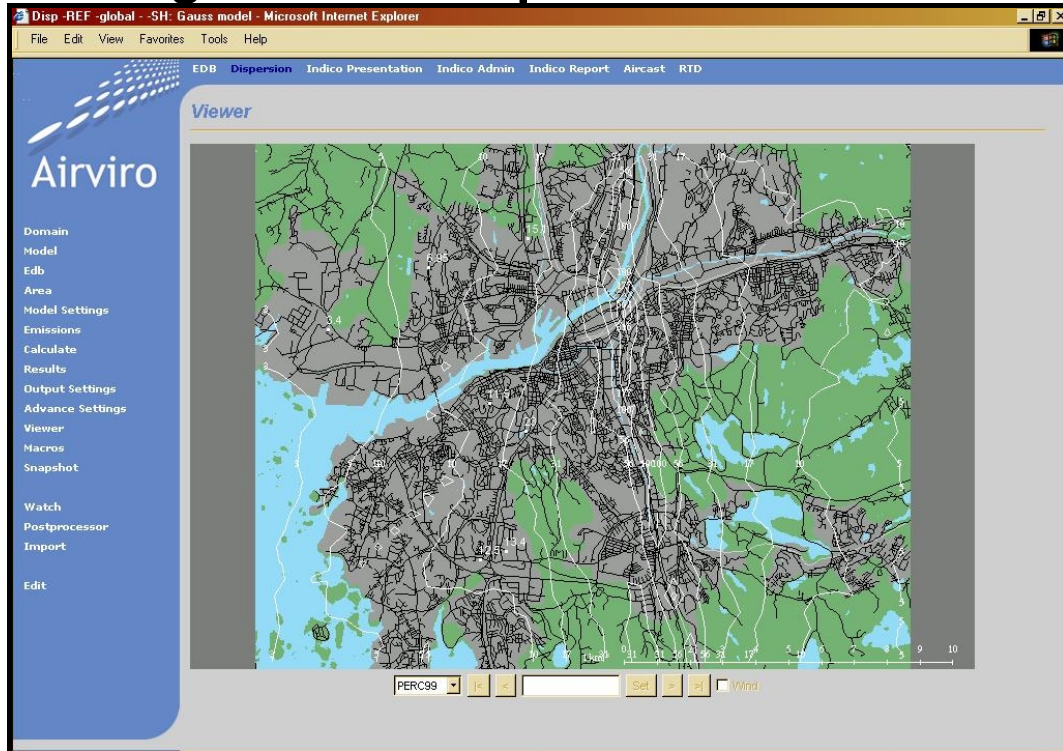


## Working with the Dispersion Module Client



**How to simulate the dispersion of pollutants**



# Contents

<b>4.1 Introduction .....</b>	<b>6</b>
4.1.1 Why You Need to Use Dispersion Models.....	6
4.1.1.1 What's the Use of Dispersion Simulations.....	6
4.1.1.2 How Can Airviro Help?.....	6
4.1.1.3 Model Assumptions .....	6
4.1.2 How does the Dispersion Module client work? .....	7
4.1.3 Overview of the Dispersion Module Main Window .....	8
4.1.3.1 Changing Weather Conditions .....	8
4.1.3.2 Specifying Source Types.....	9
4.1.3.3 Submitting a Dispersion for Calculation .....	9
4.1.3.4 Viewing Existing Dispersion Calculations .....	10
4.1.3.5 Finding Local Values .....	10
4.1.3.6 Using Receptor Points.....	10
4.1.3.7 Map Functions .....	10
4.1.3.8 Sub-menus on the left-hand side in the Dispersion main windows.....	10
4.1.4 Getting Started.....	13
<b>4.2 The Gauss Model.....</b>	<b>14</b>
4.2.1 Examples Based on the Case Weather Condition.....	14
4.2.1.1 Ordering a Calculation.....	15
4.2.2 Examples Based on Emission for a Specific Hour.....	18
4.2.3 Using Scenario Weather Conditions.....	20
4.2.4 Using the Advanced Result Options .....	23
4.2.4.1 Adding a Background Value.....	23
4.2.4.2 Conversion of NO <sub>x</sub> to NO <sub>2</sub> .....	23
4.2.4.3 Adding Various Result Files Together.....	24
4.2.4.4 Smoothing of Concentration Isolines .....	24
<b>4.3 The Street Canyon Model .....</b>	<b>25</b>
4.3.1 Street Canyon Overview.....	25
<b>4.4 The Grid Model .....</b>	<b>28</b>
4.4.1 Looking at Dispersions for a Specific Time Period .....	28
4.4.2 Looking at Dispersions for a Season .....	30
<b>4.5 The Heavy Gas Model .....</b>	<b>32</b>
4.5.1 Simulation of a Continuous Liquid Leak .....	32
4.5.2 Simulation of a Tank Burst.....	34
<b>4.6 Introduction to the Post processor.....</b>	<b>36</b>
4.6.1 Overview of the Postprocessor Main Window .....	36
4.6.2 Specifying Model Results .....	37
4.6.3 Spatial evaluation .....	37
4.6.3.1 Specifying object and method .....	37
4.6.3.2 Viewing the result .....	39

4.6.4 Time series export .....	40
4.6.4.2 Specifying object and location.....	41
4.6.4.3 Viewing the result .....	41
4.6.4 Model adjustment .....	42
4.6.4.1 Specifying object and reference.....	42
4.6.5 Split model result .....	44
4.6.6 Merge model results .....	44
4.6.7 Combined .....	45
<b>Appendix 4A:The Wind Model - Calculation of the Wind Fields.....</b>	<b>47</b>
4A.1 Principles of Wind Field Calculations .....	47
4A.1.1 Wind Model Equations .....	47
4A.1.2 Initialisation .....	48
4A.1.3 Stability and Turbulence Estimation - Preprocessing of Meteorological Data.....	48
4A.1.4 Mesoscale Interpolation .....	51
4A.1.5 Procedures for Solving the Wind Model Equations .....	52
4A.1.6 Numerical Methods .....	52
4A.1.7 Reference Literature .....	53
<b>Appendix 4B:Results from Verification Studies .....</b>	<b>54</b>
<b>Appendix 4C: The Gauss Dispersion Model .....</b>	<b>58</b>
4C.1 Introduction .....	58
4C.2 When to Use the Gauss Plume Model.....	58
4C.2.1 Source Type Definitions.....	59
4C.3 Plume Rise Formulation.....	59
4C.4 Building Downwash.....	62
4C.5 The Gaussian Plume Model.....	63
<b>Appendix 4D:The Eulerian Advection-Diffusion Grid Model .....</b>	<b>65</b>
4D.1 Introduction .....	65
4D.2 Formulation of the Grid Model.....	65
4D.2.1 Numerical Methods.....	66
4D.2.2 The Numerical Grid, Coordinate Transformations.....	67
4D.2.3 The Turbulent Exchange Coefficient .....	67
4D.2.4 The Three-Dimensional Wind Field .....	70
4D.2.5 Source Initialisation.....	70
4D.3 Particle Deposition .....	71
4D.3.1 Dry Deposition of Gases and Non-Gravitating Particles .....	71
4D.3.2 Wet Deposition .....	72
4D.3.3 Particle Settling.....	72
<b>Appendix 4E:Street Canyon Model.....</b>	<b>73</b>
4E.1 Model Description.....	73
<b>Appendix 4F:The Heavy Gas Model.....</b>	<b>75</b>
4F.1 Continuous Release or a Leakage From a "Small" Hole .....	75
4F.2 Instantaneous Release or a Tank Rupture - Emission Only from the Liquid Phase.....	77
4F.3 Substances and Coefficients .....	78

4F.3.1 Comments.....	78
<b>Appendix 4G:Scenario Calculations.....</b>	<b>79</b>
4G.1 General Principles.....	79
4G.2 A Standard Method to Generate a Statistical Sample: klmstat .....	79
4G.3 General Applications Using the Scenario Feature .....	80
<b>Appendix 4H:References .....</b>	<b>81</b>

## 4.1 Introduction

### 4.1.1 Why You Need to Use Dispersion Models

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

Measured data provides a strong argument: This is the situation at a specific place, and the results are easily understood by non-experts 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.

#### 4.1.1.2 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 informed 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 client 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 client 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 advantage of an integrated system is illustrated by the Airviro Receptor model, where measured and simulated values are statistically evaluated over a given period. Simulation models are of great value in the interpretation of measured data.

#### 4.1.1.3 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, for simulations in a complicated topography, or simulation of events where pollutants accumulate over a period of time, the advection/diffusion grid model should be used instead of the Gauss model. The grid model also permits a straightforward 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.

**Guidance for the beginner:** The dispersion chapter consists of two major parts:

- An introduction - section 4.1-4.4 - on how to operate the menus and sub-windows in the different dispersion modules, and how to run some simple examples
- A reference part collected in the appendices where 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 sub-windows in the Dispersion module client. You will find that the sub-windows 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).

### 4.1.2 How does the Dispersion Module client work?

The Dispersion Module is a JAVA-based user interface to the database and shell programs at the Airviro server. Dispersion Module client can be executed from a PC or other device running Internet Explorer 6 or Netscape Navigator 7 (or higher).

After logging in, an Dispersion user can process data from a database on the server, according to settings in Dispersion. All processing of data is done at the Airviro server. Results are transferred over a TCP/IP connection for presentation in Dispersion Client.

Output is generated to an SVGA-capable display as; a HTML-picture - including some interactive elements; a pdf-file or as plain ASCII text. Printing is generated by the web browser or with third-party software, e.g. Adobe® Reader 6. A searchable help system is provided in the form of a pdf-file.

Please be aware that the Dispersion client requires no installation at the PC side only that Internet Explorer 6 or Netscape Navigator 7 is installed. Anybody who knows the Airviro web URL may reach the database. It is therefore important to change passwords regularly and to set privilege levels for the users with great concern to limit not authorized access. Using an Intranet solution behind a firewall prevents general access from the world wide web, if properly set up. This is strongly recommended.

### 4.1.3 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:

Links

- to select the domain and a model
- to the type source and the emission
- to select hypothetical or observed weather conditions.
- to post process the results.
- to save macros with the results.

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

#### 4.1.3.1 Changing Weather Conditions

The weather plays a crucial role in dispersion calculations, and you can select weather conditions by clicking on **Model Settings**. You can choose between weather conditions in the



**Type** sub-window by using the drop-down menu. Different weather options are available, depending on the model that has been chosen.

#### 4.1.3.2 Specifying Source Types

Under **Emission** is an option menu with choices: Street, EDB, Tank data. Different options are activated depending upon the model used. If you have built an EDB then you can use combinations of EDB sources specified in the same way as emission searches in the EDB. For some models and weather conditions you are able to make one-off definitions of point, area and road sources. You cannot combine these, but within each source type you can define more than one source, e.g. you can define three different roads and calculate their joint dispersion pattern. (4.2.4 *Using the Advanced Result Options* explains how to calculate the total impact of different sources by summing up after the actual simulations have taken place.)

The **Apply** button under **Emission** saves the settings of the source specifications you have entered.

#### 4.1.3.3 Submitting a Dispersion for Calculation

When you have defined the source emissions, choose **Model Settings**, this takes you to a sub-window where you can specify the calculation height and give a name to your dispersion calculation before starting the calculation.

Once you have defined the source emissions choose **Calculate**. It is important to give a meaningful name to each dispersion calculation that you carry out, otherwise you will have trouble finding them again in the future.

After you have started a calculation, an information window automatically appears once it has finished.

#### 4.1.3.4 Viewing Existing Dispersion Calculations

**Results** allows 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 have permissions to do so).

#### 4.1.3.5 Finding Local Values

Use right 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.

#### 4.1.3.6 Using Receptor Points

**Receptors** can be activated, under **Snapshot**, to evaluate simulated concentration levels at different locations of particular interest, such as monitoring stations (including open path stations). Simulated concentration levels are shown at the receptor point locations on the map display, and are also saved in a file (receptor.pts) in the users home directory. The receptor points must have been previously defined in a specific file on **Edit, Receptors**. All point definitions start with #POINT, all line definitions start with #LINE and all station references start with #STN. A typical receptor point file could be as follows:

```
#POINT 1264626 6401932
#LINE 1274068 6396857 1274757 6397139
#STN GO1
#STN GO2
#STN GM5
```

This file contains the x and y coordinates for one point definition, the x and y start coordinates and the x and y stop coordinates for one line 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.

If the environment variable is not set, then Airviro will look for receptor point definitions in the file recpts.def .

#### 4.1.3.7 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 sub-area (this operation can be repeated), **Clear** the map of isolines and un-zoom 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.

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

More menus are found for each link.

<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.
<b>Calculate</b>	Here you can calculate the simulation.
<b>Results</b>	Here you can select the different results.
<b>Output Settings</b>	They are all toggle options, that is they only have two states (activated or inactivated).

**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, and shows the grid colours and levels used down the left hand side of the map.

**Field output configuration**

Here you have some control over what the output looks like. You can adjust the isoline frequency or choose to instead display the output as a coloured grid.

**Advance Settings**

A result is produced by each performed calculation, and is a matrix containing concentration values for each grid square. The New result option can be used in order to combine several results into a new result matrix, or to create a new matrix based on a transformation of an existing one.

**View** Here you can view you simulation 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.

	<b>Save</b>	In order to save your settings for a Dispersion macro, choose <b>Save macro</b> to define a dsp-file for the actual model type, project and user.
	<b>Delete</b>	Here you may delete saved Dispersion macros for the actual model type and project.
<b>Snapshot</b>		If you select <b>Snapshot</b> then whatever is currently displayed on the map will be copied to another window (select <b>PDF</b> or <b>GIF</b> ). 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 will be the same size as the original picture, and after it has been created it cannot be resized. With <b>Excel</b> and <b>Receptors</b> you have the concentration value at specific point on the map. <i>See 4.1.3.6. Using receptor point.</i>
<b>Watch</b>		This brings up a sub-window showing the progress of dispersion calculations.
<b>Postprocessor</b>		It is possible to make a statistical study with result dispersion
<b>Import</b>		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 <b>Extern</b> in the <b>Results</b> sub-window.
<b>Edit</b>	<b>Project</b>	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.
	<b>Receptor</b>	Here you can edit receptors.

### 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 impacts 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 the 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.

**4.1.4 Getting Started**

The best way to get acquainted with using the Dispersion module is to carry 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 sub-windows, 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 Client. Before you start trying to repeat the examples yourself you have to choose the reference database. Select **Ref** under the **Domain** on the frame.

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:

- Canyon model (CN)
- Gauss model (SH)
- Grid model (EU)
- Heavy Gas model (HG)

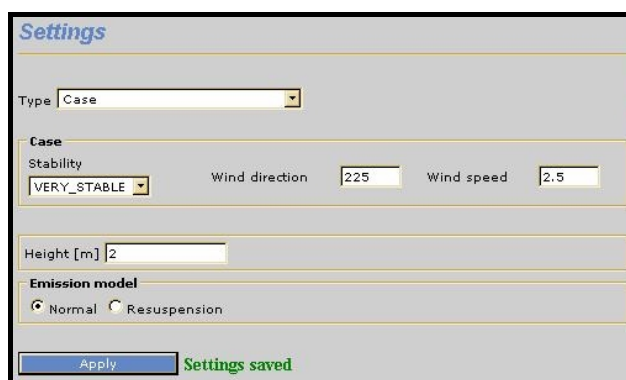
Click on the model name that you are going to use and then click on **Apply**.

## 4.2 The Gauss Model

### 4.2.1 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>.



The screenshot shows the 'Settings' window with the following configuration:

- Type: Case
- Case Stability: VERY\_STABLE
- Wind direction: 225
- Wind speed: 2.5
- Height [m]: 2
- Emission model: Normal (selected), Resuspension

Buttons: Apply, Settings saved

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** in the left hand frame. In the **Settings** sub-window use the option text box menu **Type** to choose **Case**. This enables you to enter the case conditions lower down in the sub-window. 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 prevailing wind direction 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**).

Suppose you have to give the source specifications. 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

**These point sources are saved in the EDB Client.** See *User's Reference Working with the Emission Database (EDB)*.

#### 4.2.1.1 Ordering a Calculation

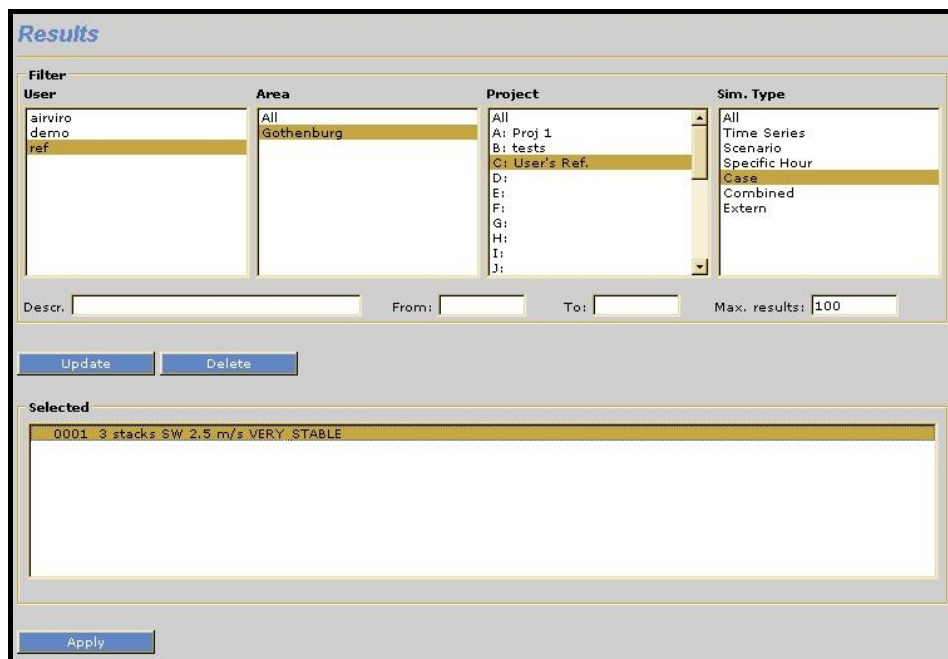
Now that you have specified weather and emission data, it's time to click on the **Calculate** to submit the batch calculation job. You will see your user name, the project under which your result files will be saved and the job number. As a user, you are allowed to store your results under whatever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



You can change the project that you are working in or create a new project name by choosing the **Project option** under the **drop down menu** 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. When this has been done, click on **Apply** and the calculation will begin.

### 4.2.1.2 Displaying Results



Now the process behind running a simulation calculation is now complete. 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. You may clear this list 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 **Filter** on the Results frame.

In order to display the results of a recent calculation, first click on the relevant user name, map area, project and simulation type. 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 the **Viewer** on the frame.



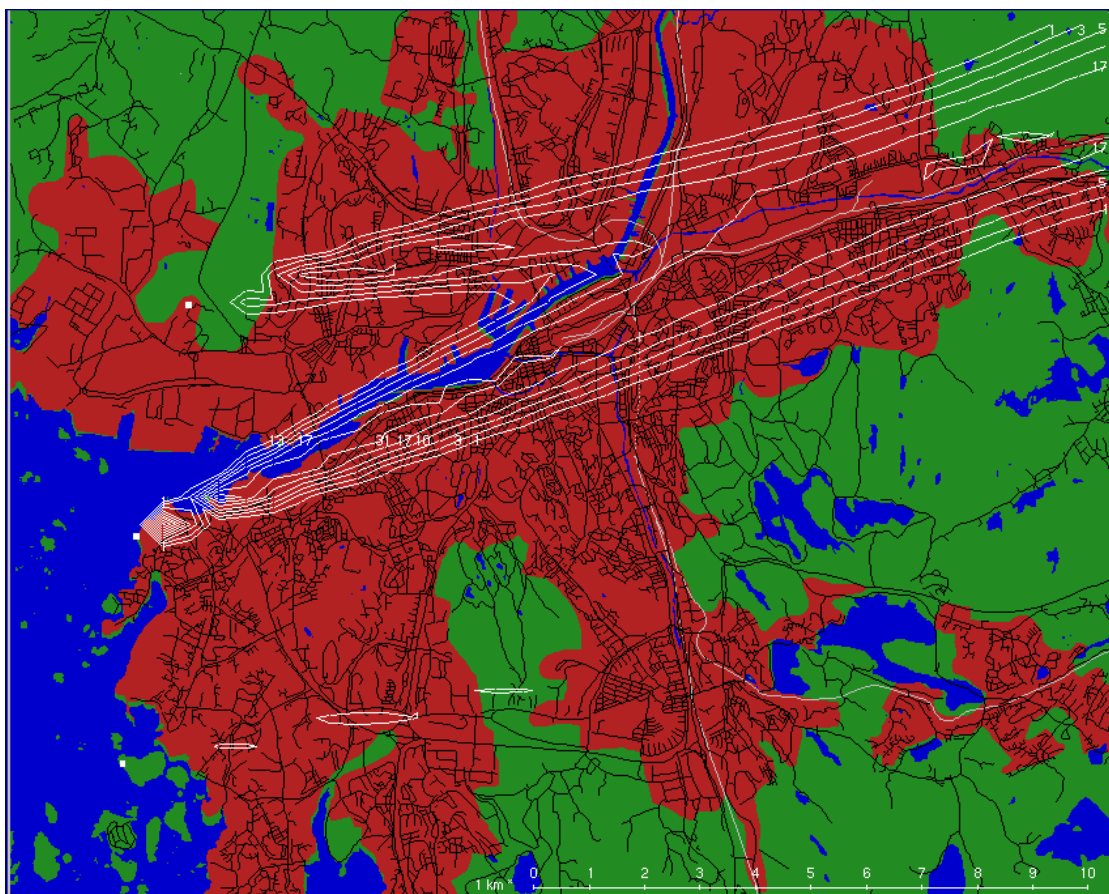


Figure 4.2.1 Three stacks with a 2.5 m/s SW wind

The Result View Control options appears automatically when you show a result. This enables you to view multiple fields (if the calculation had more than one result field) or, to view the wind field (if one was produced by the calculation).

**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 4.2.1*. 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  $\mu\text{g}/\text{m}^3$ ). **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 *4.1.2.6 Specifying Source Types*.

## 4.2.2 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 a 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 cross hair 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 4.2.2* is source 1).

Now, you set the model using Model Setting (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** sub-windows.

- choose the relevant **Substance (VOC)**
- click on **Apply**

The calculation is submitted in the **Calculate** sub-window, after editing the description text. When you display the result (*Figure 4.2.2*), you will notice a much stronger impact close to the area sources as compared to the point sources in *4.2.1 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 explain 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. 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.

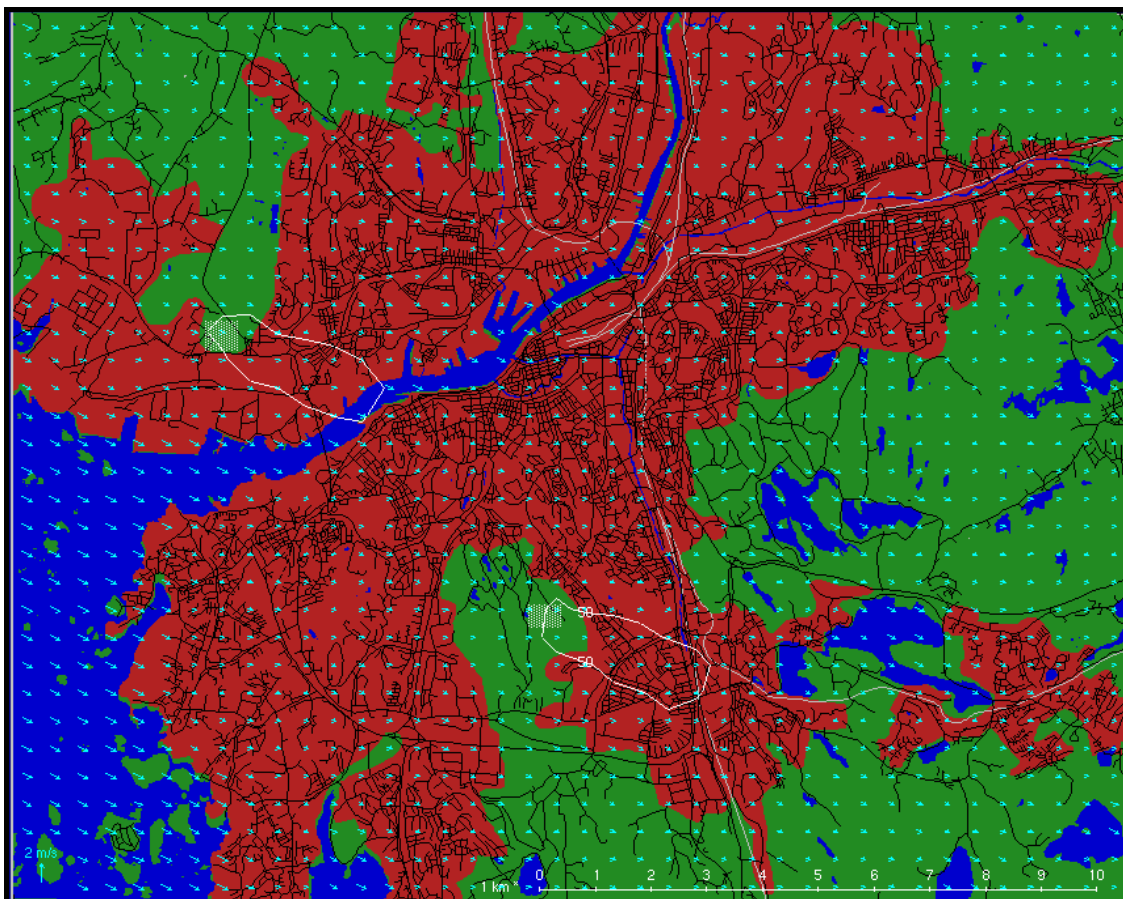


Figure 4.2.2 Two area sources together with the wind field

Figure 4.2.2 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** under **Field output configuration** in the **Output settings** Airviro 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 lines and/or the grid points to be displayed above your map area. The size and number of grid squares used in the calculation is also shown in the right part of the information 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 activating the **Wind** toggle button in the Viewer window. 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).

### 4.2.3 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** sub-window.

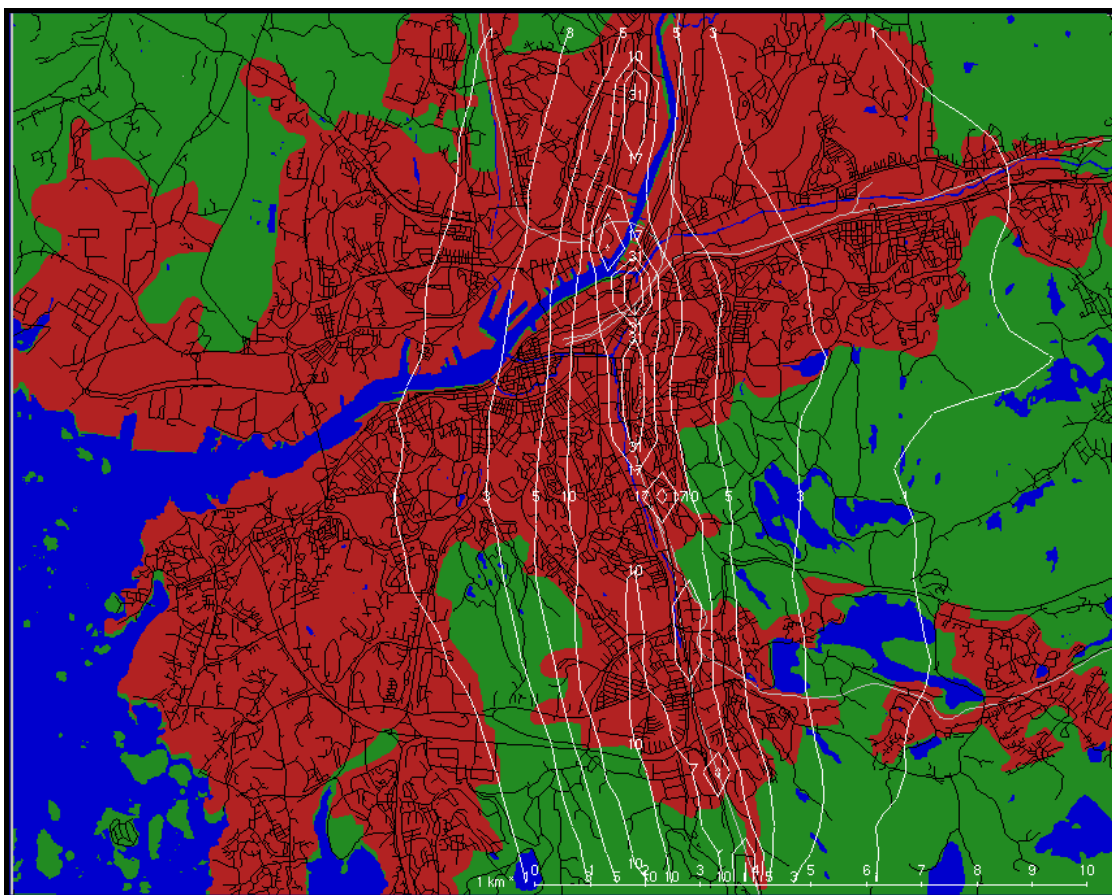
Now select the weather conditions to use in the **Settings** (Model settings) sub-window. Chose Type: **Scenario** and select the scenario called **WINTER**.

Enter the search conditions to find all road sources containing the string E6. Use the settings shown in the sub-window above. It is advantageous to use EDB search macros for complicated queries. See *User's Reference Volume 3: 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** sub-window. 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 airviro 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 4G: 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** sub-window 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.

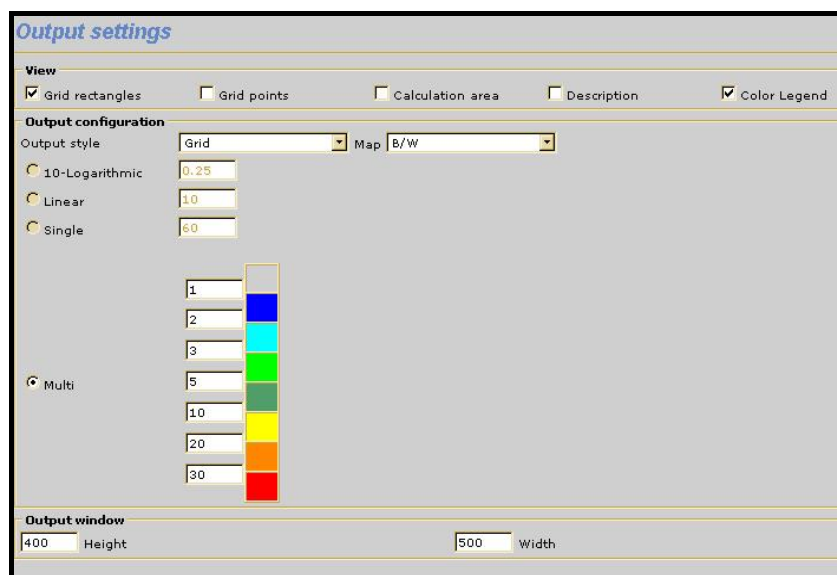


*Figure 4.2.3 The E6 through Göteborg with winter mean weather conditions*

The result in *Figure 4.2.3* 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 sub area).

Select **Output configuration** under the **Output Settings** sub-windows.



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.

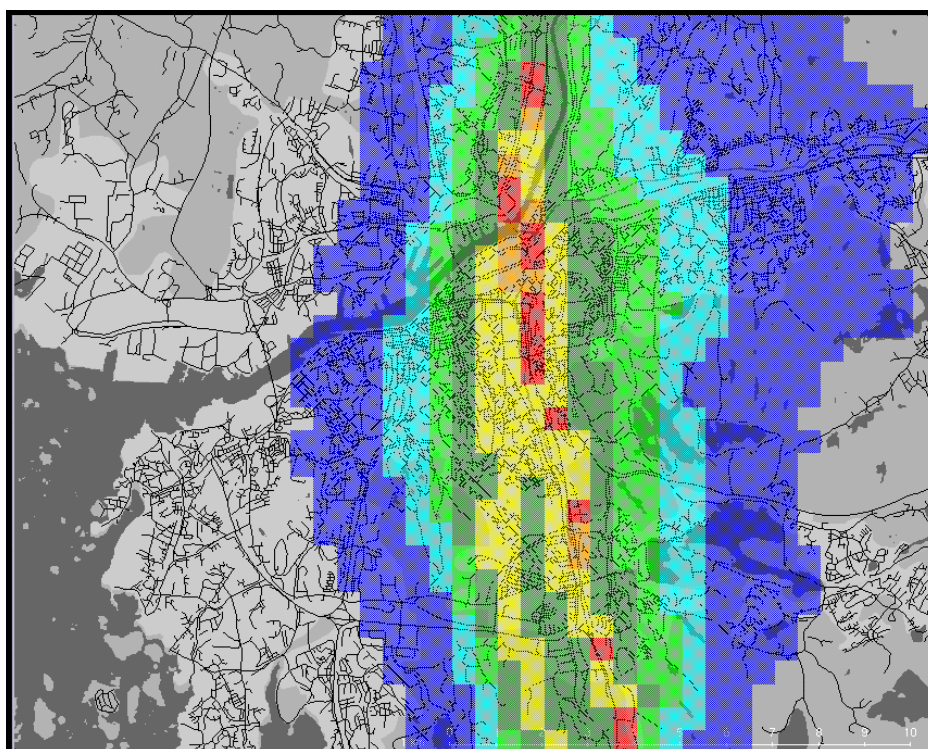


Figure 4.2.4 E6 through Göteborg with winter mean weather conditions, shown as a grid.

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** sub windows.

## 4.2.4 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.

### 4.2.4.1 Adding a Background Value

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.

### 4.2.4.2 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>.
- 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 *4.2.3 Using Scenario Weather Conditions*, i.e. the effect of the European highway passing Göteborg:
- Select the line source result file and click on **Advanced...**
- Click on 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

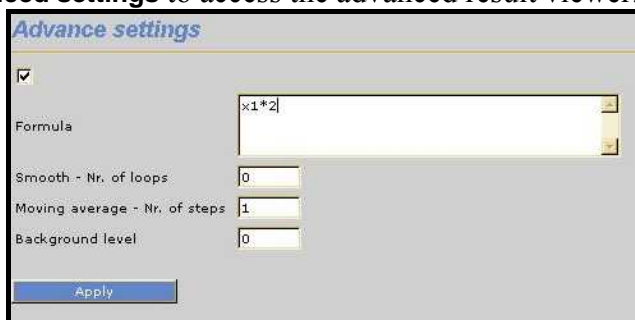
The displayed isolines will now be considerably lower than those from the NO<sub>x</sub> result file itself (Figure 4.2.3). The formula is based on the existence of a statistical relation between the NO<sub>2</sub>/NO<sub>x</sub> ratio to the absolute NO<sub>x</sub> level, in that the ratio normally is higher for low NO<sub>x</sub> concentration values.

#### 4.2.4.3 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** sub-windows, 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 2: Working with Indico Presentation*).

As an exercise, assume that the VOC emissions of the area sources in 4.2.2 *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.

#### 4.2.4.4 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 iterations are asked for. Test the output by a stepwise increase in the number of iterations.



## 4.3 The Street Canyon Model

### 4.3.1 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 4E: 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 (*4.2 The Gauss Model*). Other model specifications are given in the **Emission** sub-window.

The screenshot shows the 'Emission' sub-window with the following details:

- Substances List:** Methanol, Mn, N2O, NH3, NO, NO2, NOx (highlighted), Naphthalene, Ni, Nitrate, O3, PAC, PAH, PAN, PCB, PCDD, PCDF, Pb, PetroleumSpirit, Phenantrene, 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 (selected), Roadtype; Emission [microg/m,s] = 100.

Start by choosing a substance from the list under **Substances**. Then work down the right side of the sub-window, 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 **Pos. 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 mg/m,s) .

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

### 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 (In Sweden, nobody would eat his meal outside in the street during wintertime!).

Choose the following weather settings:

**Type (Model Settings):** Time period

**Period:** 990802 17 - 990802 20

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** sub window, 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

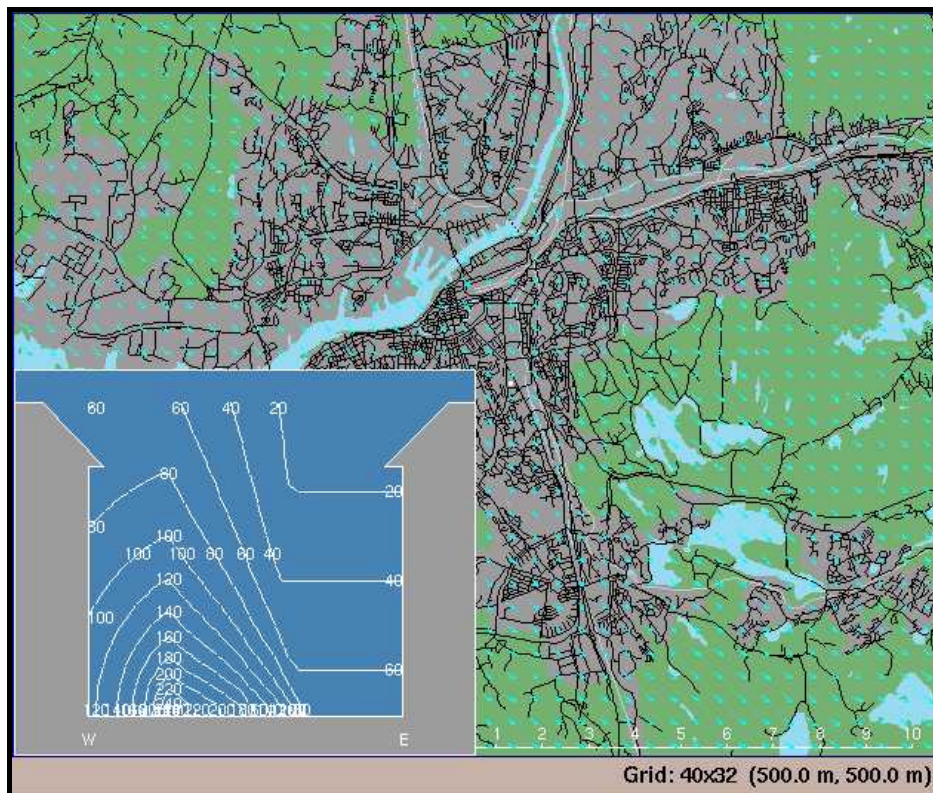
The position of the Linnégatan model section is shown as a white rectangle on the map to the left of the result shown in *Figure 4.3.1*. Use the cross hair to locate the position where you want your simulation to be performed.

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 4.3.1*. 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 below sub-menu.



*Figure 4.3.1 Canyon model of a typical summer west wind across Linnégatan*

## 4.4 The Grid Model

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** sub-window found on the frame. Then you must make sure that you are working with the correct EDB. This is done in the **Select EDB** sub-window 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).

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

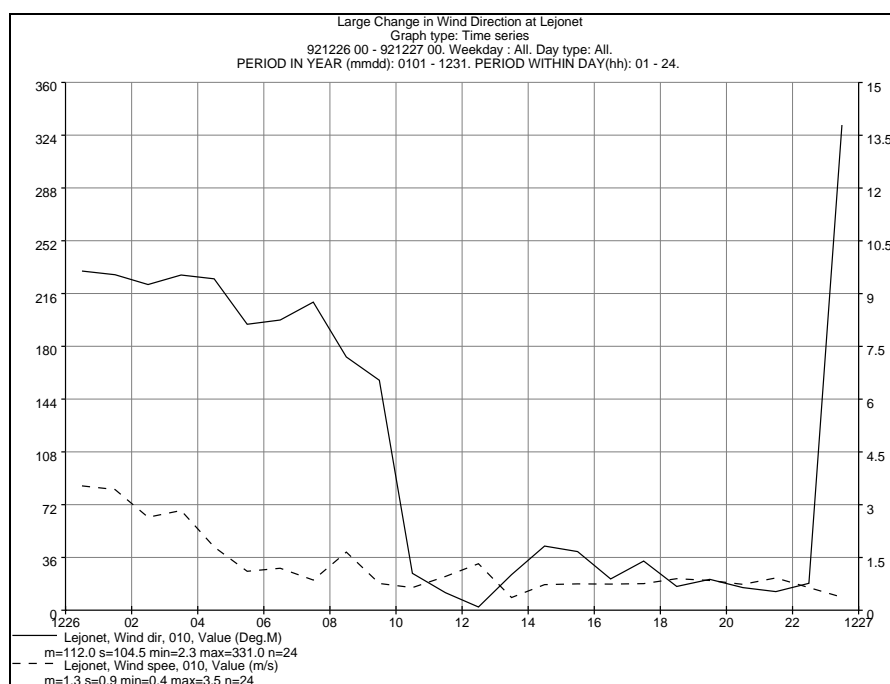


Figure 4.4.1 Wind speed and direction at Lejonet 921226

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.

EDB sources are needed as input to a dispersion calculation. 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 **Type** choose Time period and enter the period 921226 07 to 921226 15.

Under **Edb** select the EDB and choose Large NO<sub>x</sub> as search key 1. Remember that EDB search macros may be loaded from the menu under **Macros**.

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 finished dispersion result consists of several fields, one for each hour chosen. When you select the result the **Result View Controller** automatically appears and you can use the arrows under **Time** to step through the calculations. If you activate **Show Wind** then you will also be able to see the way 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** output option (under **output configuration** in the **Output Settings** menu).

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 4.4.2* 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 4.4.2* 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.

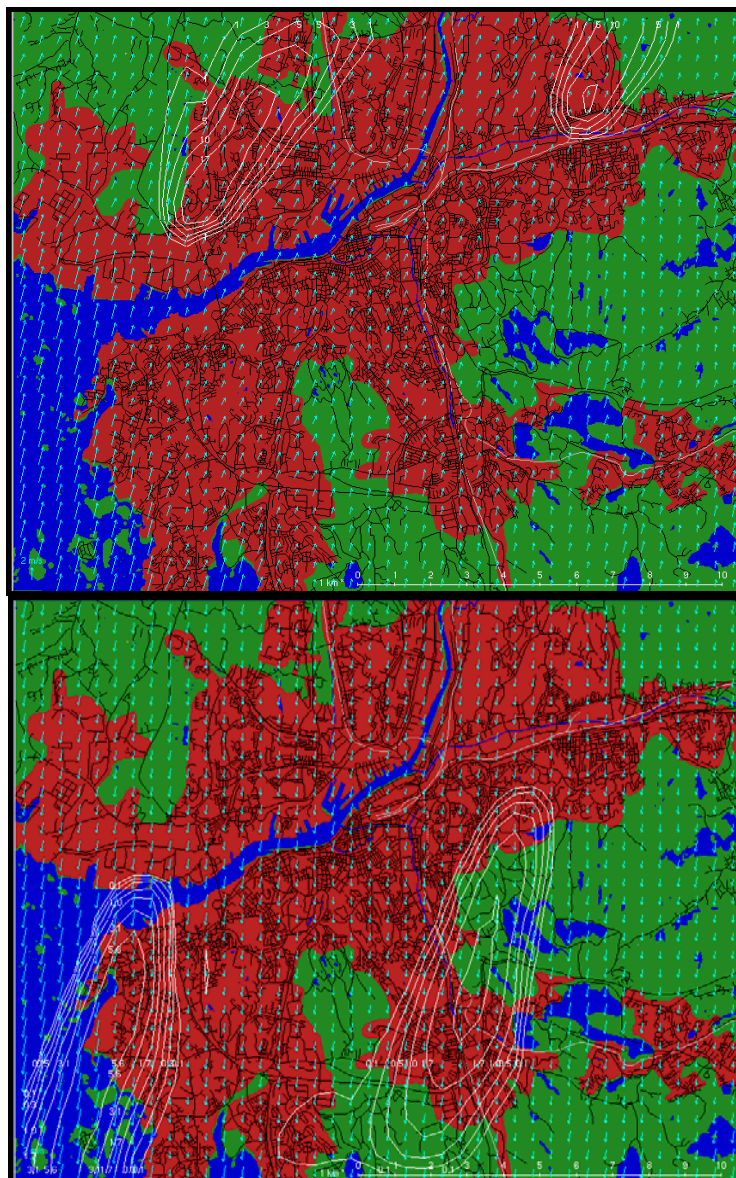
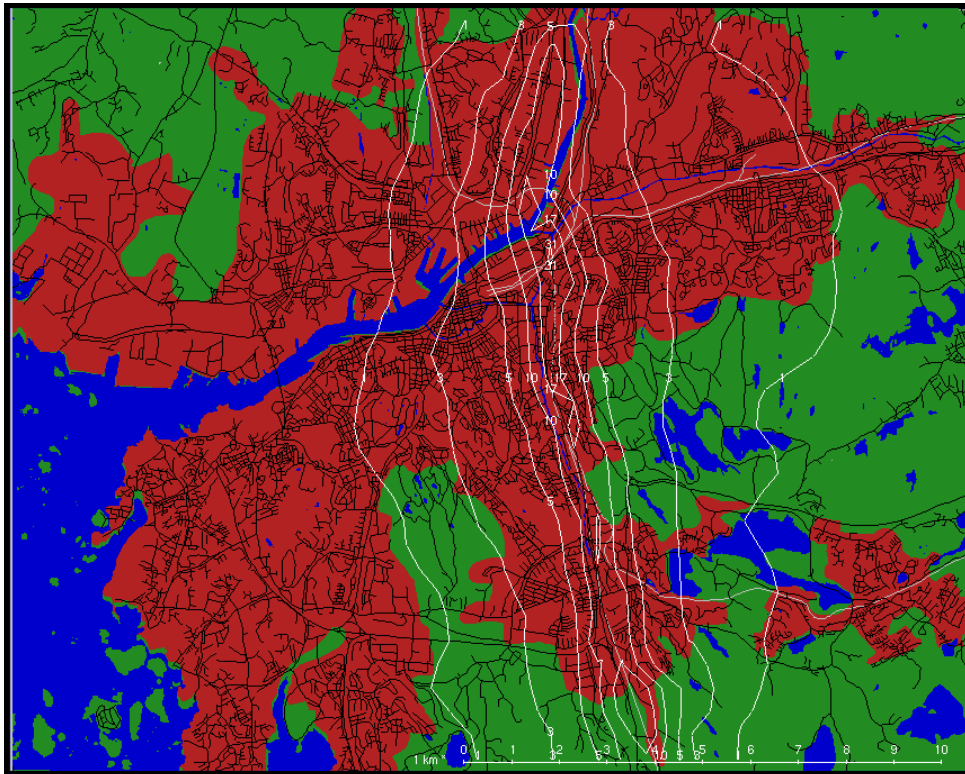


Figure 4.4.2 The two  $\text{NO}_x$  plumes and the wind field at 921226 08 and 921226 12

#### 4.4.2 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 4.2.3 *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 4.4.3.



*Figure 4.4.3 Winter mean scenario from the E6 highway*

## 4.5 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

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** in the menu.

### 4.5.1 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.

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

Zoom into an area of about 2\*2 km in the middle of the map. Use the scale shown in the bottom right corner of the map to get an idea of the size of the area you have chosen.



**Emission**

**Pos. of source**

Continuous Liquid leak

Ammonia  
**Chlorine**  
 SO2  
 Propane  
 Vinyl Chloride  
 Methane  
 Methane Pipe

**Default values**

**Tank data**

Pipe length [m] 0.1

Pipe diameter [m] 0.025

Tank contents [Kg] 10000

Tank pressure [KPa] 0

Tank temperature [C] 0

**Source information**

Source location 1275083 9608125

Apply

Under **Edb** you can enter the criteria for the heavy gas emission. Enter the following information:

**Events:** Continuous Liquid Leak  
**Substances:** Chlorine  
**Tank data:** Pipe length:0.1 m  
**Pipe diameter:** 0.025 m  
**Tank contents:** 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** sub-window are not available to you, so save your settings and close the sub-window by clicking on the **Apply** button.

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

*Figure 4.5.1* 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.

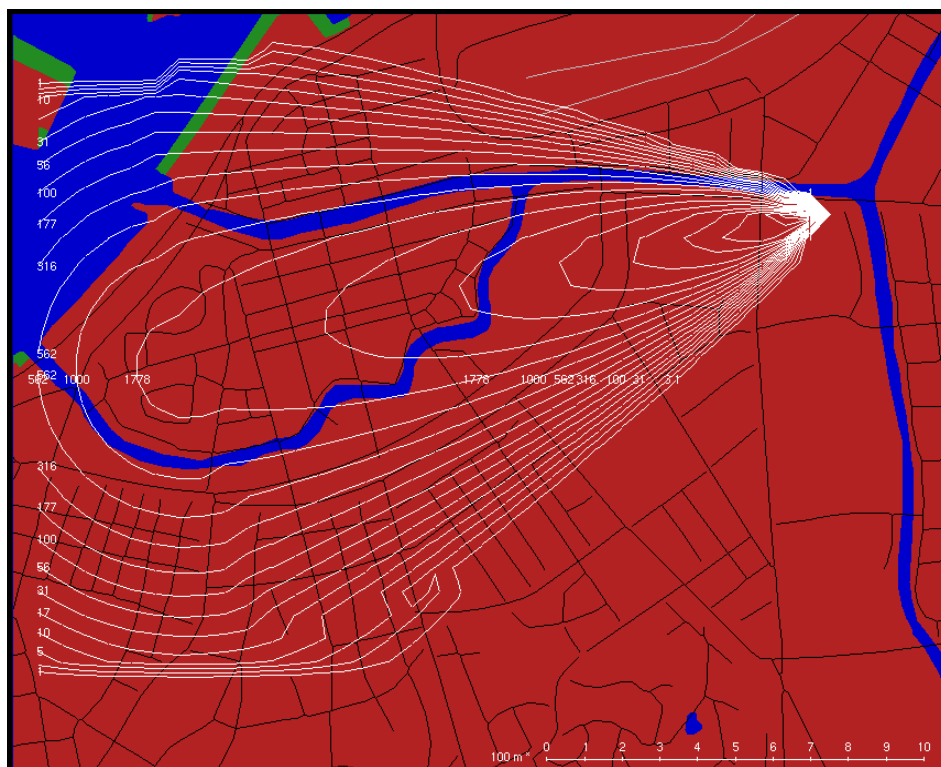


Figure 4.5.1 Simulation of Chlorine levels from 920524 12, 10 minutes after a leak began

## 4.5.2 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 **Type** 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** sub-window 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
<b>Air Data:</b>	15 degrees C

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

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

Figure 4.5.2 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.

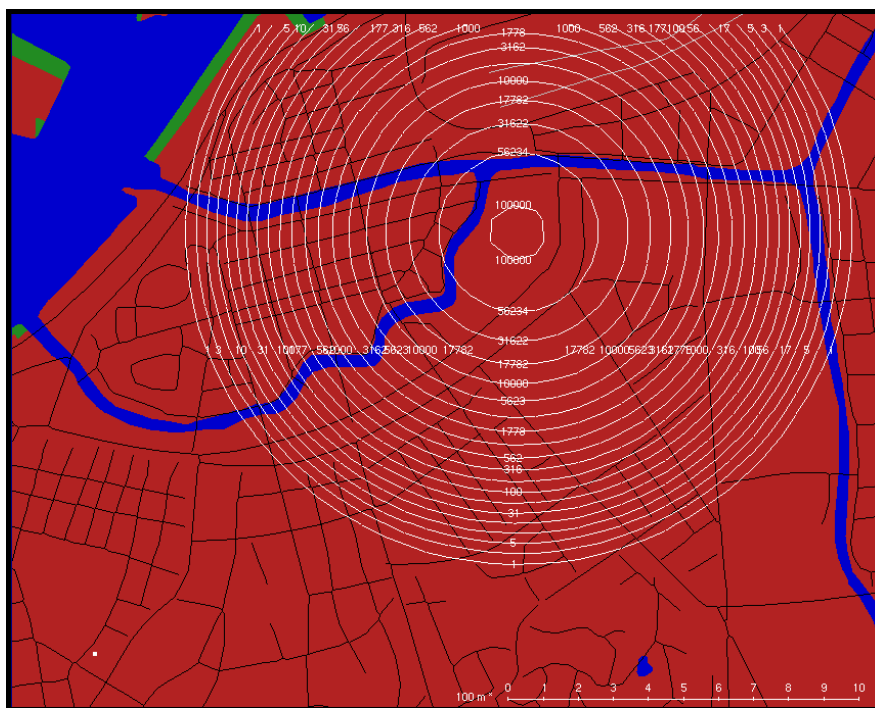


Figure 4.5.2 Ammonia leakage from a tank burst, 10 minutes after the burst.

## 4.6 Introduction to the Post processor

The Post processor operates on results from the Dispersion Module. The main functionality of the Postprocessor lies in the treatment of results from time period calculations, but there are also some functions that may operate on other dispersion calculations like Specific Hour or Case weather conditions.

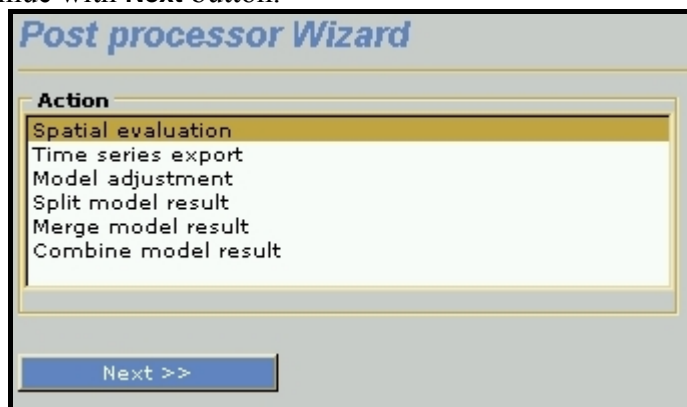
The characteristic result from the dispersion is one or more fields with hourly mean concentrations (except for Scenario, which is a weighed field for many hours). In order to evaluate the results, it is often necessary to either make a statistical study of the results or to use a diagram presentation for some point in the field.

With the Postprocessor, it is possible to make a statistical study or to create a new time period. It is also possible to export the simulated concentrations to the time series database for a station in the calculation grid, in order to make comparisons between measured and simulated concentrations in a diagram within Indico Presentation Client.

### 4.6.1 Overview of the Postprocessor Main Window

The Postprocessor is started from the Dispersion Module Main Window by clicking on the **Postprocessor** (on the frame).

The Post processor Wizard window consists simply of an **Action** option menu button and the possibility to continue with **Next** button.



The first alternative is **Spatial evaluation**, which is a process that calculates statistics for a time period or creates a new, processed time period for viewing in **Results**.

Second is the **Time series export**, which is a process that collects the simulated model result at the position of a predefined monitoring station within the calculation domain and exports it to the time series database. The simulated time series may be viewed in Indico Presentation Client.

The **Model adjustment** alternative is a process that compares the model result with a set of predefined monitoring stations within the calculation domain. Using station data as reference, the model result is adjusted to fit with measured data in the entire calculation domain. The adjusted result may be viewed in **Results**.

**Split model result** is simply a process that creates a new time period as a contiguous subset of the original model time period. The splitted model time period may be viewed in **Results**.

**Merge model result** is a process that creates a new time period by merging original model results into a longer time period.

**Combined model result** is a process that creates a new result applying one formulates constant to an entire dispersion result.

When you have chosen an ACTION, click the **Next** button to proceed in the actual process.

## 4.6.2 Specifying Model Results

All processes share a common path for specification of model results. The common path includes specification of model type, user identity and model result.

The window for choice of model type includes a **Model** option button with a pull-down menu, which includes all configured models for your installation. Choose the model type that you have used to make your dispersion calculations with.

In this window, and all subsequent windows, there is a **Prev** button, which takes you back to the previous window. The Back button can be used if you want to change your selection in a previous window.

When you have chosen a model type, click **Next** to proceed.

The window for choice of user includes a **user** option button with a pull-down menu, which includes all defined Airviro users in your system. Choose the user identity you used to make your Dispersion calculations with.

The window for choice of result includes a **result** option button with a pull-down menu, which includes all saved calculation results for the chosen model, by the chosen user. Choose the result you want to post-process.

If some error should occur, you may view the log file at `/usr/airviro/log/tscalcul.log`.

## 4.6.3 Spatial evaluation

The Spatial evaluation action is a process, which calculates descriptive statistics, frequency statistics and exceeded statistics upon request for a model time period.

The name Spatial evaluation emanates from the fact that the statistical treatment is grid based. For instance, in a 70x70 square horizontal calculation grid, the mean value for the time period is calculated in every grid square. The result of the calculation yields a 70x70 matrix with mean values for the calculation domain.

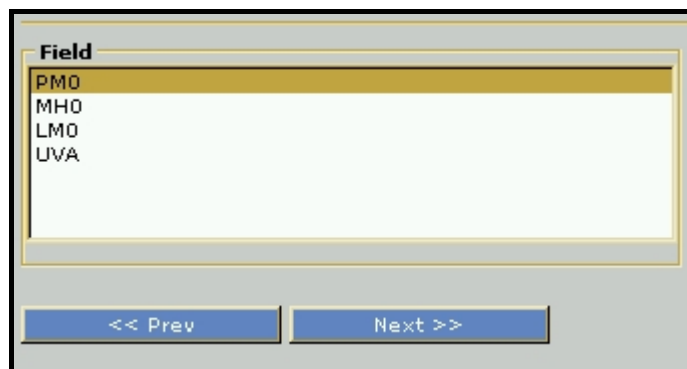
The matrix can be analysed in the same manner as an hourly modelled concentration field. The isoline analysis is made in the Dispersion Module Client.

In addition to calculating statistical fields, the Spatial evaluation module can create new results for longer sampling times (daily averages, 8 hourly or 24 hourly running mean).

### 4.6.3.1 Specifying object and method

Spatial evaluation operates on a scalar variable, usually a mass concentration field from the dispersion result. The window for choice of field variable includes a time series option button with a pull-down menu, which includes all field variables for your dispersion calculation.

Choose the field that you want to post process.



When you have chosen a field, click **Next** to proceed.

If you would attempt to operate Spatial evaluation on any other weather conditions than Time period or Forecast, there would be very little functionality in the subsequent menu.

The window for choice of methods is the core of the Spatial evaluation and includes many statistical measures that can be toggled on or off.

The average value, minimum, maximum and standard deviation are descriptive statistics, which always are calculated. To allow for missing values in the time period, there is a **Percentage** toggle button, which eventually opens a window where the required data capture is specified. As a rule of the thumb, the data capture should be kept high; at least seven out of eight hours should be included. If the data capture is less than specified in Percentage, the average, daily average or running average will not be calculated.

Frequency statistics can be calculated as **Percentiles** in the interval 90-100. The 98<sup>th</sup> percentile of some period, say the monthly 98<sup>th</sup> percentile of hourly mass concentrations is the value below which 98% of the hourly values during that month fall.

Exceeded statistics can be calculated from the **Exceeded limit** toggle button, which eventually opens a window where the threshold limit is specified. The resulting field shows the percentage of values that exceed the specified limit.

In addition to the statistical measures, the Spatial evaluation module has the ability to create new results based on other sampling periods. Under **Running averages**, an average based on 8 hours, 24 hours or one year of hourly values will be calculated to deliver a result for the last valid hour in the sampling period.

The **Daily average** check box will trigger a calculation of daily averages of the chosen field. The resulting average will be written to the noon hour each calendar day with valid data.

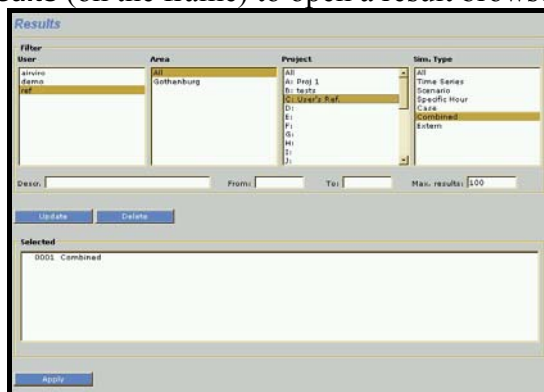
In the **Correction factors** you may enter peak-to-mean correction factors for 15-minute averages. The values of the correction factors may vary depending on the source distribution and on atmospheric stability. If you monitor the concentrations of the actual substance, you may have the possibility to estimate correction factors from your monitoring data.

In the **Description** field, you can enter a name to identify the Spatial evaluation calculation. It is strongly recommended to enter a unique name in the Description field, to simplify the presentation of results in **Results**.

#### 4.6.3.2 Viewing the result

When all calculations have been performed, a message box appears to inform that Spatial evaluation was executed.

In order to view the result, select the model whose result you post processed with Spatial evaluation. Click on **Results** (on the frame) to open a result browser.



Select the user identity, calculation domain and project that you used for your Dispersion calculations. You can find your post processed results under the **Combined** simulation type.

With **Viewer** you can see the result the post processor.

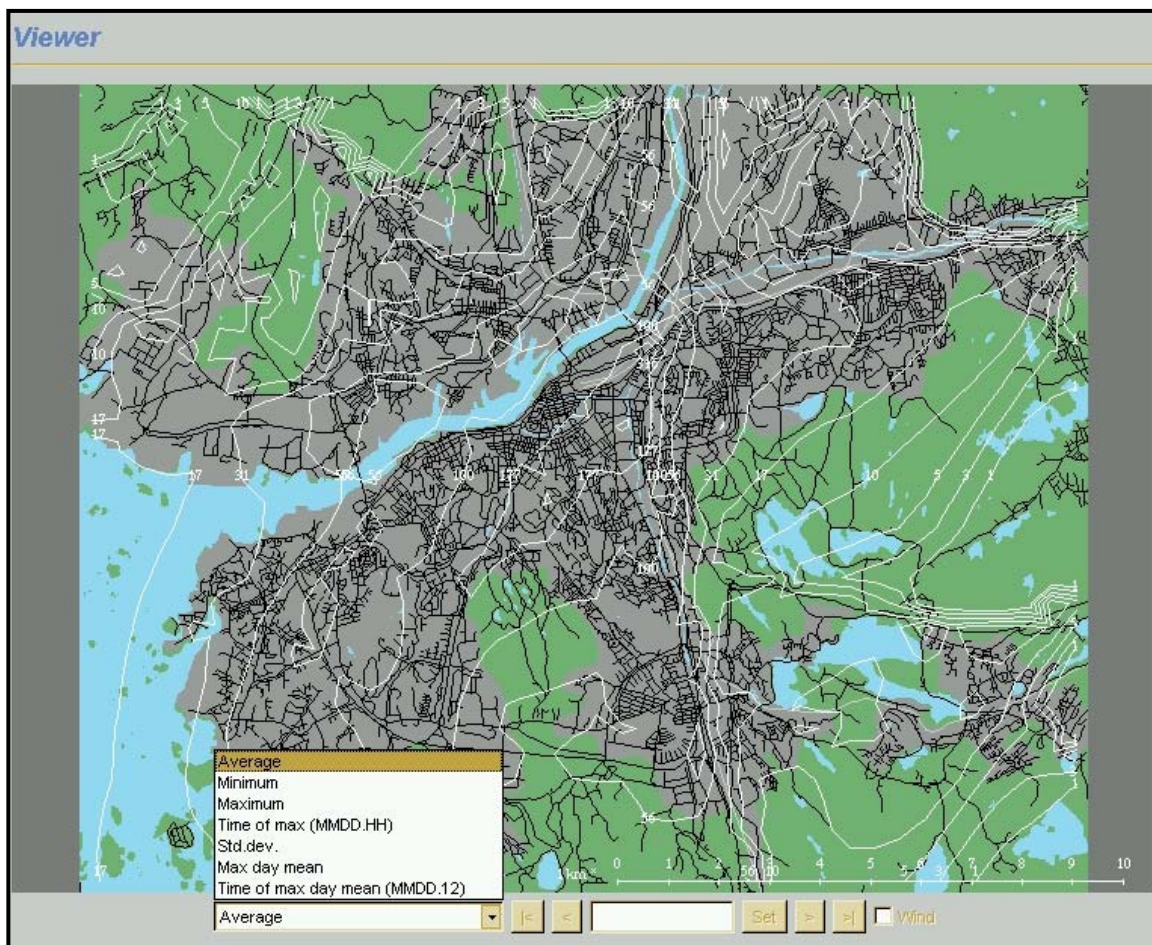


Figure 4.6.3 Example Spatial Evaluation

#### 4.6.4 Time series export

The Time series export action is a process, which creates a focused time series with simulated data for a particular grid square in the calculation area. The purpose of Time series export is to allow simulated data to be stored in the time series database.

The time series database requires that data is stored with station and parameter as reference. Stations are defined in the station database and parameters are defined in the parameter database.

If you want to store some simulated results in the time series database, you must have defined a monitoring station. Time series export will select data from the grid square closest to the monitoring station for export.

You must also define a parameter in the parameter database, which can be used for storing simulated results. Make sure that the prefix 'sim' is included in the name of the parameter, to avoid confusion with measured parameters.



#### 4.6.4.2 Specifying object and location

Time series export operates on a scalar variable, usually a mass concentration field from the dispersion result.

The window for choice of field variable includes a time series option button with a pull-down menu, which includes all field variables for your Dispersion calculation. Choose the field that you want to post process.

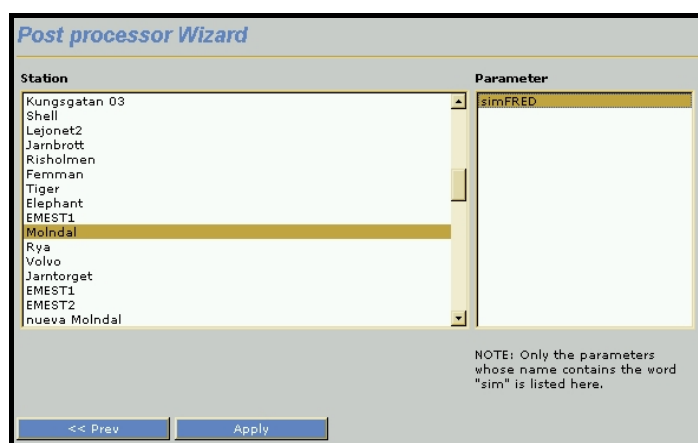
The window for choice of station includes a **station** option button with a pull-down menu, which includes all active stations within the calculation area and within the installed database project. Choose the station for which you want to store simulated results.

If the list of Station options becomes too long, the **More stations** button will appear to let you choose from more monitoring stations.

When you have chosen a station, click **Next** to proceed.

The window for choice of parameter includes a **parameter** option button with a pull-down menu, which includes all available parameters from the parameter database. Choose the parameter that you want to use as reference for the simulated variable.

If none of the available parameters are applicable, consider creating a new parameter in Indico Administration. Make sure that the prefix 'sim' is included in the name of the parameter, to avoid confusion with measured parameters.



#### 4.6.4.3 Viewing the result

When all calculations have been performed, a message box appears to inform that the Time series export was executed. Clicking **Apply** ends the Post processor module.

In order to view the result, you must start Indico Presentation Client from the Airviro main window.

Select the station and parameter that you used for your post processing. Make sure that you have selected the correct time period. Proceed as usual in Indico Presentation Client.

## 4.6.4 Model adjustment

The Model adjustment action is a process, which compares a model time period with one or more measured time series from stations within the calculation area. Using station data as reference, the model result is modified to fit with measured data in the entire calculation area. Model adjustment should be used with caution, because a poor agreement between measured and modelled data indicates that the knowledge about emissions is limited or that there is some other systematic error in the modelling. There is also the possibility that measurements are inaccurate.

The influence of a monitoring station on the model result depends on how many stations are located within the calculation area. If only one station is within the area, the adjustment to the model result will be applied over the whole area. The adjustment is function both of the difference between modelled values and the measured values and of the distance from the station to the actual grid square.

The model adjustment operates at one time step at a time. The process does not assimilate corrections from one time step to another.

If you want to use Model adjustment, you must first define a macro within Indico Presentation Client. The macro should include selection of all the monitoring stations and data that you want to use as reference.

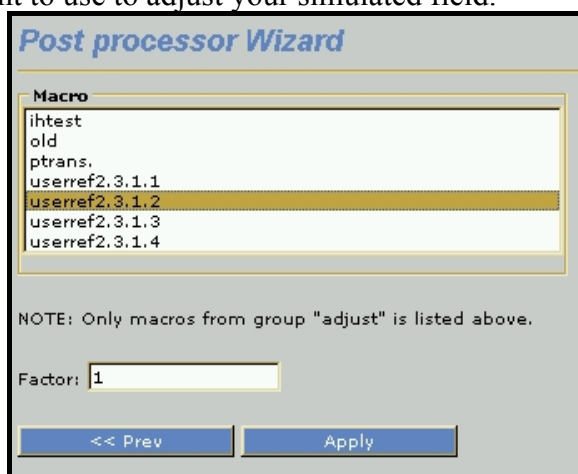
### 4.6.4.1 Specifying object and reference

Model adjustment operates on a scalar variable, usually a mass concentration field from the dispersion result.

The window for choice of field variable includes a time series option button with a pull-down menu, which includes all field variables for your dispersion calculation. Choose the field that you want to post process.

When you have chosen a field, click **Next** to proceed.

The window for choice of macro includes a **macro** option button with a pull-down menu, which includes all available macros from the adjust group in Indico Presentation Client. Choose the macro that you want to use to adjust your simulated field.



If no macro is available, check first if the adjust directory exists (usr/airviro/data/project\_name/indico/adjust/). If it doesn't exist, simply create a new adjust folder for the project. Next, you must create a macro within Indico Presentation Client, which has the prefix health\_ and place it under the user adjust. The macro should include selection of

all the monitoring stations and the pollutant that you want to use to correct the simulated values. The type of Indico graph is not essential, neither the time period.

You may enter an optional factor in the **Factor** field. This may be used if you compare modelled data for another species than that measured, but only if the two species are covariant, i.e. if they are emitted from the same sources and with the same pattern of variation. If you want to correct the level of monitored data for some station, it is also possible to define correction factors for individual stations in the macro.

Click **Apply** to complete the specification of Model adjustment.

When all calculations have been completed, a message box appears to inform that Model adjustment was executed. Clicking **Apply** ends the Post processor.

In order to view the result, click on **Results** to open a result browser.

Select the user identity, calculation area and project that you used for your Dispersion calculations. You can then find your post processed results under the **Combined** simulation type. The name is “Adjusted data” with a new file number.

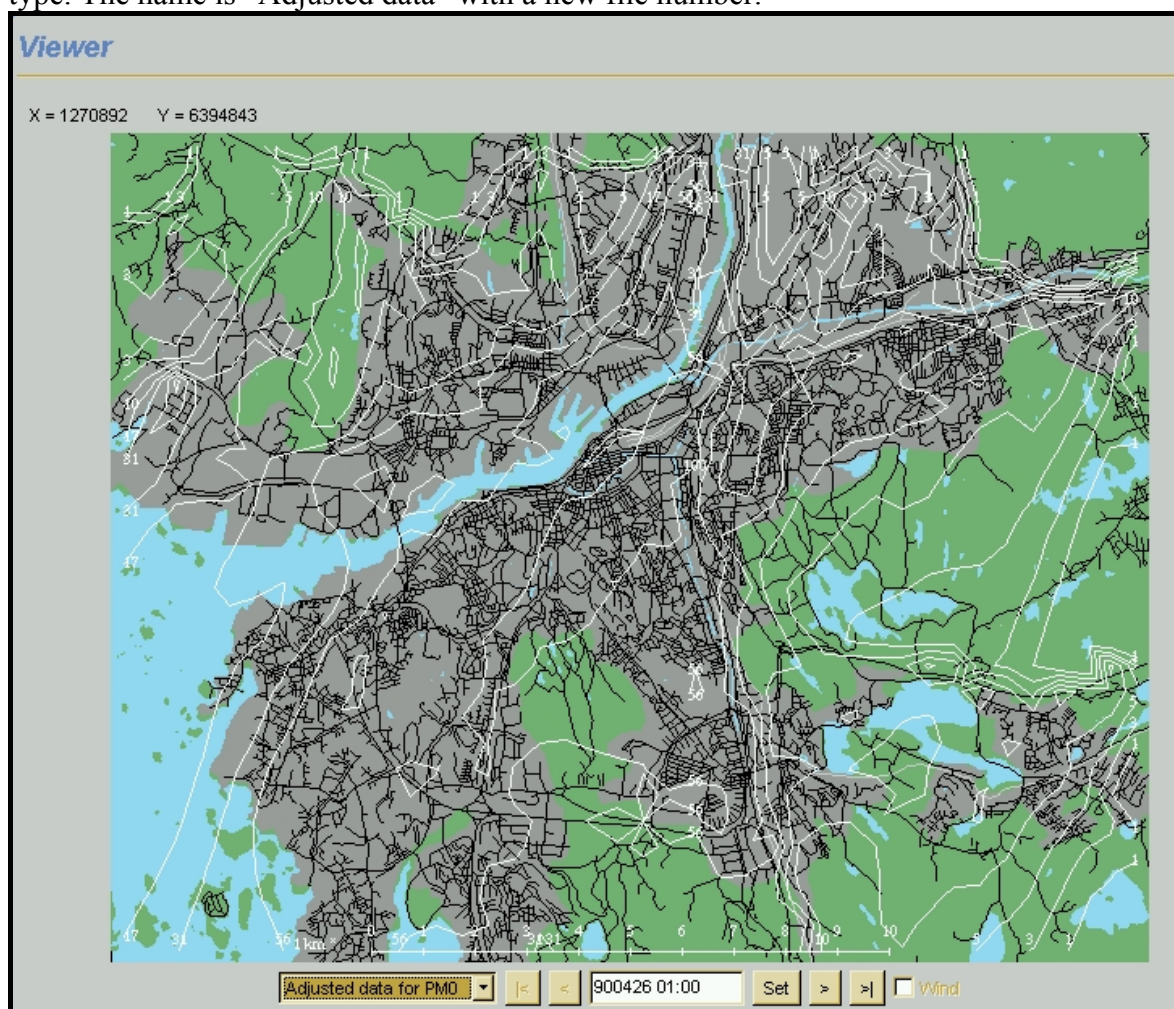


Figure 4.6.4.1. Example Adjusted model

## 4.6.5 Split model result

The Split model result action is a process, which extracts a shorter time period from a model result. The purpose may be to highlight an interesting episode or to split a long time period into shorter ones for further processing.

Split model result operates on the entire model result from the dispersion.



The window for choice of **time period** includes a Start date and a Stop date field. Enter date and time for the time period subset in the specified format.

When you have entered the values, click **Apply** or << **Prev** to alter your choices.

When the extraction is completed, a message box appears to inform you that the Split model result was executed. Clicking **Apply** ends the Post processor windows.

In order to view the result, you must start the Dispersion module from Airviro Main window. Select the model whose result you post processed with Split model result. Click on **Results** to open the result browser.

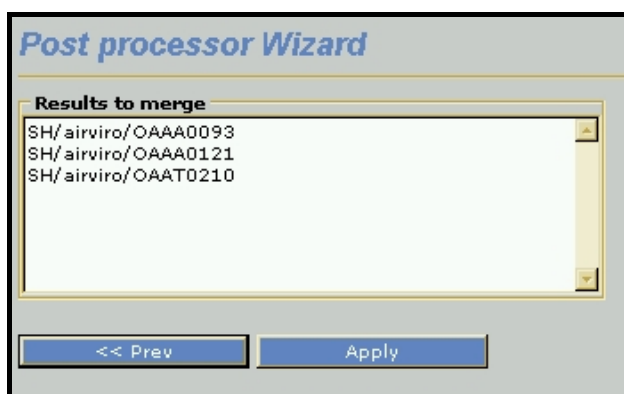
Select the user identity, calculation area and project that you used for your Dispersion calculations. You can find your post-processed results under the **Time period** simulation type. The name is "Splitted data from XXXXnnnn.REX".

Use the normal procedure in Dispersion to view the results..

## 4.6.6 Merge model results

The Merge model results action is a process, which merges two or more model results into a longer time period. If you, for instance, have twelve monthly results and you want to calculate yearly statistics, you could use Merge model results to create a yearly model result and then apply Spatial evaluation on the merged result.

Merge model results operates on the entire model results from the dispersion.



The window for choosing results for merging includes a **result** option button with a pull-down menu, which includes all saved calculation results for the chosen model, by the chosen user. Choose the result you want to post process.

If you want to select more results, click on **Select another** to choose from more model results. When you have selected all results for merging, click **Apply** to complete the specification of Merge model results.

When the merging is completed, a message box appears to inform you that Merge model results was executed. Clicking **Apply** ends the post processor.

In order to view the result, select the model whose result you post processed with Merge model results. Click on **Results** to open the result browser.

Select the user identity, calculation area and project that you used for your Dispersion calculations. You can find your post-processed results under the **Time period** simulation type. The name is "Merged data from XXXXnnnn.RES".

Use the normal procedure in Dispersion to view the results..

#### 4.6.7 Combined

The combined result action is a process, which to apply one formulates to a dispersion result.

For example: To add a background to 10 to the concentration result.

The screenshot shows a dialog box titled "Post processor Wizard". It has several sections:

- Results to combine:** A dropdown menu showing "SH/airviro/OAAT0210" and a list of options: "CONC", "CONC", "MIXH", and "LMO". The first "CONC" is selected.
- Formula:** A text box containing "x1".
- Project:** A dropdown menu showing "C: User's Ref.".
- Description:** A text box containing "Combined".
- Buttons:** "<< Prev" and "Apply".

Click on **Results** to open the result browser, and then click on **Viewer**.

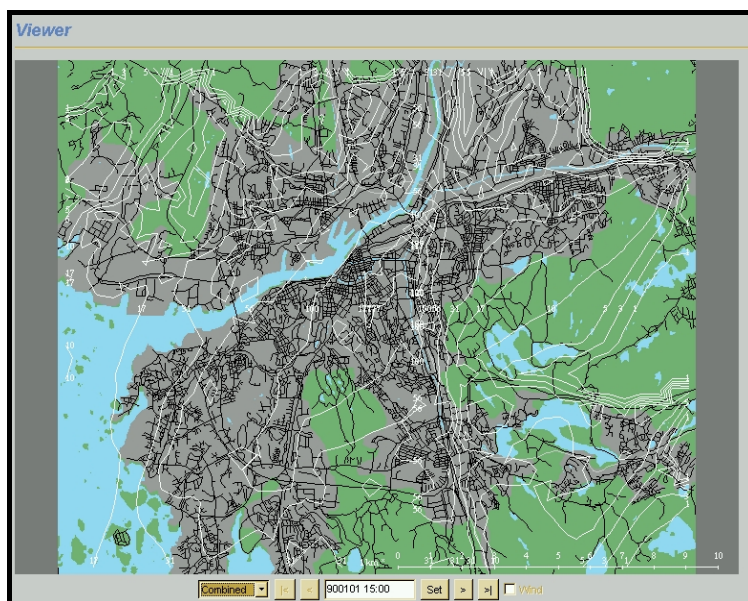


Figure 4.6.7.1. Example Combined

## Appendix 4A: The Wind Model - Calculation of the Wind Fields

### 4A.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.

#### 4A.1.1 Wind Model Equations

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

$$\frac{\partial V_s}{\partial t} = -V_s \cdot \nabla V_s - (g \nabla Z_s + R T_s \nabla \ln p_s) - f K \times V + F + K_m \nabla^2 V \quad (\text{eq 4A.1.1})$$

$$\frac{\partial \Theta_s}{\partial t} = -V \cdot \nabla \Theta_s + K_t \nabla^2 \Theta_s + Q / C_p \quad (\text{eq 4A.1.2})$$

$$\frac{\partial p_s}{\partial t} = \frac{g}{R \Theta_s T_s} \cdot \int_0^H \frac{\partial \Theta}{\partial t} dz \quad (\text{eq 4A.1.3})$$

$V$  = 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)

#### 4A.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 *4A.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 4A.1.1) until two successive estimations of the average wind component do not differ by more than 2%.

#### 4A.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

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

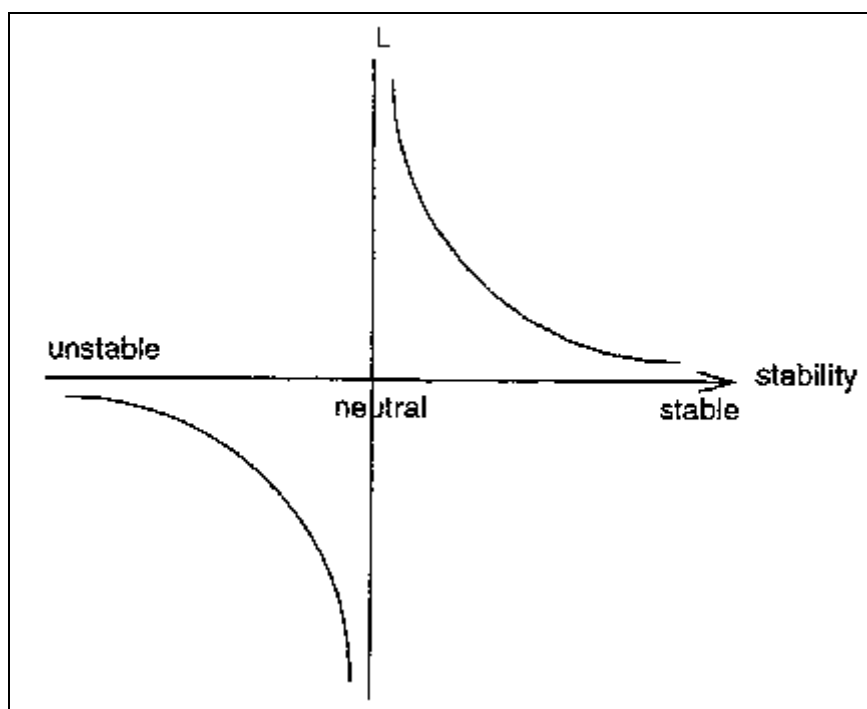


Figure 4A.1 The Monin-Obukhov length ( $L$ ) behaviour as a function of stability

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:

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

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

*Figure 4A.2 Recommended values of  $T_i$  according to Draxler (1976). Sources higher than 30 m are considered as elevated.*

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

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

#### 4A.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:

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

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

$d_k(i,j)$  = 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 ( $Z_i$ ) and mixing height ( $mixh$ ) are treated in much the same way.

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

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

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

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

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

### **Free wind**

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

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

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

## **4A.1.5 Procedures for Solving the Wind Model Equations**

When the initial conditions have been estimated, the thermodynamic equation (eq 4A.1.2) is used to estimate the local change in potential temperature. The tendency equation (eq 4A.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 4A.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.

## **4A.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.

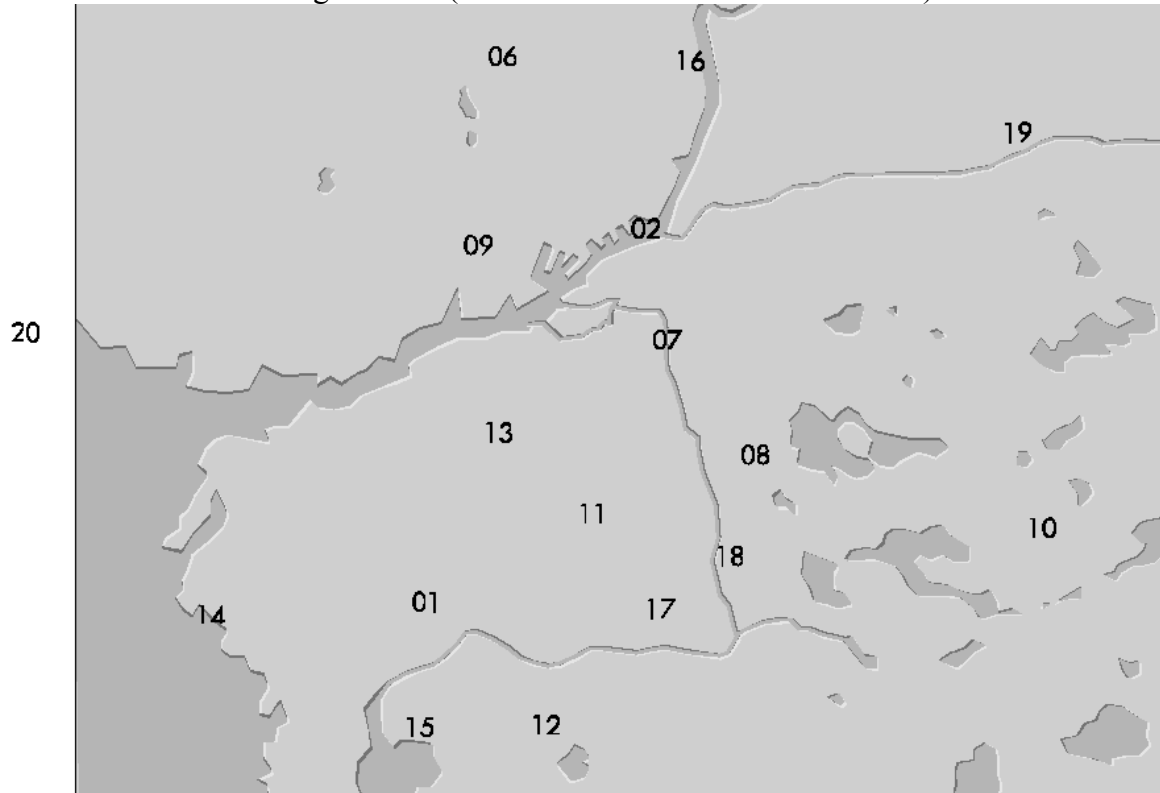
Consequently, the total adaption period in this case is 4 minutes.

#### **4A.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 4B: Results from Verification Studies

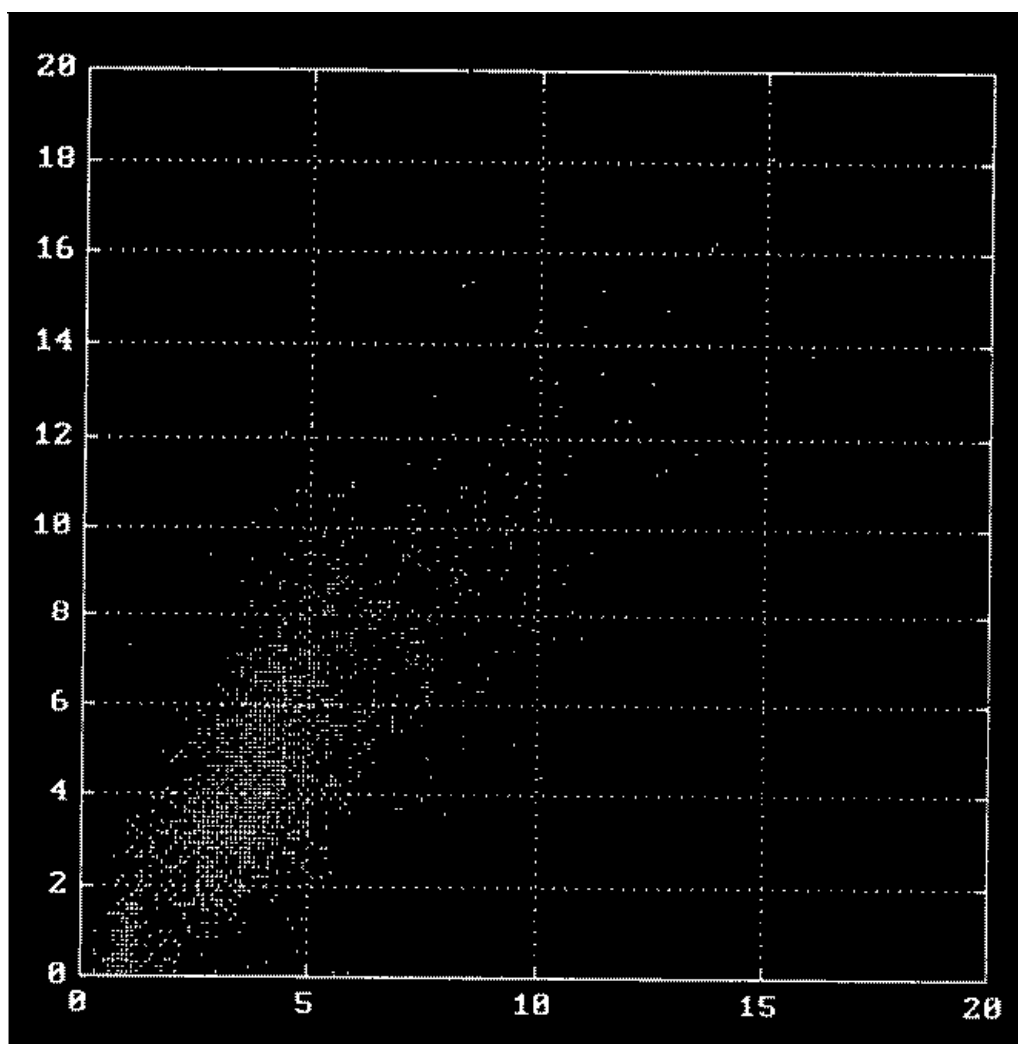
During the period 25 January to 25 March 1990 a wind experiment was performed in the Göteborg area. A total of 18 wind monitoring stations were located in the area. At these locations wind speed and direction were measured at approximately 10 m from ground level. Data was collected as 15 minute average 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 4B.1 (the Jarnbrott station is station no. 01).



*Figure 4B.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 4B.2* a scatter diagram is presented showing the measured winds compared to the modelled winds at all locations during the two month period.



*Figure 4B.2*

In *Figure 4B.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 4B.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.

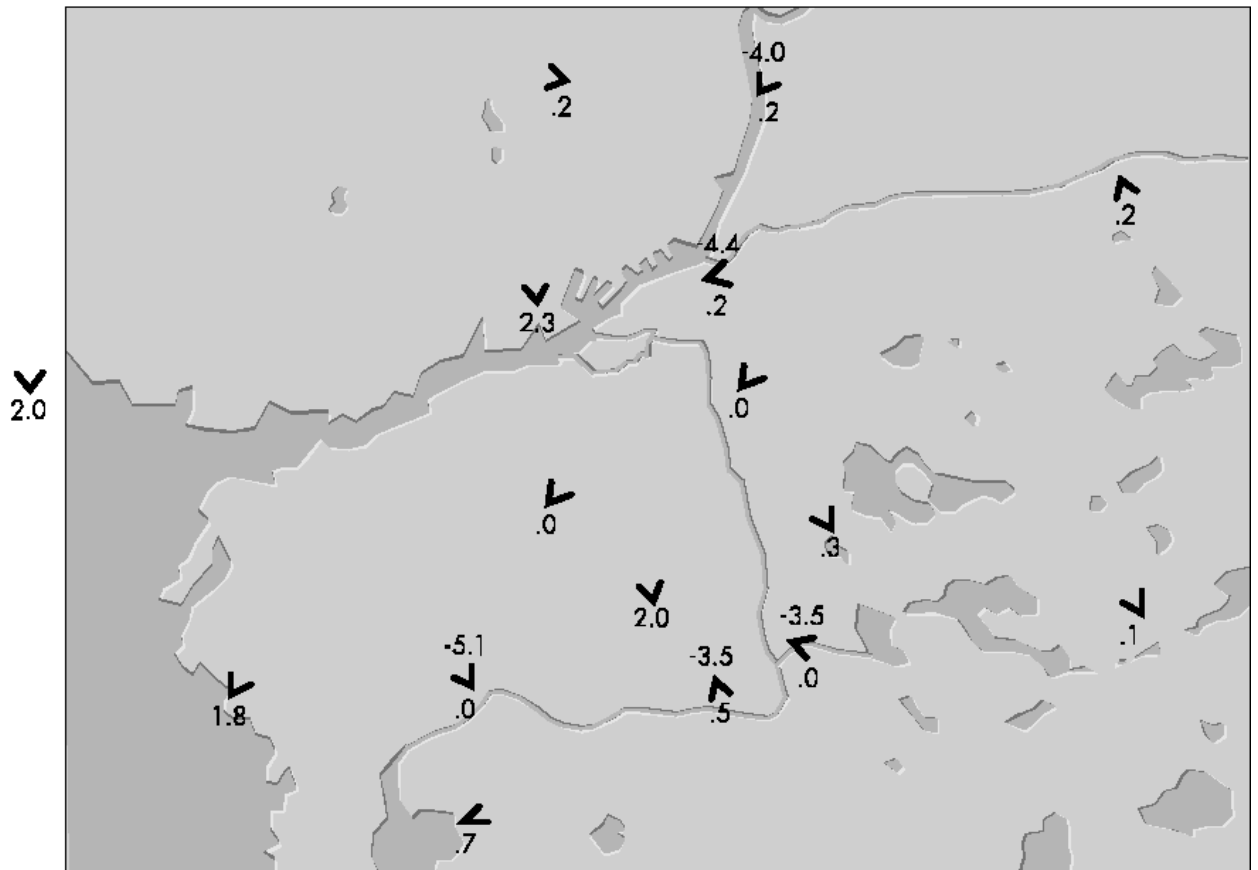


Figure 4B.3

In *Figure 4B.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.



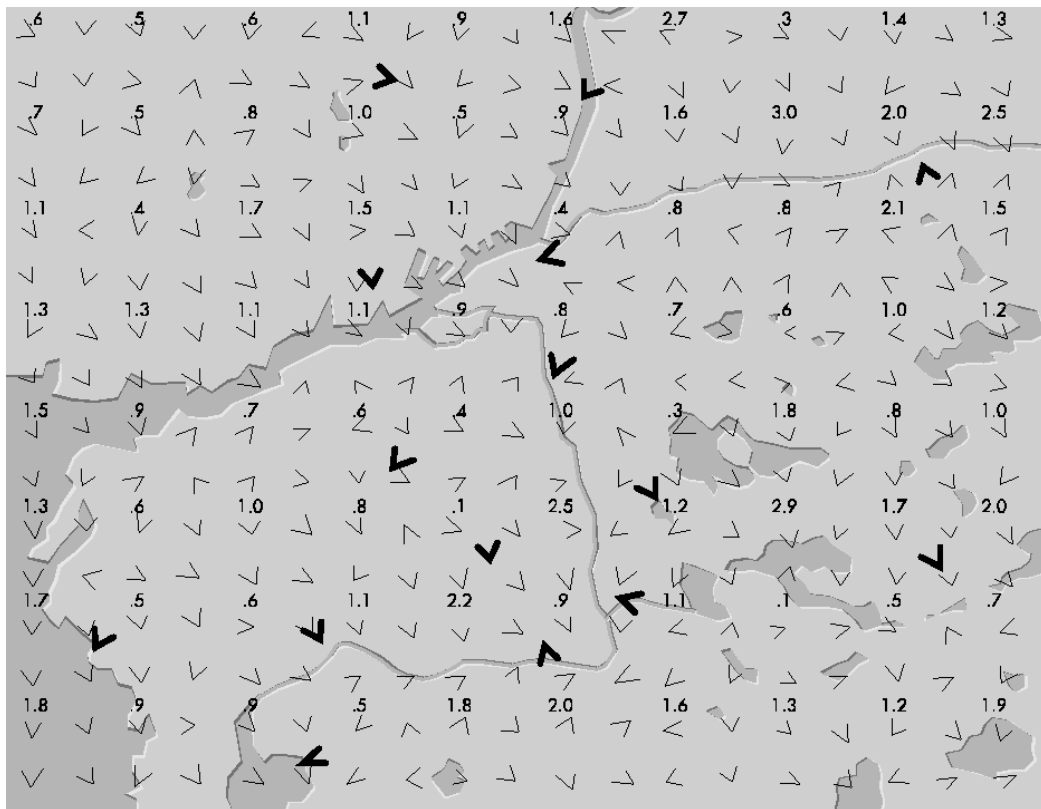


Figure 4B.4

## Appendix 4C: The Gauss Dispersion Model

### 4C.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 4G: 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 4G: 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.

### 4C.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 4A:*). 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 4E: 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.

#### 4C.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).

#### 4C.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.

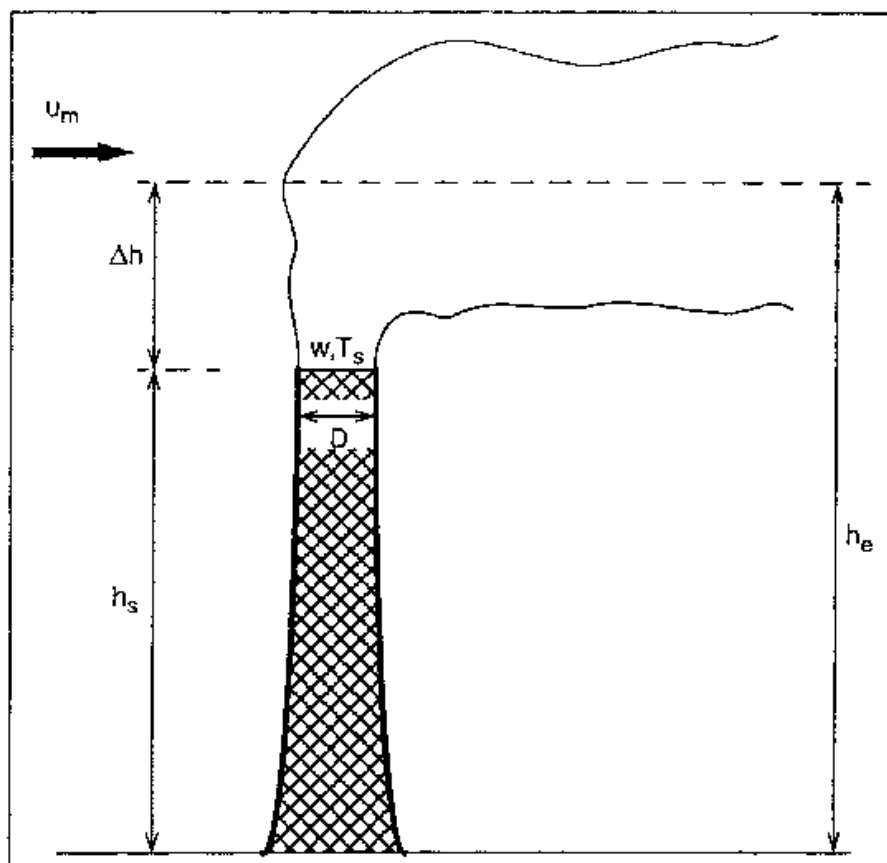


Figure 4C.1 Explanation of the different heights relevant for the plume rise calculation. The initial plume path height may be described as a function of horizontal distance from the source ( $X$ ):

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

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:

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

#### 4C.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).

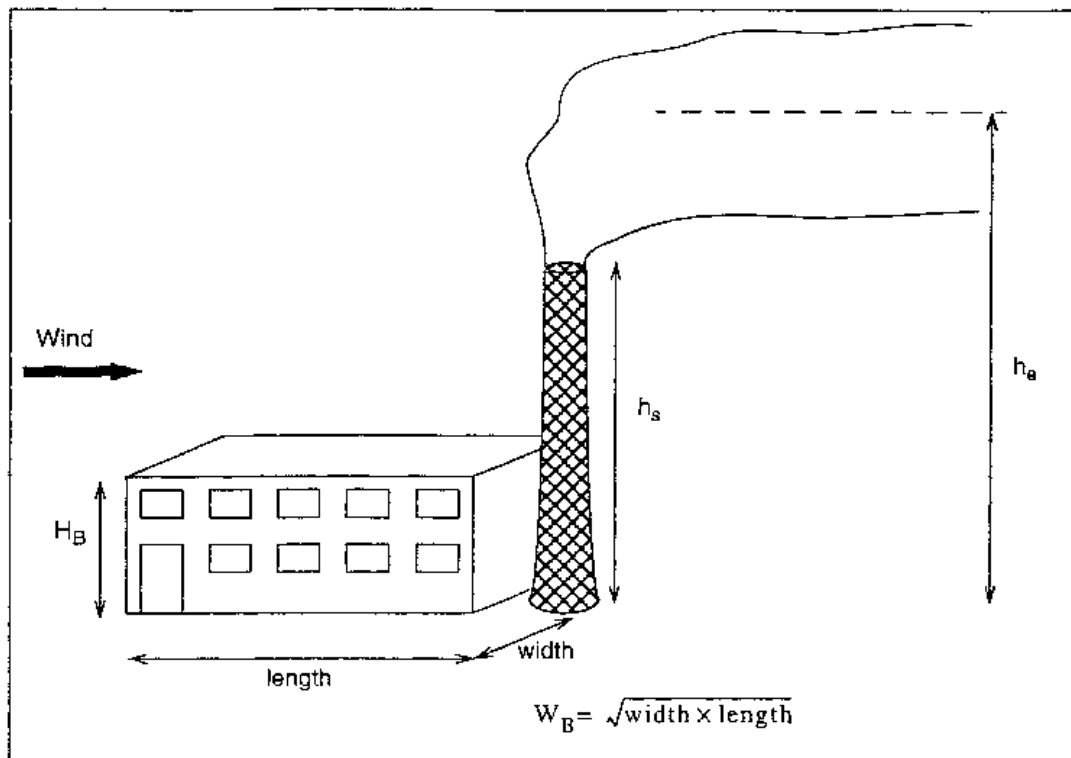


Figure 4C.2 Parameters of interest in the downwash calculation. Find  $\xi = \min(H_B, W_B)$ .

## 4C.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 and: 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

<sup>2</sup> 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  $\max[(3.57 - 0.53U), (0.667 \times \text{building height})]$ . The advection of the polluted air will follow trajectories in the wind field. For each emission point source, such a trajectory will constitute the plume centre line, i.e. a transformation to a Lagrangean coordinate system takes place. The Gaussian plume equation is solved along the trajectories (the standard plume model may be found in any textbook on atmospheric dispersion, e.g. Hanna et al., 1982):

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

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



## Appendix 4D: The Eulerian Advection-Diffusion Grid Model

### 4D.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 4A*). 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 4E: Street Canyon Model*).

### 4D.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

ρ = density of air, a function of height

u, v, w = wind velocity components

x, y, z = cartesian coordinates

w<sub>s</sub> = 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.

#### 4D.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:

$$c^* = A_x c^{t-1}$$

$$c^{**} = A_y c^*$$

$$c^{***} = A_z c^{**}$$

$$c^t = (A_c A_c) c^{***}$$

$$c^{t+*} = A_z c^t$$

$$c^{t+**} = A_y c^{t+*}$$

$$c^{t+1} = A_x c^{t+**}$$

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.

#### 4D.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.

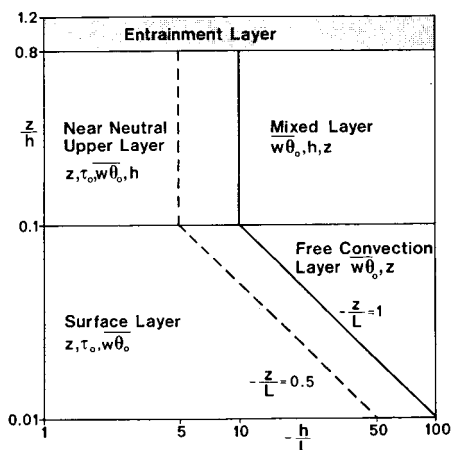
$$\zeta(\sigma) = a \left[ \frac{1}{\kappa} \ln \left( \left( \frac{\sigma + z_0}{z_0} \right) + \frac{\sigma}{b} \right) \right] + 1$$

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.

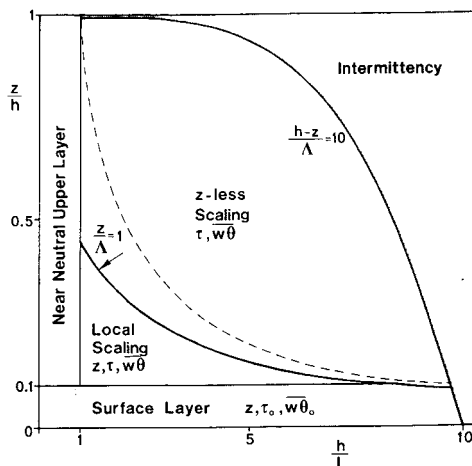
#### 4D.2.3 The Turbulent Exchange Coefficient

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

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

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

$$K_z(z) = 0.4u_{*l}\Lambda$$

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:

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

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

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

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

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

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

#### 4D.2.4 The Three-Dimensional Wind Field

The construction of the surface (two-dimensional) wind field is described in section *Appendix 4A: 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 another section. The profiles are distributed through the boundary layer up to the height  $mixh$ , the mixed layer height. Above  $mixh$  a free wind field, constant up to the top of the calculation domain, is assumed to prevail.

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

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

or, if the horizontal wind fields are evaluated directly in the  $\zeta$ -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.

#### 4D.2.5 Source Initialisation

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

The sources are distributed in the three-dimensional grid according to type and size. The source strength for a 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 *4C.3 Plume Rise Formulation*.

## 4D.3 Particle Deposition

### 4D.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

#### 4D.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).

#### 4D.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 *4D.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 4E: 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 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.

### 4E.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 lee wind 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 lee wind 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

$L_0$  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).

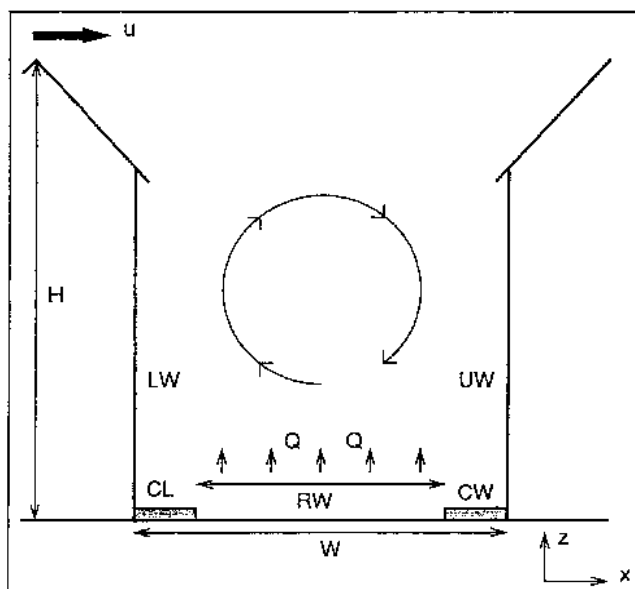


Figure 4E.1 Principles of air circulation within a street canyon (the upwind side is denoted  $UW$ , the leeward side  $LW$ , see also notations for house height ( $H$ ), street width between houses ( $W$ ) and road width ( $RW$ )).

## Appendix 4F: 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.

### 4F.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:

$$q_0 = A c_f G_0 \quad (\text{kg/s}) \quad (\text{eq 4F.1.1})$$

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

$$G(p) = \sqrt{\frac{P_0 - P}{v(p)}} \quad (\text{kg/s,m}^2) \quad (\text{eq 4F.1.2})$$

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:

$$M = q_0 u_0 + A(p - p_a) \quad (\text{N}) \quad (\text{eq 4F.1.3})$$

where  $u_0$  is the outlet velocity.

$$u_0 = \frac{q_0}{Av(p)} \quad (\text{m/s}) \quad (\text{eq 4F.1.4})$$

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

$$\text{- massflow } q(x) = C_1 \sqrt{M \rho_a x} \quad (\text{kg/s}) \quad (\text{eq 4F.1.5})$$

$$\text{- centre velocity } u_c(x) = C_2 \sqrt{\frac{M}{\rho_a}} \frac{1}{x} \quad (\text{m/s}) \quad (\text{eq 4F.1.6})$$

$C_1$  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 mass flow at that distance are given by equations 4F.1.6 and 4F.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  $p_0$ :

$$\frac{p_a}{p_0} \leq \left( \frac{2}{\kappa + 1} \right)^{\frac{\kappa}{\kappa + 1}}; \kappa = \frac{c_p}{c_v} \quad (\text{eq 4F.1.7})$$

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:

$$\text{- velocity } u_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} p_0 v_0} \quad (\text{m/s}) \quad (\text{eq 4F.1.8})$$

$$\text{- mass flux } q_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} \left( \frac{2}{\kappa + 1} \right)^{\frac{2}{\kappa - 1}} \frac{p_0}{v_0}} \quad (\text{kg/s}) \quad (\text{eq 4F.1.9})$$

otherwise, if condition 4F.1.7 is not fulfilled,

$$\text{- velocity } u_0 = \sqrt{2 \frac{\kappa}{\kappa + 1} \left[ 1 - \left( \frac{p_a}{p_0} \right)^{\frac{\kappa - 1}{\kappa}} \right]} \quad (\text{m/s}) \quad (\text{eq 4F.1.10})$$

$$\text{- mass flux } q_0 = \sqrt{2 \frac{\kappa}{\kappa - 1} \left[ \left( \frac{p_a}{p_0} \right)^{\frac{2}{\kappa}} - \left( \frac{p_a}{p_0} \right)^{\frac{\kappa + 1}{\kappa}} \right] \frac{p_0}{v_0}} \quad (\text{kg/s}) \quad (\text{eq 4F.1.11})$$

Using the jet equations 4F.1.3 to 4F.1.6, with the initial values given by equations 4F.1.8 to 4F.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:

$$u_g = C_3 \sqrt{gH \frac{\rho_p - \rho_a}{\rho_p}} \quad (\text{m/s}) \quad (\text{eq 4F.1.12})$$

$C_3$  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 an other place in this documentation, takes over and proceeds with the dispersion calculations (see appendix E3.2 in Airviro Specification Part II).

## 4F.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)):

$$A = C_4 V^{\frac{2}{3}} \quad (\text{m}^2) \quad (\text{eq 4F.2.13})$$

where  $V$  is the tank volume and  $C_4$  is a coefficient. The emission phase follows equations 4F.1.1 to 4F.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)):

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

$C_5$  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:

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

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.

### 4F.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):

Ammonium	$C_1 =$	0.284
Chlorine	$C_2 =$	7.21
Sulphur dioxide	$C_3 =$	1.0
Propane	$C_4 =$	0.05
Vinyl chloride	$C_5 =$	2.9
Methane	$C_6 =$	1.7

#### 4F.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 4G: Scenario Calculations

### 4G.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. 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).

### 4G.2 A Standard Method to Generate a Statistical Sample: **klmstat**

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

In order to achieve a climatology that reflects the local variation of weather conditions, more than one, preferably five years of monitoring data of the horizontal wind vector, the air temperature and the vertical temperature gradient from a meteorological mast is necessary. However, additional measurements of the standard deviation of the horizontal wind direction and of the vertical wind velocity, the solar radiation and the precipitation, are recommended. Provided that the monitoring data (described above) is available in the time series database, the **klmstat** program will extract a representative sample using the following technique:

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

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

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

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

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

### 4G.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.



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