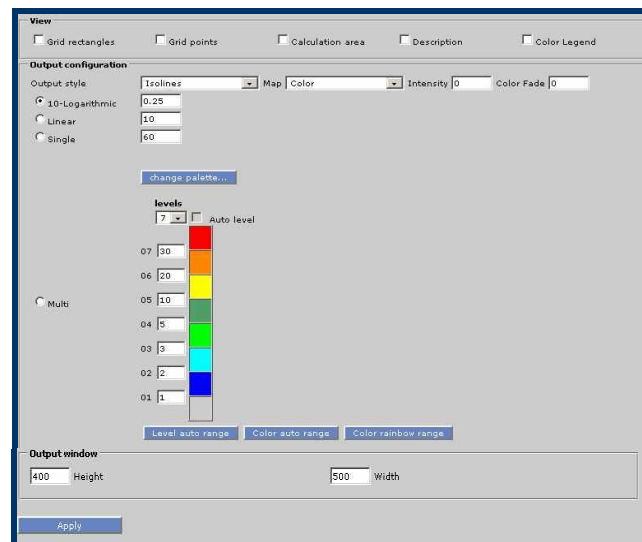


Figure 2.8.2. Emission. OS Model.

Now you are ready to submit the calculation. Now the user proceed in the same way as with the other Models. Click on **Calculate** and enter a proper description including date and times for the time period selected. Start the calculation.

**Output Settings** can be used when the output configuration format has been set to grid or isocolour, and shows the grid colours and levels used down the left hand side of the map. The colour palette can be changed, see *Figure 2.8.3*.



*Figure 2.8.3. Output Settings*

When you select the **Results** and click on **Viewer**, the Result View Controller automatically appears and you can use the arrows under **Time** to move through the calculations. If you **select Wind10m** then you will also be able to see how the wind field changes from hour to hour. Looking more carefully at the wind field, you will see how it is affected by both topography and ground type.



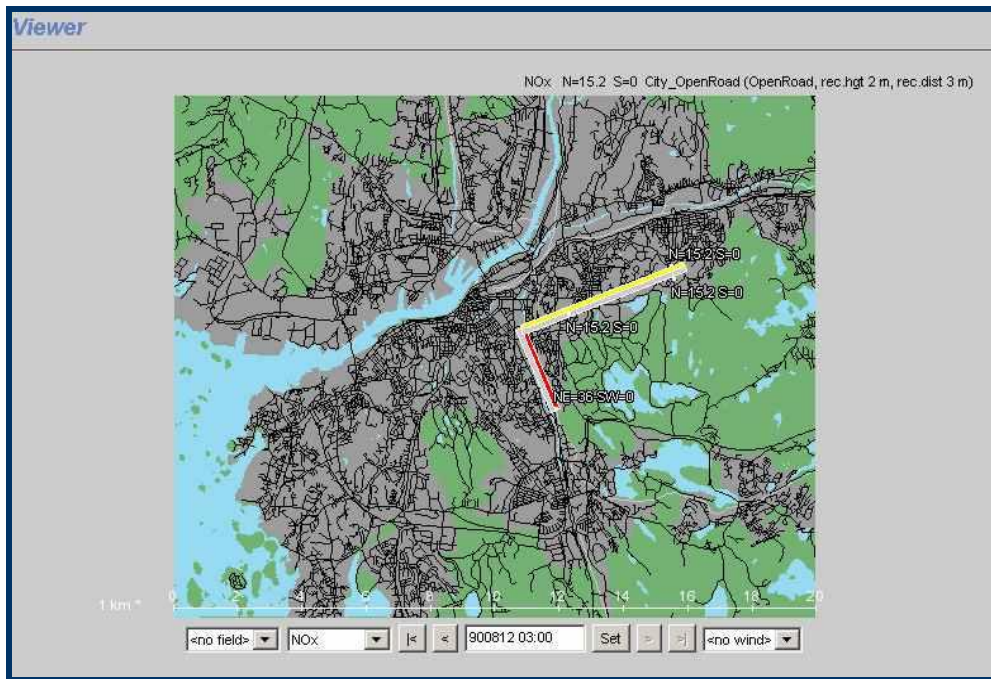


Figure 2.8.5. Viewer. Example Open Road

The examples result file will be presented as in *Figure 2.8.4.* y 2.8.5.. Note the pollution levels along the hours in the roads. The colour grid is configured in **Output Settings**.

The concentration in the road is shown as  $\mu\text{g}/\text{m}^3$ .

The Viewer window shows the description of the source and concentration by clicking on the result. Concentrations are given for both sides of the road, e.g. E means concentration on the east side of the road and W means the concentration on the west side.

## 2.9 MATCH Model

MATCH is the acronym for Multiscale Atmospheric Transport and Chemistry Model. MATCH models the basic processes of atmospheric transport, governing sources, sinks and transformation of atmospheric trace constituents in a three-dimensional framework. This is an Eulerian model that can be configured with an arbitrary number of layers in the vertical axis and for different geographical areas with different resolution. Depending on the application, specific modules describing physical or chemical transformation processes are added to the basic model. The model is driven by meteorological data taken from operational numerical weather prediction models such as HIRLAM or ECMWF, objective analyses such as MESAN or a combinations of them.

For this model all windows are similar to those already explained and showed for other models, except for Model Settings windows. All functionalities are the same as for other models, several the model settings.

First select **Match model (MA)** under **Model** on the frame. The definition of the weather conditions is different than for Gauss model. Now you can select your type settings. Other model specifications are given in the **Emission** subwindow. You will use the emission database of our dispersion calculations.

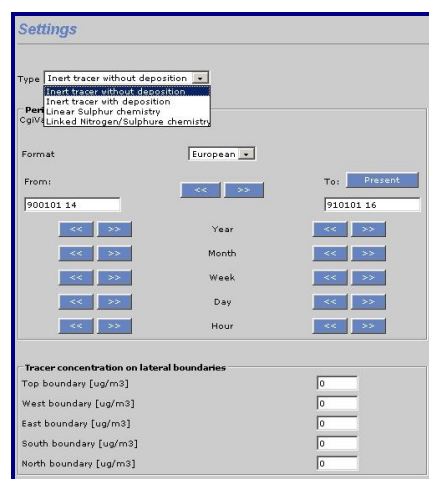


Figure 2.8.1. Settings

The type options available are:

- Inert tracer without deposition.  
The user must enter the following characteristics:
  - TRACER CONCENTRATION ON LATERAL BOUNDARIES  
Top boundary (ug/m3)

West boundary (ug/m3)  
East boundary (ug/m3)  
South boundary (ug/m3)  
North boundary (ug/m3)

- Inert tracer with deposition  
The user must enter the following characteristics:
  - DEPOSITION
    - Scavenging coefficient (h/(mm s))
    - Dry deposition velocity to water surfaces (cm/s)
    - Dry deposition velocity to urban areas (cm/s)
    - Dry deposition velocity to forests (cm/s)
    - Dry deposition velocity to low vegetation (cm/s)
    - Dry deposition velocity to bare soils (cm/s)
  - TRACER CONCENTRATION ON LATERAL BOUNDARIES
- Linear sulphur chemistry
  - 3-dimensional background values on lateral boundaries
- Linked nitrogen/sulphur chemistry
  - 3-dimensional background values on lateral boundaries

Now you can start the calculation. Do not forget to enter a precise description of the calculation in the **Start calculation** subwindow. Include information about which EDB sources are included and what weather conditions were specified

When the calculation is ready you will see that you have actually obtained several calculation results for both the mean conditions and also some of the percentile conditions. Select the **MEAN** result field.

This Advance Result options function allows you to perform some very useful operations with your dispersion result files created in the earlier examples. The function is activated in the **Advance settings** menu, and does not modify the stored result files in any way.

## Appendix 2A: The Wind Model - Calculation of the Wind Fields

### 2A.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 parameterised 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 breeze) information from more than one meteorological station is needed. The data from these stations will then pass through a mesoscale interpolation before entering the wind model.

#### 2A.1.1 Wind Model Equations

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

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

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

$$\frac{\partial p_s}{\partial t} = \frac{g}{R \Theta_s T_s} \cdot \int_0^H \frac{\partial \Theta}{\partial t} dz \quad (\text{eq 2A.1.3})$$

$V$  = 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)

### 2A.1.2 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 ( $\Theta_s$ ). Physiographical information (surface characteristics) is used for area interpolation of H, Q and  $\Theta_s$ . 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 *2A.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 (eq 2A.1.1) until two successive estimations of the average wind component do not differ by more than 2%.

### 2A.1.3 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  $\bar{T}$  is the average surface air temperature, g is gravity,  $\kappa$  is the von Kármán constant and  $\rho c_p$  is the specific heat capacity. In the Airviro dispersion models, the Monin-Obukhov length is extensively used as a discriminator of different meteorological regimes.

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 ( $\Delta q$ ) 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):

$$u_* = \frac{\kappa(U_{z_2} - U_{z_1})}{\ln\left(\frac{z_{u2} - \Psi_{m2} + \Psi_{m1}}{z_{u1}}\right)}$$

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

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 similarity functions  $\Psi_m$  and  $\Psi_H$  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

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

and

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

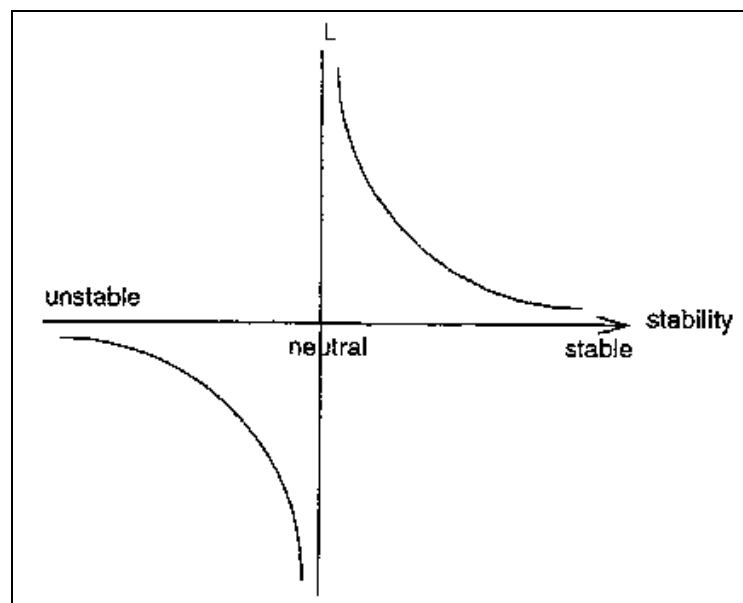


Figure 2A.1 The Monin-Obukhov length ( $L$ ) behaviour as a function of stability

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

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

Note that  $mixh$  varies with latitude.

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  $\sigma_y$  and  $\sigma_z$  that regulate lateral and vertical diffusion of the Gaussian plume. The measured quantities are the standard deviation of wind direction ( $\sigma_\alpha$ ) and vertical wind speed ( $\sigma_\omega$ ). 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  $\sigma_\alpha$  the standard deviation of the horizontal wind direction.

A similar expression is used for the vertical coefficient:

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

where  $\sigma_\omega$  is the standard deviation of the vertical wind speed.

*Figure 2A.2 Recommended values of  $T_i$  according to Draxler (1976). Sources higher than 30 m is 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.

## 2A.1.4 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  $a_k(n)$ , 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 in Airviro Specification Part II). For every grid point (i,j) a value is interpolated from all observation places:

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

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

$d_k(i,j)$  = 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\*, Zi and mixh

The Monin-Obukhov length (L), friction velocity ( $u_*$ ), temperature scale ( $T_*$ ), convective velocity scale ( $w_*$ ), boundary layer (Zi) 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 Zi. It is also possible for Zi 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 in Airviro Specification Part II.

The location of this effect is given in a grid, see appendix D3.3 in Airviro Specification Part II.

### 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 Zi 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.

### 2A.1.5 Procedures for Solving the Wind Model Equations

When the initial conditions have been estimated, the thermodynamic equation (eq 2A.1.2) is used to estimate the local change in potential temperature. The tendency equation (eq 2A.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 2A.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.

### 2A.1.6 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 ( $\Delta t$ ) depends upon the resolution of the grid ( $\Delta s$ ) 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.

### 2A.1.7 Reference Literature

Readers that are interested in further theories and experience with the Danard model are referred to: Danard (1977), Mass (1981), Mass (1984), Alpert and Getenio (1988). Numerical methods can be found in: Richtmeyer and Morton (1967), Messinger and Arakawa (1976).

## Appendix 2B:Results from Verification Studies

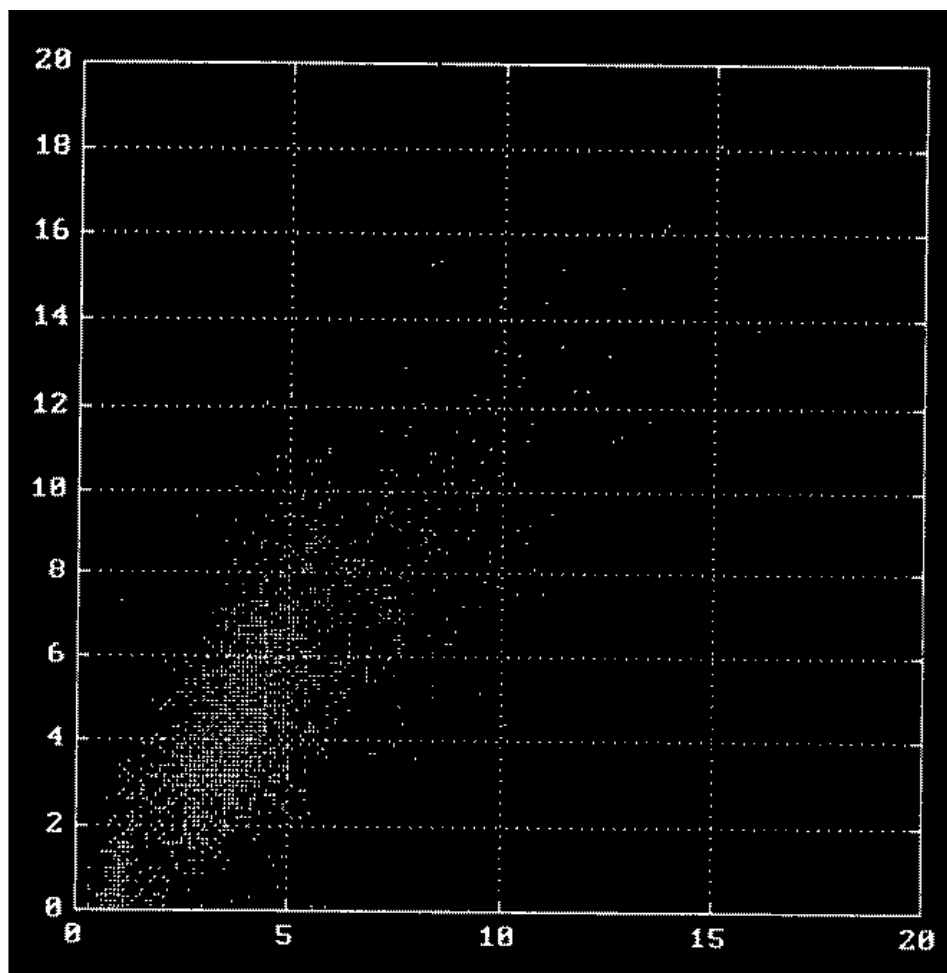
During the period 25 January to 25 March 1990 a wind experiment was performed in the Göteborg area. A total of 18 wind monitoring stations were located in the area. At these locations wind speed and direction were measured at approximately 10 m from ground level. Data was collected as 15 minute average winds once per hour during the period. In addition, at one location (Jarnbrott) a 130 m mast was equipped with wind and temperature sensors at 4 levels (2m,10m,60m and 130m). The size of the area was 20\*16 km and the locations of the stations can be seen in Figure 2B.1 (the Jarnbrott station is station no. 01).



Figure 2B.1

The area was digitised as a grid with a resolution of 500\*500m. Input data for the estimation of boundary scaling parameters, mixing height, large scale winds, etc. was taken from the profile measurements at Jarnbrott.

In Figure 2B.2 a scatter diagram is presented showing the measured winds compared to the modelled winds at all locations during the two-month period.



*Figure 2B.2*

In *Figure 2B.3* the very complex situation from March 3 at 05.00 is presented. The temperature and wind profiles taken from the mast at Jarnbrott are shown in *Figure 2B.3* below. A strong surface temperature inversion had developing during the night, and the upper wind at 130m (wind speed: 6 m/s) cannot penetrate through the inversion layer. The 10 metre winds are weak and are mainly driven by the fluxes from the ground, and the wind pattern in the area is extremely complex. This is a typical situation during winter time when severe pollutant episodes occur.

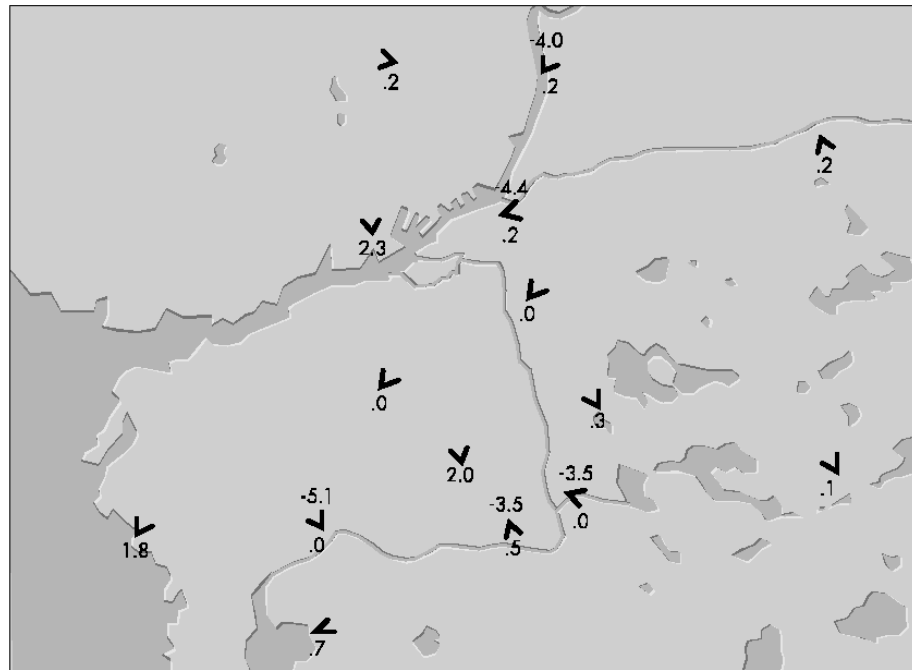


Figure 2B.3

In *Figure 2B.4* the model simulation is presented. Although, the resolution is low (500\*500m) it is clearly shown that the main part of the local wind pattern is described.

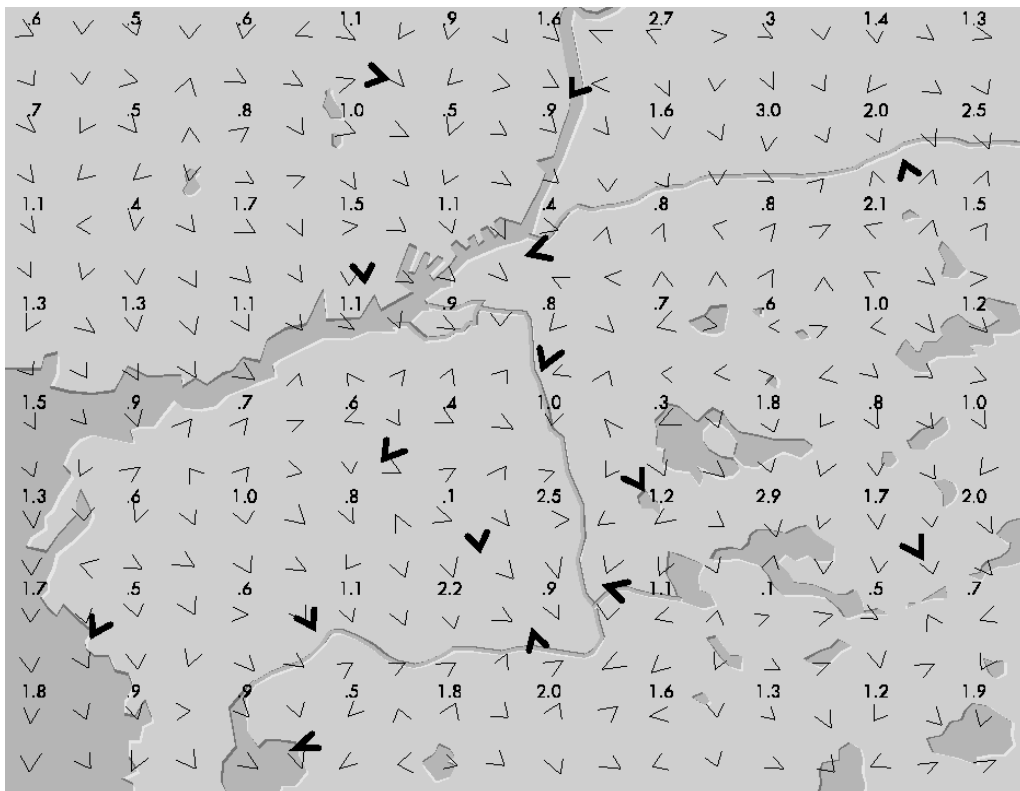


Figure 2B.4

## Appendix 2C: The Gauss Dispersion Model

### 2C.1 Introduction

This section describes the details of the dispersion calculation. The user can choose to use it during different weather conditions. The Reference database includes

- Winter season: A statistical sample of meteorological data between 1st October and 31st March is extracted from the time series database (see *Appendix 2G: Scenario Calculations*)
- Summer season: A statistical sample of meteorological data between 1st April and 31st September is extracted from the time series database (see *Appendix 2G: Scenario Calculations*)
- Case: A homogeneous wind field is used that is not based on any real data. Instead the user can enter the wind speed and direction to use as well as stability conditions
- Specific hour: The weather data for a specific date and time is fetched from the time series database

When using a scenario (season) or specific hour the wind field for the whole area is calculated for the whole map area when you start the dispersion calculation. For this reason you cannot view the wind field until the calculation is finished.

### 2C.2 When to Use the Gauss Plume 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 Gaussian 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 Gaussian 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 Gaussian dispersion 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 *Appendix 2A:*). 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 *Appendix 2E: 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 the Airviro system 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.

### 2C.2.1 Source Type Definitions

The source emission data may be described as coming from a point, a line or an area or from the EDB. From a model point of view, these are all treated as point emissions (except EDB sources): A line (normally 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 input data is obtained from the EDB, then the area, line 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 line source is assumed to be identical with traffic emissions from roads (at ground level).

### 2C.3 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.

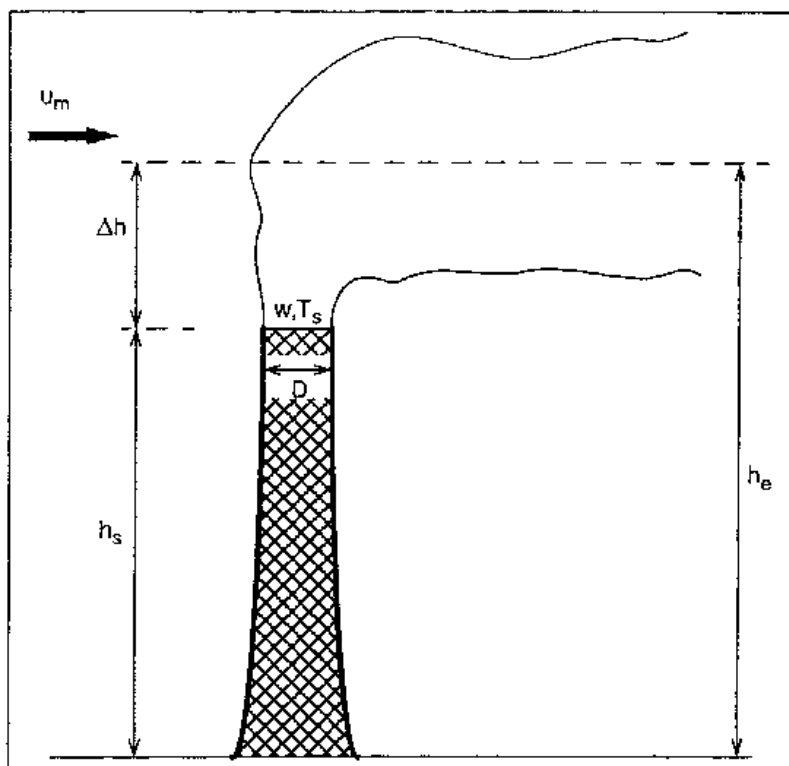


Figure 2C.1 Explanation of the different heights relevant for the plume rise calculation

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)<sup>2</sup>, which means that a factor  $\pi$  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  $\alpha$  and  $\beta$  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 might 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 ( $\Delta h$ ) 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  $\Delta h_d$  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  $h_e'$ , that is:

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

## 2C.4 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  $\Delta h_d$  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

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

(actually it is the crosswind width that is of importance, but we simplify this to a typical width). The relevant length scale ( $\xi$ ) 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:

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

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

$$h_s + \Delta h_d < H_b \Rightarrow h_e = h_s + \Delta h_d - 1.5\xi \quad ^{2(2)}$$

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

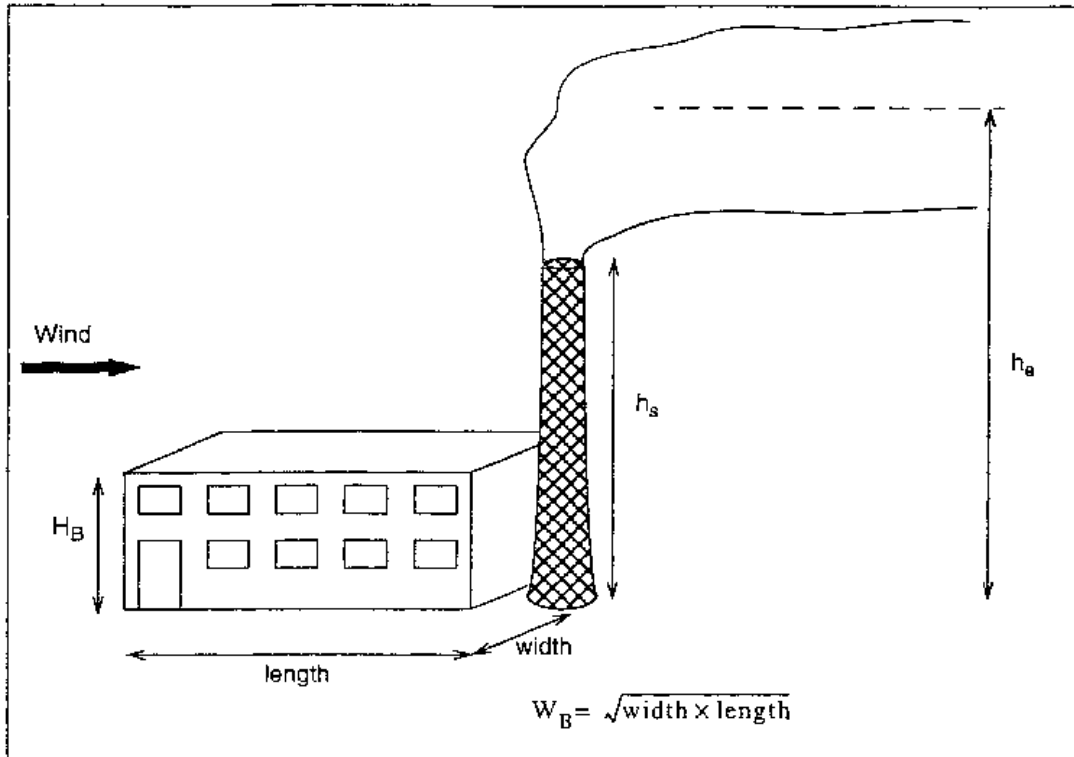


Figure 2C.2 Parameters of interest in the downwash calculation. Find  $\xi = \min(H_B, W_B)$ .

## 2C.5 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  $\sigma_y$  and  $\sigma_z$ :

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

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

1

2 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.

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

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

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

However, in built up areas where the Gauss model calculations are evaluated at roof level,  $\sigma_y$  is set to 0.667\*building height. The building heights are specified in a grid, see appendix D3.3 in Airviro Specification Part II.

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  $\Delta xy_{em}$ . The corresponding values of  $\sigma_y$  will be  $0.5 \times \Delta xy_{em}$  and  $0.5 \times \Delta xy_{em} \sigma_z$  is set to  $\max[(3.57 - 0.53U), (0.667*\text{building height})]$ .

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):

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

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.

## Appendix 2D: The Eulerian Advection-Diffusion Grid Model

### 2D.1 Introduction

The grid dispersion model built into the Airviro system 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 *Appendix 2A*). 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 *Appendix 2E: Street Canyon Model*).

### 2D.2 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

$\rho$  = 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.

### 2D.2.1 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 one big 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.

### Boundary Conditions

At the lateral boundaries constant inflow and gradient outflow conditions are applied (see Pielke (1984)). A Laplace 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.

### 2D.2.2 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,

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

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  $\sigma$  is transformed to a logarithmic-linear vertical co-ordinate.

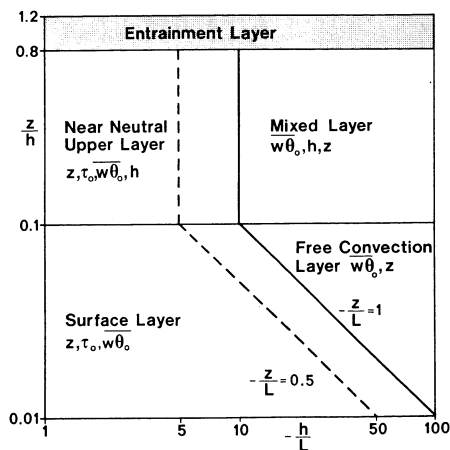
$$\zeta(\sigma) = a \left[ \frac{1}{\kappa} \ln \left( \left( \frac{\sigma + z_0}{z_0} \right) + \frac{\sigma}{b} \right) \right] + 1$$

where  $z_0$  is the surface roughness. For a certain choice of the coefficient  $a$ , the  $\zeta$ -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.

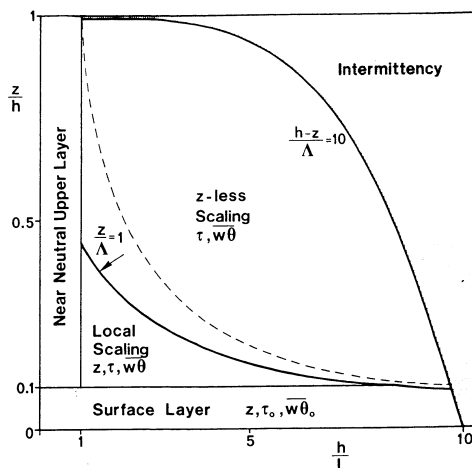
### 2D.2.3 The Turbulent Exchange Coefficient

The parameterisation of the vertical turbulent exchange coefficient,  $K_z$ , is prescribed according to the following classification:

A state of the art classification of the different scaling regions in the boundary layer, shown below for unstable and stable conditions, respectively, has been introduced.  $z$  is distance above ground,  $h$  is the height of the boundary layer and  $L$  is the Monin-Obukhov 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 absent.



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.

*Stability regimes under **unstable** conditions (from Holtslag, 1987)*

*Stability regimes under **stable** conditions (from Holtslag, 1987)*

Models for the formulation of the vertical turbulent exchange coefficient,  $K_z$ , were discussed in Yamartino et al (1992). The formulas for  $K_z$  in the different regimes indicated in the diagrams above are:

**Unstable case  $L < 0$ :**

Surface layer ( $z/h \leq 0.1; -z/L \leq 1.0$ ):

$$K_z(z) = \frac{u_* k z}{\Phi_h\left(\frac{z}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74\left(1 - 9\frac{z}{L}\right)^{-\frac{1}{2}}$$

Free convection layer ( $z/h \leq 0.1; -z/L > 1.0$ ):

$$K_z(z) = w_* z$$

Near neutral upper layer ( $z/h > 0.1; z/h \leq 1.0; -h/L > 1.0; -h/L \leq 10.0$ ):

$$K_z(z) = \frac{u_* k h}{\Phi_h\left(\frac{0.1h}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74\left(1 - 9\frac{z}{L}\right)^{-\frac{1}{2}}$$

Mixed layer ( $z/h > 0.1; z/h \leq 1.0; -h/L > 10.0$ ):

$$K_z(z) = 0.1 w_* h$$

Entrainment layer ( $z/h > 1.0; -h/L > 1.0; -h/L \leq 10.0$ )

$$K_z(z) = \frac{0.01 u_* k h}{\Phi_h\left(\frac{0.1h}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74\left(1 - 9\frac{z}{L}\right)^{-\frac{1}{2}}$$

Entrainment layer ( $z/h > 1.0; -h/L > 10.0$ )

$$K_z(z) = 0.01w_*h$$

**Stable case  $L \geq 0$ :**

Surface layer ( $z/h \leq 0.1$ ;  $h/L \geq 0.0$ ;  $(h-z)/\Lambda \leq 10.0$ ):

$$K_z(z) = \frac{u_*\kappa z}{\Phi_h\left(\frac{z}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74 + 4.7z/L$$

Near neutral upper layer ( $z/h > 0.1$ ;  $z/h \leq 1.0$ ;  $h/L > 0.0$ ;  $h/L \leq 1.0$ ):

$$K_z(z) = \frac{u_*\kappa h}{\Phi_h\left(\frac{0.1h}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74 + 4.7z/L$$

Local scaling layer ( $z/h > 0.1$ ;  $h/L > 1.0$ ;  $z/\Lambda \leq 1.0$ ;  $(h-z)/\Lambda \leq 10.0$ ):

$$K_z(z) = \frac{u_*\kappa z}{\Phi_h\left(\frac{z}{\Lambda}\right)} \quad \text{where } \Phi_h\left(\frac{z}{\Lambda}\right) = 0.74 + 4.7z/\Lambda$$

Z-less scaling layer ( $z/\Lambda > 0.1$ ;  $h/L > 0.0$ ;  $(h-z)/\Lambda \leq 10.0$ ):

$$K_z(z) = 0.4u_*\Lambda$$

Intermittency layer ( $(h-z)/\Lambda > 10.0$ ;  $z/h \geq 0.0$ ;  $h/L \leq 1.0$ ):

$$K_z(z) = \frac{0.1u_*\kappa h}{\Phi_h\left(\frac{0.1h}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74 + 4.7z/L$$

Layer above ( $h/L > 0.0$ ;  $h/L \leq 1.0$ ;  $z/h > 1.0$ ):

$$K_z(z) = \frac{0.1u_*\kappa h}{\Phi_h\left(\frac{0.1h}{L}\right)} \quad \text{where } \Phi_h\left(\frac{z}{L}\right) = 0.74 + 4.7z/L$$

where:

$u_*$  = friction velocity ( $= \sqrt{\tau_0/\rho}$ )

$u_{*1}$  = local friction velocity ( $= u_*(1-z/h)^{3/4}$ )

$w_*$  = convective velocity scale ( $= (gh\overline{w\theta_0}/T)^{1/3}$ )

$w_{*1}$  = local convective velocity scale ( $= (gh\overline{w\theta_0}(1-z/h)/T)^{1/3}$ )

$\overline{w\theta_0}$  = surface heat flux

T = air temperature

g = gravitational acceleration

$\rho$  = density of air

$c_p$  = specific heat of air at constant pressure

$\kappa$  = von Kármán's constant ( $= 0.4$ )



$z$  = height above the surface

$L$  = Monin-Obukov length scale ( $= -(u_*^3 / (\kappa \frac{g}{T} \overline{w\theta_0}))$  )

$\Lambda$  = local Monin-Obukov length scale ( $= -(u_*^3 / (\kappa \frac{g}{T} \overline{w\theta_0}(1 - z/h)))$  )

$h$  = height of the mixed layer

## 2D.2.4 The Three-Dimensional Wind Field

The construction of the surface (two-dimensional) wind field is described in section *Appendix 2A: The Wind Model - Calculation of the Wind Fields*. 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 an other 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  $\zeta$ -system:

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

where  $w^\zeta$  = vertical velocity in the  $\zeta$ -system.

## 2D.2.5 Source Initialisation

The Grid model only uses the EDB to obtain emission input data. Points 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 line 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 *2C.3 Plume Rise Formulation*.

## 2D.3 Particle Deposition

### 2D.3.1 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 Sehmel (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

$\nu$  = 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

### 2D.3.2 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 the surrounding is relatively fast and therefore in equilibrium.

The wet deposition is modelled as

$$-\lambda c$$

where  $\lambda$  is a washout coefficient defined as:

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

Both  $l$  and  $c$  are functions of the height,  $\lambda$  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:

$$\int_0^h \lambda(z)c(z)dz = \bar{\lambda} \bar{c} mixh = \bar{\lambda} c_0 mixh \Rightarrow \bar{\lambda} = \frac{W_r P}{mixh}$$

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).

### 2D.3.3 Particle Settling

Particles in a certain size range are affected by gravitational forces, without being big enough to be ballistic. 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 *2D.2 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.

## Appendix 2E: Street Canyon Model

Both the Gaussian 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 Gaussian 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.

### 2E.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):

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

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

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

L<sub>0</sub> 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 gridpoints, a summation of  $CL$  values takes place, implying a contribution from each emitting segment situated upwind the gridpoint itself (no impact from an emitting segment situated downwind).

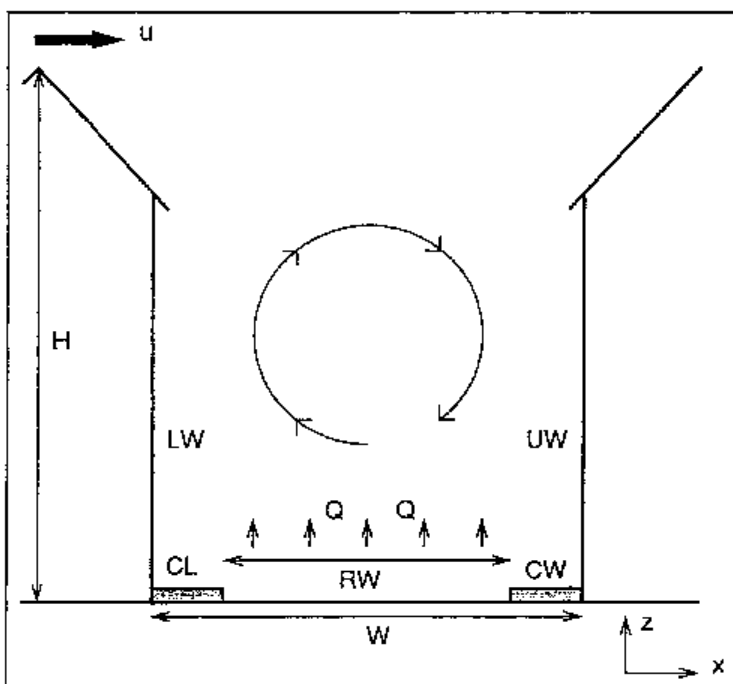


Figure 2E.1 Principles of air circulation within a street canyon (the upwind side is denoted  $UW$ , the leewind side  $LW$ , see also notations for house height ( $H$ ), street width between houses ( $W$ ) and road width ( $RW$ )).

## Appendix 2F: 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 that 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 is given below.

### 2F.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:

$$q_0 = A c_f G_0 \quad (\text{kg/s}) \quad (\text{eq 2F.1.1})$$

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

$$G(p) = \sqrt{\frac{p_0 - p}{v(p)}} \quad (\text{kg/s,m}^2) \quad (\text{eq 2F.1.2})$$

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:

$$M = q_0 u_0 + A(p - p_a) \quad (\text{N}) \quad (\text{eq 2F.1.3})$$

where  $u_0$  is the outlet velocity.

$$u_0 = \frac{q_0}{Av(p)} \quad (\text{m/s}) \quad (\text{eq 2F.1.4})$$

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

$$\text{- massflow } q(x) = C_1 \sqrt{M \rho_a x} \quad (\text{kg/s}) \quad (\text{eq 2F.1.5})$$

$$\text{- centre velocity } u_c(x) = C_2 \sqrt{\frac{M}{\rho_a}} \frac{1}{x} \quad (\text{m/s}) \quad (\text{eq 2F.1.6})$$

$C_1$  and  $C_2$  are coefficients and  $\rho_a$  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 2F.1.6 and 2F.1.5 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  $p_0$ :

$$\frac{p_a}{p_0} \leq \left( \frac{2}{\kappa + 1} \right)^{\frac{\kappa}{\kappa + 1}}; \kappa = \frac{c_p}{c_v} \quad (\text{eq 2F.1.7})$$

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:

$$\text{- velocity } u_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} p_0 v_0} \quad (\text{m/s}) \quad (\text{eq 2F.1.8})$$

$$\text{- mass flux } q_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} \left( \frac{2}{\kappa + 1} \right)^{\frac{2}{\kappa - 1}} \frac{p_0}{v_0}} \quad (\text{kg/s}) \quad (\text{eq 2F.1.9})$$

otherwise, if condition 2F.1.7 is not fulfilled,

$$\text{- velocity } u_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} \left[ 1 - \left( \frac{p_a}{p_0} \right)^{\frac{\kappa - 1}{\kappa}} \right]} \quad (\text{m/s}) \quad (\text{eq 2F.1.10})$$

$$\text{- mass flux } q_0 = \sqrt{2 \frac{\kappa}{\kappa - 1} \left[ \left( \frac{p_a}{p_0} \right)^{\frac{2}{\kappa}} - \left( \frac{p_a}{p_0} \right)^{\frac{\kappa+1}{\kappa}} \right]} \frac{p_0}{v_0} \quad (\text{kg/s}) \quad (\text{eq 2F.1.11})$$

Using the jet equations 2F.1.3 to 2F.1.6, with the initial values given by equations 2F.1.8 to 2F.1.11, 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:

$$u_g = C_3 \sqrt{gH \frac{\rho_p - \rho_a}{\rho_p}} \quad (\text{m/s}) \quad (\text{eq 2F.1.12})$$

$C_3$  is a coefficient, here equal to 1.0.  $g$  is the gravitational acceleration,  $H$  is the cloud height and  $\rho_p$  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 another place in this documentation, takes over and proceeds with the dispersion calculations (see appendix E3.2 in Airviro Specification Part II).

## 2F.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 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)):

$$A = C_4 V^{\frac{2}{3}} \quad (\text{m}^2) \quad (\text{eq 2F.2.13})$$

where  $V$  is the tank volume and  $C_4$  is a coefficient. The emission phase follows equations 2F.1.1 to 2F.1.6. 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)):

$$x = C_5 \left( \frac{u(x) T \tau}{\rho_a} \right)^{\frac{1}{4}} \quad (\text{m}) \quad (\text{eq 2F.2.14})$$

$C_5$  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:



$$Vol = C_6 \left( \frac{u(x)T\tau}{\rho_a} \right)^{\frac{3}{4}} \quad (\text{m}^3) \quad (\text{eq 2F.2.15})$$

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.

## 2F.3 Substances and Coefficients

Currently the following substances can be handled by the model:

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

### 2F.3.1 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.



## Appendix 2G: Scenario Calculations

### 2G.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).

### 2G.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  $6^\circ$ . 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.

## 2G.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 SO<sub>2</sub>.** Examine the last 5 years measurements of SO<sub>2</sub> 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 of the event.

## Appendix 2H: A Method to Locate Dominating Sources

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 center (i.e. 24 x 20 sources). All sources emit according to

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

where  $a_h$  is the emission amplitude as specified by a normalized 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  $\sigma_{yinit}$  and  $\sigma_{zinit}$  - depends on the horizontal dimensions of the calculation grid ( $dxy$ ):

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

The simulation uses the Gaussian plume model, using the mast data for the estimation of stability, mixing height and plume growth coefficients  $\sigma_y$  and  $\sigma_z$ . 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  $j=1, \dots, m$  hourly values, and the measured concentrations are given at  $k=1, \dots, l$  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  $j=1, \dots, m$  hours and  $k=1, \dots, l$  stations.

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

The interpretation of the result should concentrate on the isoline pattern that is the distribution of maximum and minimum, and not in absolute values. This is because one dominating source will yield a higher correlation coefficient compared to the case of various and geographically dispersed sources, even if each of the latter sources is as strong a contaminator as the first, single source.

## Appendix 2I: A Method to Estimate Emissions from Dominating Sources

The method assumes the same kind of data as for the location 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 various monitor stations (point or open path measurements). It is preferable to have more than one time series for concentration values.

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 and this is explained in section *2.I.1 Monitor Option for a Time Varying Background Concentration*.

As a starting point, each specified area source will be divided into 9 sub areas and the emission represented by 9-point sources. The initial diffusion is as described in *Appendix 2H: A Method to Locate Dominating Sources* (where  $dx_y$  is now the dimensions of the 9 sub areas). All sources are assumed to emit with a normalized, default emission rate, as an average over the specified period. During the period, each area source may have a unique variation specified by a normalized 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 *Appendix 2H: A Method to Locate Dominating Sources*.

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 normalized 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 predicted). The regression method - stepwise regression with a forward selection principle - is described in *Exploiting the Regression Models in User's Reference Volume 3: Working with Indico Presentation*.

The multiple regression analysis will optimize 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  $\varepsilon$  is the (minimized) estimation error. The stepwise regression uses two criteria,  $F_{in}$  and  $F_{out}$ , that regulate the risk (in percent) that you are willing to take in the inclusion or exclusion of an individual source  $i$ . The user can specify the values to use in the emission estimation but something similar to  $F_{in}=0.05$ ,  $F_{out}=0.10$  is recommended.

If the impact of the sources to be estimated gives a clear signal in the measured concentration data, the method will yield a coefficient  $b_i$  that scales the normalized simulation time series. If, as an example, the normalized emission is set to 1 g/s, the  $b_i$  value will express the estimated emission for source  $i$  directly in g/s.

The multiple correlation coefficient is the overall measure of how good your source assumptions are. You should always try to maximize it, either by running individual or combined source estimates. Typical tests are:

- changing area sizes (e.g. half, double)
- changing plume heights
- changing emission variations (EDB formulas)

For a given number of sources, the source specific standard error (the standard deviation of the estimated error in the emission estimation for a particular source) is the measure of how good a source estimate is. Assuming the estimate error to be normally distributed, it gives the interval of 67% confidence level (twice times the estimate error gives 95% confidence level).

The part of the monitored pollution data that is not explained by the impact of the specified sources will fall into the (constant) background value.

## 2.1.1 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.



## Appendix 2J: The OSPM Model

- Description

### OSPM is a practical street pollution model

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

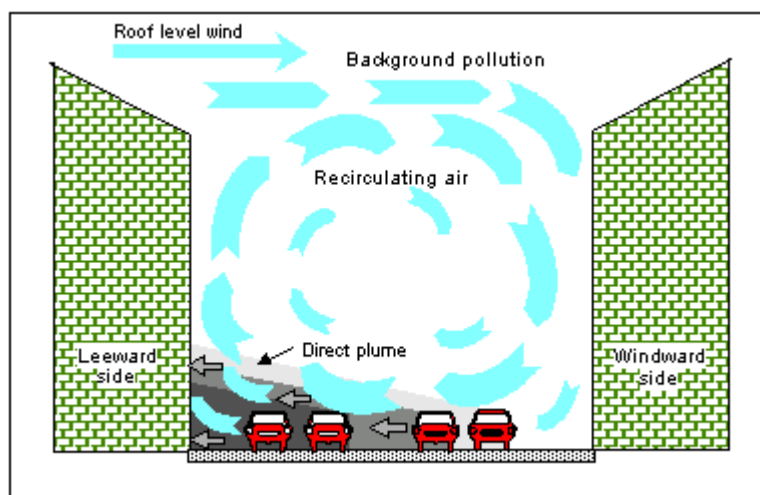


Figure 2J.1. Description

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.

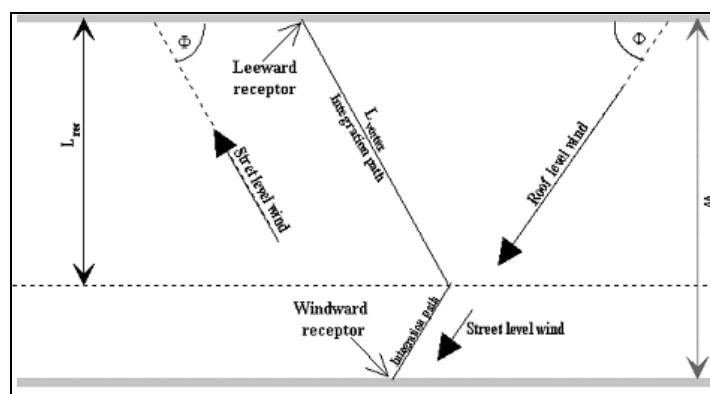
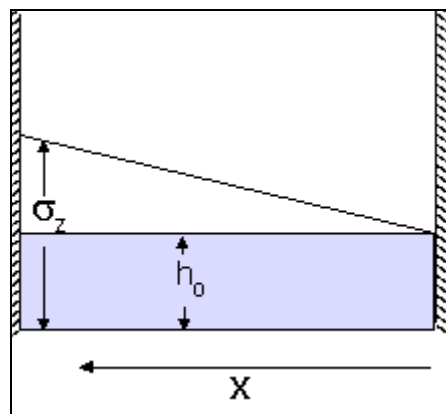


Figure 2J.1. OSPM

- 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.



**Vertical dispersion:**

$$\sigma_z(x) = \sigma_w \frac{x}{u_b} + h_0$$

**The direct contribution:**

$$C_d = \sqrt{\frac{2}{\pi}} \frac{Q}{W \sigma_w} \exp\left[-\frac{h_0 + (\sigma_w / u_b) W}{h_0}\right]$$

**Initial dispersion:**

$$h_0 = 2 \sim 4 \text{ m (depends on wind speed)}$$

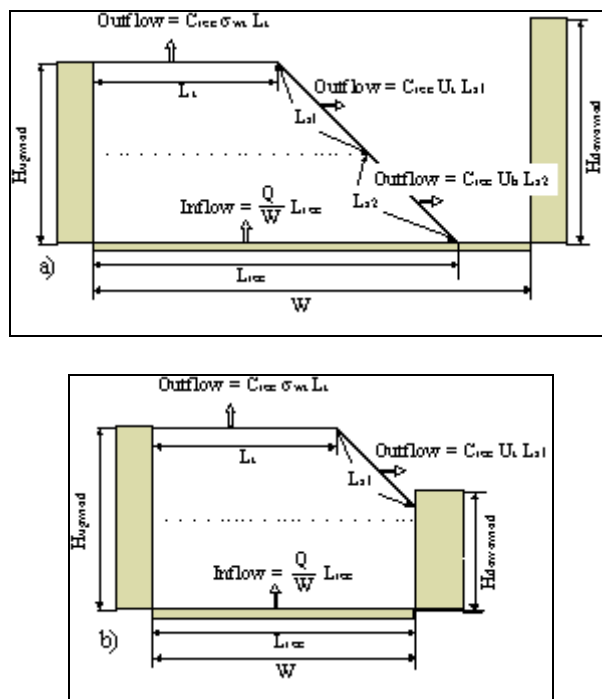


Figure 2J.3. Recirculation

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.

## NO<sub>2</sub> chemistry

The NO<sub>2</sub> concentrations are calculated taking into account NO-NO<sub>2</sub>-O<sub>3</sub> chemistry and the residence time of pollutants in the street.

The presence of NO<sub>2</sub> in ambient air is mainly due to the chemical oxidation of the emitted NO by background ozone. Under sunlight conditions, photo dissociation of NO<sub>2</sub> leads to partial reproduction of NO and O<sub>3</sub>.

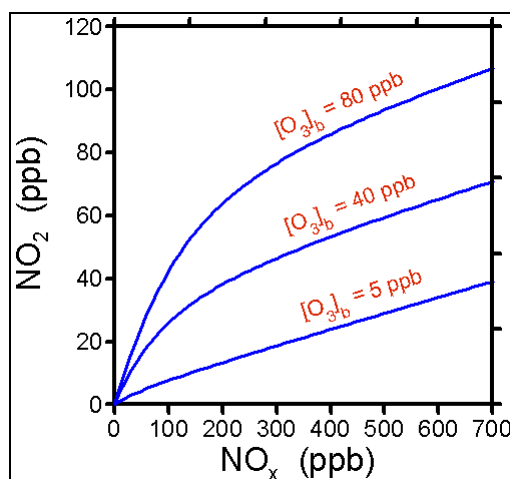
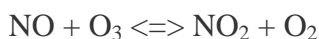


Figure 2J.4. Relation NO<sub>2</sub>-NO<sub>x</sub>

The relationship between NO<sub>2</sub> and NO<sub>x</sub> 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 NO<sub>2</sub> formation.

- **Model structure**

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

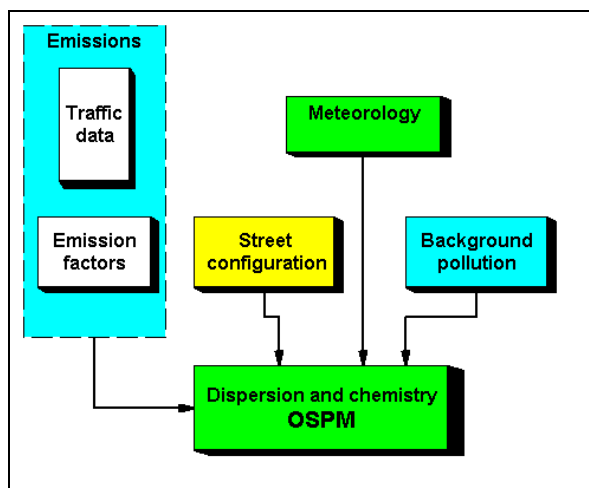


Figure 2J.5. Model structure

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-NO<sub>2</sub>-O<sub>3</sub>. 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.

## Appendix 2K : References

### **Alpert, P., Getenio, B. (1988)**

One-Level Diagnostic Modelling of Mesoscale Surface Winds in Complex Terrain. Part I: Comparison with Three-Dimensional Modelling in Israel.  
*American Meteorological Society*, 116, 2025-2046.

### **Bahe, F.C., Schurath, U. and Becker, K.H. (1980)**

The frequency of NO<sub>2</sub> photolysis at ground level, as recorded by a continuous actinometer.  
*Atmospheric Environment*, 14, 711-718

### **Berkowicz, R. and Prahm, L. P. (1982)**

Evaluation of the Profile Method for Estimation of Surface Fluxes of Momentum and Heat  
*Atmos. Environ.* 16, 2809-2819

### **Briggs, G. A. (1973)**

Diffusion Estimation for Small Emissions  
*ATDL Contribution File No. 79, Atmospheric Turbulence and Diffusion Laboratory*

### **Businger, J. A., Wyngaard, J. C., Izumi, Y. and Bradley, E. F. (1971)**

Flux profile Relationships in the Atmospheric Surface Layer.  
*J. Atmos. Sci.*, 28, 181-189

### **Cats, G. J. (?)**

A Simple Method for Quick Estimates of Frequency Distributions of Air Pollution Concentrations from Long-Term Average Concentrations  
*Proceedings....*

### **Chock, D.P. and Dunker, A.M. (1983)**

A comparison of numerical methods for solving the advection equation.  
*Atmospheric Environment, Vol., 17, No.1, 11-22.*

### **Danard, M. (1977)**

A Simple Model for Mesoscale Effects of Topography on Surface Winds.  
*Monthly Weather Review.*,99,831-839

### **Draxler, R. (1976)**

Determination of Atmospheric Diffusion Parameters.  
*Atmospheric Environment*, 10, 95-105

### **Dyer, A. J. (1974)**

A Review of Flux-Profile Relationships.  
*Boundary Layer Meteorology.*, 7., 363-372

**Eliassen, A. and Saltbones, J. (1983)**

Modelling of the long range transport of sulphur over Europe: A two-year model run and some modelling experiments.

*Atmospheric Environment*, 17, 1457-1473

**Hanna, S. R., Briggs, G. A. and Hosker Jr, R. P. (1982)**

Handbook on Atmospheric Diffusion

*Technical Information Center, U. S. Department of Energy*

**Hanna, S.R. and Drivas, P.J. (1987):**

Guidelines for use of Vapor Cloud Dispersion Models,

*American Institute of Chemical Engineers, ISBN 0-8169-0403--0*

**Hildemann, L.M., Russel, A.G. and Cass, G.R. (1984)**

Ammonia and nitric acid concentrations in equilibrium with atmospheric aerosols: Experiment vs theory.

*Atmospheric Environment*, 17, 1737-1750

**Holtslag A. A. M. (1984)**

Estimates of Diabatic wind Speed Profiles from Near Surface Weather Observations.

*Boundary Layer Meteorology* 29, 225-250.

**Iversen, T., Saltbones, J., Sandnes, H., Eliessen, A. and Hov, O. (1989)**

Airborne transboundary transport of sulphur and nitrogen over Europe - model description and calculations.

*EMEP MSC\_W report 2/89*

**Laurin, S. And Omstedt, G. (1987)**

En modell för beräkning av bilavgaser i gatumiljö.

*Swedish Meteorological and Hydrological Institute (SMHI)*

**Long, P.E.Jr. and Pepper, D.W. (1976)**

A comparison of six numerical schemes for calculating the advection of atmospheric pollution.

*Am. Meteor. Soc. Symp. Atmos. Turbul. Diffus. Air Qual. Prepr. 3rd, 181-187.*

**Lyons, T. J. and Scott, W. D. (1990)**

Principles of Air Pollution Meteorology

*Belhaven Press, London*

**Marchuk, G.I. (1975)**

Methods of Numerical Mathematics.

*Springer, New York.*

**Mass, C. (1981)**

A Single-Level Numerical Model Suitable for Complex Terrain.

*Proceedings of the Fifth Conference on Numerical Weather Prediction, American Meteorological Society, Boston, MA 02108, 316-319.*

**Mass, F. (1984)**

Simple Mesoscale Models for Operational Use in Regions of Topographic and Thermal Forcing: Development and Evaluation.  
*Contractor report CR 84-05, Naval Environmental Predictions Research Facility, Monterey, CA 93943*

**McMahon, T. A. and Denison, P.J. (1979):**

Empirical Atmospheric Deposition Parameters-A survey,  
*Atmospheric Environment, 13: 571-585.*

**McRae, G.J., Goodin, W.R. and Seinfeld, J.H. (1982)**

Numerical solution of the atmospheric diffusion equation for chemically reacting flows.  
*Journal of Computational Physics, 45., 1-42*

**Messinger, F., and A. Arakawa. (1976)**

Numerical Methods Used in Atmospheric Models.  
*Vol I. GARP Publications Series No. 17.*

**Nielsen, S. P., Gryning, S. E., Karlberg, O., Lyck, E. and Thykier-Nielsen, S. (1986)**

A Field Experiment to Validate Atmospheric Dispersion and Dose Models.  
*Risø National Laboratory, DK-4000 Roskilde, Denmark*

**Omstedt, G. (1984)**

An Operational Air Pollution Model using Routine Meteorological Data.  
*SMHI Report RMK 39, Norrköping, Sweden.*

**Panofsky, H. A. and Dutton, J. A. (1984)**

Atmospheric Turbulence.  
*John Wiley & Sons, Inc.*

**Paulson, C. A. (1970)**

The Mathematical Representation of Wind Speed and Temperature Profiles in the Unstable Atmospheric Surface Layer.  
*J. Appl. Meteorol., 9, 857-861.*

**Pielke, R.A. (1984)**

Mesoscale meteorological Modelling.  
*Academic Press, ISBN 0 12 554820 6.*

**Richtmeyer, D. R., Morton, K. W. (1967)**

Difference Methods for Initial-Value Problems.  
*Interscience, 405 p.*



**Russel, A., McRae, G. J. and Cass, G. C. (1983)**

Mathematical modelling of the formation and transport of ammonium nitrate aerosol.  
*Atmospheric Environment*, 17, 949-964

**Sehmel, G.A. (1980):**

Particle and Gas Dry Deposition - A review,  
*Atmospheric Environment*, 14:983-1012.

**Sherman, C. A. (1978)**

A Mass-Consistent Model for Wind Fields over Complex Terrain.  
*J. Appl. Meteor.*, 17, 312-319.

**SNV**

Bilavgaser i Gatumiljö - Modell och Modell Test  
*SNV PM 891, Bilagor 1977*

**Stelson, A. W. and Senfeld, J. H. (1982)**

Relative humidity and temperature dependence of the ammonium nitrate dissociation constant.  
*Atmospheric Environment*, 16, 983-992

**van Stijn, Th.L., van Eijkeren, J.C.H. and Praagman, N. (1987)**

A comparison of numerical methods for air quality models.  
*Scientific Reports/ KNMI WR 876, ISSN 0169 1651.*

**Winter, S., Nyrén, K. and Karlsson, E. (1984):**

Uppkomst och utbredning av explosiva eller giftiga gasmoln,  
*FOA rapport E 40011.*

**Yamartino, R.J., Scire, J.S., Carmichael, G.R., Chang, Y.S. (1992):**

The CALGRID Mesoscale Photochemical Grid Model – I. Model Formulation  
*Atmospheric Environment*, Vol 26A, No 8, pp. 1493-1512.

**Yanenko, N.N. (1971)**

The Method of Fractional Steps.  
*Springer, New York.*

**Zilitinkevich, S. S. (1972)**

On the Determination of the Height of the Ekman Boundary Layer.  
*Boundary Layer Meteorol.*, 3, 141-145