Castor-AIR

Version 5.0

Air pollution dispersion modeling software

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IMPORTANT. READ ATTENTIVELY

Castor-AIR 5.0 FOR WINDOWS 95

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The CASTOR-AIR software estimates the dispersion of pollutants in the air. These types of numeric simulations are a method to estimate the contamination in an approximate way. Castor Software doesn't guarantee that the results obtained by this program coincide with the real concentrations that we can find in the air. The software, the used algorithms and the manual have been conscientiously examined of the possible existence of errors or omissions. Although we have checked the operation of CASTOR-AIR keeping in mind the results that we can find in the existent scientific literature on the area, Castor Software is not responsible for errors or omissions that we can find in the software, in the used calculation algorithms and in this manual. Castor Software is not responsible for losses or damages caused by the use of this software or of the user's manual. This software has been conscientiously examined of the possible existence of computer virus before its distribution.

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FOREWORD

The numeric algorithms that CASTOR-AIR uses gives us the possibility to study a great quantity of air pollutants that we find in our environment. The numerical method uses a equation that estimates the dispersion of the pollutants in the air.

The software admits meteorological data to establish the form of the polluting plume. The software calculates the pollutant concentration that is produced by each one of the sources and it considers the estates of the pollutant and the state of the winds. CASTOR-AIR carries out temporary averages (daily, monthly or annual) so that you can calculate the concentration average in each point of the affected area.

The system of simulation of processes of dispersion that CASTOR-AIR has, offers to the beginner and the expert programmer, a quick and practical system to evaluate the dispersion of pollutants in the air. The program is based on the operating system Microsoft WINDOWS where one works intensively with the mouse and the graphic windows. The bars of icons facilitate the realization of the different tasks of the program. We can say, with a certain security that the software CASTOR-AIR is one of the best tools, to carry out numeric simulations of air pollution processes. Without considering the experience that the user possesses in programming languages or in the use of simulation tools, in few minutes he will be able to have the first results.

This manual will describe the use and the possibilities of CASTOR-AIR that we will show with the use of examples. It is not strictly necessary possessing knowledge on the handling of the operating system of Microsoft WINDOWS although it is advisable. Along the user's manual we will simulate some air pollution processes whose development will illustrate the use of the program in the case of complex systems. We will describe the necessary steps for the study of a air pollution process with the software.

Finally, we will say that they exist in the scientific literature a great quantity of models to evaluate the dispersion of pollutants in the air. In this way, we will obtain numeric differences among the results of the program and the results of other numeric models. This is not strange since there are numeric differences among the different models of the scientific literature. The problem is that the dispersion is a complex physical phenomenon (that involves turbulences, non-linear dynamics and thermodynamic of the irreversible processes) and we want to simplify it with a simple equation. On the other hand, we will add that this approach type is, today per today, the most reasonable that we can think about to evaluate the air pollution.

1. Introduction

Our planet is fragile and limited as for its potential of generating the resources that the humanity requests and her capacity to absorb the residuals that we emit. The precariousness of the ecological and environmental resistance of the earth can end up threatening the humanity's development. IUICN, PNUMA, WWF and Agenda 21 plead insistently to reach the sustainable development. This admits a growth and an evolution of the carrying capacity of the ecosystems, without committing the necessities of the future generations, by means of the environmental administration of the different places of the Planet.

2. Administration and Environmental Impact

The environmental administration is based on two fundamental tools: the planning and the evaluation of the environmental impact. These two instruments are fundamental to coordinate the human activity and to maintain the quality of the environmental resources. The process of environmental planning combines the characteristics of each place with the possibilities of economic development. We will define administration objectives that will achieve the optimization of the use of the resources minimizing the impact generated on the environment. We will define the environmental impact that suffers a certain region as the difference among the future environmental situation of the place, after the realization of a project, and the environmental state of the area if this project had never taken place. The correct diagnosis of the impact demands to know all the elements implied in the environmental process. A study of environmental impact will also include a planning of the environmental surveillance of the project.

One of the fundamental physical systems for the study of the environmental quality of a region is the atmosphere. The atmosphere play a fundamental paper in the development of the life. In this software, we will center ourselves in the study and in the administration of the air quality.

3. The Atmosphere

The atmosphere supports photosynthesis and respiration. It is a source of nitrogen for nitrogen-fixing plants and nitrogen-fixing bacteria. The atmosphere transports air vapour and protect the Earth from cosmic rays and UV radiation. The atmosphere absorbs much of the infrared radiation, thus stabilising the Earth's temperature at a level which will support life. Short-term changes are described as weather and long-term changes as climate. The movement of masses of air that occurs horizontally is called wind. It takes place from regions of high pressure to regions of lower pressure. The movement of air masses transfer heat from the ocean to land. The temperature of the atmosphere varies with height and forms the basis for one classification of the atmosphere into layers.

3.1 The Greenhouse effect

Energy is received by the Earth from the Sun and is radiated back into space. Earth temperature is maintained at an average of 15 degrees. A mechanism for doing this is the greenhouse effect. Energy is lost from the Earth by conduction and radiation. In fact, about half of the solar radiation which enters the atmosphere reaches the Earth surface. An increase in the carbon dioxide level of the atmosphere could prevent sufficient energy loss and cause a damaging increase in the Earth temperature. Other greenhouse gases are methane, dinitrogen oxide, carbon monoxide, ozone and CFCs.

3.2 The Ozone layer

There is a layer of ozone in the Stratosphere and there is a natural balance which keeps the ozone layer at a constant thickness. It is effective in filtering out dangerous UV-B radiation (290-320 nm). Ozone is destroyed by chemical reactions with a number of substances that occur naturally in the Stratosphere. Man-made substances are now attacking the ozone layer and reducing its thickness.

4. Air pollution

Waste matter is released into the atmosphere from a variety of pollutant sources. Atmospheric pollutants area serious threat to health. The pollutants present in the atmosphere are: particulate solids, droplets of liquids and gases. It is convenient to classify pollutants as primary pollutants which are emitted directly into atmosphere and secondary pollutants which are formed in the atmosphere from primary pollutants.

4.1 Particles

Parcicules, alternately referred to as Particle Matter (PM). Aerosols or fine particles are tiny particles of solid or liquid suspended in the air. They range in size from 10 nm (nanometer) to 100 um (micrometer) in diameter. The composition of fine particles depends on the source. The deposition site is a function of particle size. Larger particles are generally filtered by the nose and do not cause problems, but particulate matter smaller than about 10 micrometres (PM_{10}) can settle in the lungs and cause health problems. Particles emitted from modern vehicle engines are typically in the size range of 100 nanometres.

4.2 Lead

Lead enters the air from lead tetraethyl which is added to petrol as an antiknock. Lead from atmosphere pollutes the land. Vehicles exhausts are the chief source of lead pollution.

4.3 Carbon monoxide

Carbon monoxide, which is primarily emitted from combustion process, particularly from vehicle exhausts; the highest concentrations are generally found at roadside locations. Inhalation of high levels of carbon monoxide can cause headaches and respiratory problems. Carbon monoxide has many common sources. The exhaust of the internal combustion engine, when burning a carbon-based fuel contains carbon monoxide. In the home, carbon monoxide (CO) gas forms when fuels like natural gas or wood do not burn completely in appliances such as air heaters, ranges and ovens.

4.4 Sulphur dioxide

Sulfur oxides, which causes acid rain is caused from the burning of fuel containing sulfur, mostly at power plants. Sulphur dioxide reacts with air doplets to form acid rain.

4.5 Oxides of nitrogen

Emissions are primarily in the form of NO, which is oxidised by ozone (O3) from nitric oxide to NO2. Nitrogen dioxide (NO2) is the primary concern for effects on health. The various oxides of nitrogen can also react with hydrocarbons in the atmosphere to contribute to photochemical smog. Oxides of nitrogen can also affect ecologically sensitive sites through deposition, causing acidification. The term nitrogen oxide can be used to refer to any of these oxides (oxygen compounds) of nitrogen: Nitric oxide (NO); Nitrogen dioxide (NO_2); Dinitrogen oxide (N_2O) (Nitrous oxide); Dinitrogen trioxide (N_2O_3); Dinitrogen tetroxide (N_2O_4); Dinitrogen pentoxide (N_2O_5). A mixture is often formed in chemical reactions that produce nitrogen oxides, with the proportions depending on the specific reaction and the conditions it is performed in. When dissolved in atmospheric moisture the result can be acid rain which can damage both trees and entire forest ecosystems.In atmospheric science the term NOx is used to mean the total concentration of NO plus NO2. During daylight NO and NO2 are in equilibrium with the ratio NO/NO2 determined by the intensity of sunshine (which converts NO2 to NO) and ozone (which reacts with NO to give back NO2). Three primary sources of Oxides of nitrogen formation in combustion processes are: prompt NO, fuel NO and thermal NO. Thermal NO_x formation is recognized as the most relevant source when combusting natural gas.

4.6 Acid rain

Acid rain is defined as rain with a pH of below 5.6. Normal rain has a pH of slightly under 6, which is slightly acidic. This natural acidity is caused by dissolved carbon dioxide. Acid rain is caused by sulfur from impurities in fossil fuels and nitrogen from the air combining with oxygen to form sulfur dioxide and nitrogen oxides. These diffuse into the atmosphere and react with air to form sulfuric and nitric acids which are soluble and fall with the rain. Some The resulting increased acidity in soil has proven to be harmful to vegetation. Principal sources are industrial and power-generating plants and transportation vehicles. The gases may be carried hundreds

of miles in the atmosphere before they are converted to acids and deposited.Since the industrial revolution, emissions of sulfur and nitrogen oxides to the atmosphere have increased. Industrial and energy-generating facilities that burn fossil fuels, primarily coal, are the principal sources of increased sulfur oxides. The toxic ions released due to acid rain form the greatest threat to humans.

4.7 Organic pollutants

Volatile organic compounds are organic chemical compounds that have high enough vapour pressures under normal conditions to significantly vaporize and enter the atmosphere. A wide range of carbon-based molecules, such as aldehydes, are volatile organic compounds. Common artifical sources of volatile organic compounds include paint thinners, dry cleaning solvents, and some constituents of petroleum fuels. Volatile organic compounds are an important outdoor air pollutant. In this field they are often divided up into the separate categories of methane (CH4) and non-methane. Methane is an extremely efficient greenhouse gas which may contribute to enhanced global warming. Within the non-methanes, benzene may lead to leukaemia through prolonged exposure. 1,3-butadiene is another dangerous compound which is often associated with industrial uses. Volatile organic compounds are often used in paint, plastics, and cosmetics.

4.8 Photochemical smog

Photochemical smog is caused when two kinds of air pollution combine in the presence of sunlight. The first kind is the particulates and nitric oxides from the exhaust of fossil fuel-burning engines in cars and coal power plants. The second kind is the emission of volatile organic compounds from paints, solvents, and other chemicals. Smog is a problem in a number of cities and continues to harm life. High levels of smog aggravate and even cause human respiratory problems.

5. Air quality and pollutant emissions

CASTOR-AIR software uses g/m3 in the input data window. If the pollutant concentrations are in parts per million (ppmv), we can change to ug/m^3 as follows:

(c in micrograms per cubic meter)=M/0,02404 (c in ppmv)

being M the molecular mass of the pollutant. At 20C (Celsius degrees) and at 1 atm, we have the next relations that can be useful:

pollutant	*ppmv*	*micrograms/m^3*
SO_2	*1*	*2610*
CO	*1*	*1140*
NO_2	*1*	*1880*
H_2S	*1*	*1390*

5.1 Air quality indexes

There are different air quality indexes in the world. The ORAQI air quality index has the next upper limits:

Pollutant	SO_2	*Particulate matter*	NO_2	C_xH_y	CO	Pb
concentration (ug /m^3)	*350*	*250*	*200*	*140*	*20,000*	*4*

The World Health Organization, Federal and Germany air quality indexes have the next upper limits:

Pollutant	Period	Federal	WHO	Ta Luft (Germany)
CO	15 min 30 min 1 h 8 h	 40,000 ug/m³ 10,000 ug/m³	100.000 ug/m³ 60.000 ug/m³ 30.000 ug/m³ 10.000 ug/m³	 30.000 ug/m³ 10.000 ug/m³
NO_2	1 h 24 h annual	 100 ug/m³	400 ug/m³ 150 ug/m³	200 ug/m³ 80 ug/m³
O_3	1 h 24 h 100 days	235 ug/m³	200 ug/m³ 65 ug/m³ 60 ug/m³	
SO_2	10 min 1 h 3 h 24 h annual	 1,300 ug/m³ 365 ug/m³ 80 ug/m³	500 ug/m³ 350 ug/m³ 125 ug/m³ 40 - 60 ug/m³	 400 ug/m³ 140 ug/m³ 60 ug/m³
PM-10	24 h anual	150 ug/m³ 50 ug/m³	125 ug/m³ 50 ug/m³	150-300 ug/m³
SO_2+PM-10	annual		60 - 90 ug/m³	
Pb	3 months anual	1,5 ug/m³	 0,5 - 1 ug/m³	 2 ug/m³
PM + PM-10	24 h annual	260 ug/m³ 75 ug/m³		
Hydrocarbons	3 h	160 ug/m³		

5.2 Pollutant emissions

In this section, we will show typical emission values that can be used as input data in the CASTOR-AIR software:

Typical coal boiler emissions:

Coal boiler power	Coal kg per second (kg/s)	SO_x	NO_x	CO
100 MW	3,3 g/s	201 g/s	48 g/s	0,8 g/s
500 MW	16,5 g/s	1.005 g/s	240 g/s	4 g/s
1.000 MW	33 g/s	2.010 g/s	480 g/s	8 g/s
1.500 MW	49,7 g/s	3.023 g/s	721 g/s	12,4 g/s
2.000 MW	66 g/s	4.020 g/s	960 g/s	16 g/s

Typical fuel oil boiler emissions:

Boiler power	Fuel oil liters per second (L/s)	SO_2	NO_x	CO
50 MW	1,2 g/s	72 g/s	6,7 g/s	0,7 g/s
100 MW	2,4 g/s	144 g/s	13,4 g/s	1,4 g/s
150 MW	3,6 g/s	210 g/s	20,2 g/s	2,1 g/s
200 MW	4,8 g/s	280 g/s	26,8 g/s	2,8 g/s
300 MW	7,2 g/s	432 g/s	40,2 g/s	4,2 g/s

Typical butane boiler emissions:

Boiler power	Liters of butane per second (L/s)	SO_x	NO_x	CO
3 MW	0,11 g/s	0,0079 g/s	0,28 g/s	0,047 g/s
10 MW	0,37 g/s	0,027 g/s	0,93 g/s	0,159 g/s
20 MW	0,74 g/s	0,053 g/s	1,86 g/s	0,32 g/s
30 MW	1,1 g/s	0,079 g/s	2,77 g/s	0,47 g/s

Typical road emision:

Number of vehicles per hour	CO (g/ms)	NO_x (g/ms)	C_xH_y (g/ms)
100	0,00028	0,00009	0,000028

1.000	0,0028	0,0009	0,00028
5.000	0,014	0,0042	0,0014
10.000	0,028	0,009	0,0028
50.000	0,135	0,042	0,0135
100.000	0,28	0,09	0,028

Number of vehicles per day	CO (g/ms)	NO_x (g/ms)	C_xH_y (g/ms)
1.000	0,000116	0,0000375	0,0000116
5.000	0,00058	0,00019	0,000058
10.000	0,00116	0,000375	0,000116
50.000	0,0058	0,0019	0,00058
100.000	0,0116	0,00375	0,00116

6. Before you begin

Welcome to CASTOR-AIR - software for air dispersion modeling. The CASTOR-AIR software allows you to create robust and useful numeric simulations that fully make use of the graphical user interface. This chapter show you how to sep up CASTOR-AIR on your computer.

We can say, with a certain security that the software CASTOR-AIR are one of the best tools, if not the best and simpler, to carry out numeric simulations of pollutant emissions into the air. It takes just a few minutes to build your first numerical simulation.

Due to the features of the software that allows to simulate the process of air pollution dispersion immediately, the numeric simulation is carried out with a remarkable speed.

You create the graphical interface for your pollutant stacks by drawing point sources in a graphical way. You create the simulation process by drawing point sources, such as stacks, on the CASTOR-AIR window. Next, you set properties for the point sources and ambient data to specify such values as temperature, pollutant concentration,… Finally, the numeric simulation is carrier out.

6.1 CASTOR-AIR Software

Before you attempt to install and use the program, make sure your personal computer meets the hardware and software requirements shown in the following table.

- System requirements: Windows 95, 98, 2000 and XP
- CD-ROM drive
- RAM Memory: 16MB or higher

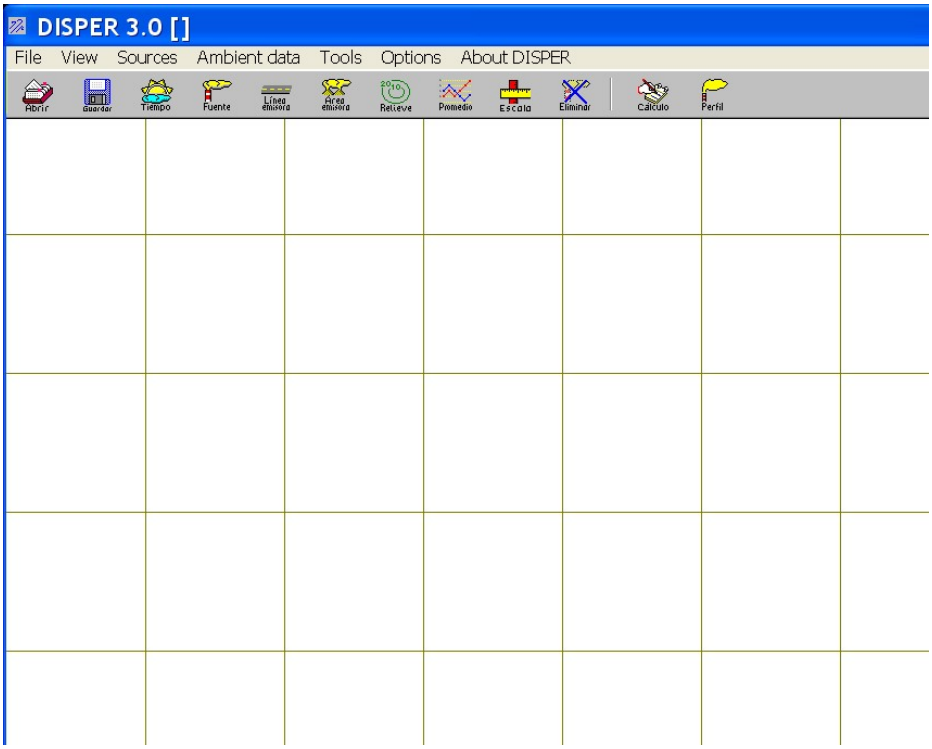
6.2 Installation

- Insert the CD. The CASTOR-AIR CD window appears on your screen.
- Click the button labeled **SETUP** and follow the instructions on the screen.

If the CASTOR-AIR CD window does not appear, the CD autorun feature might be disabled on your computer. To install CASTOR-AIR, open the CD-ROM drive icon, open the PC directory, and double-click the Installer icon.

6.3 Starting CASTOR-AIR

Click Start, go to Programs, and choose CASTOR-AIR 5.0. Here is the program window after startup.



The window has a Menu bar at the top, a Status bar at the bottom and a basic tool bar in the window. The program commands are available through the menus and toolbar buttons. Some commands have associated dialog boxes which you can choose additional options.

7. Understanding the Workplace

The MS Windows bar doesn't appear. In this way, you have more space to draw. However, and if you want, you can modify the properties of the MS Windows bar in the Microsoft Windows system. The program window size is fixed and it cannot modify. The menu bar lists the menus shown above. When you choose one of the menus, the program displays a pull-down list of available commands. The menu bar lists: **File**, **View**, **Sources**, **Ambient data**, **Tools**, **Options** and **About CASTOR-AIR**. The program window has a basic tool bar at the top.

In the center of the program window, we will draw and we will calculate the different polluting processes. We can draw using two different planes: parallel to the land surface (XY) and perpendicular to the land surface (XZ). There is a grid in the XY-plane. The coordinate origin is on the left bottom corner (X=0, Y=0) in XY-planes (parallel to the land surface). In addition, the coordinate origin is on the left bottom corner (X=0, Z=0) in XZ-planes (perpendicular to the land surface).

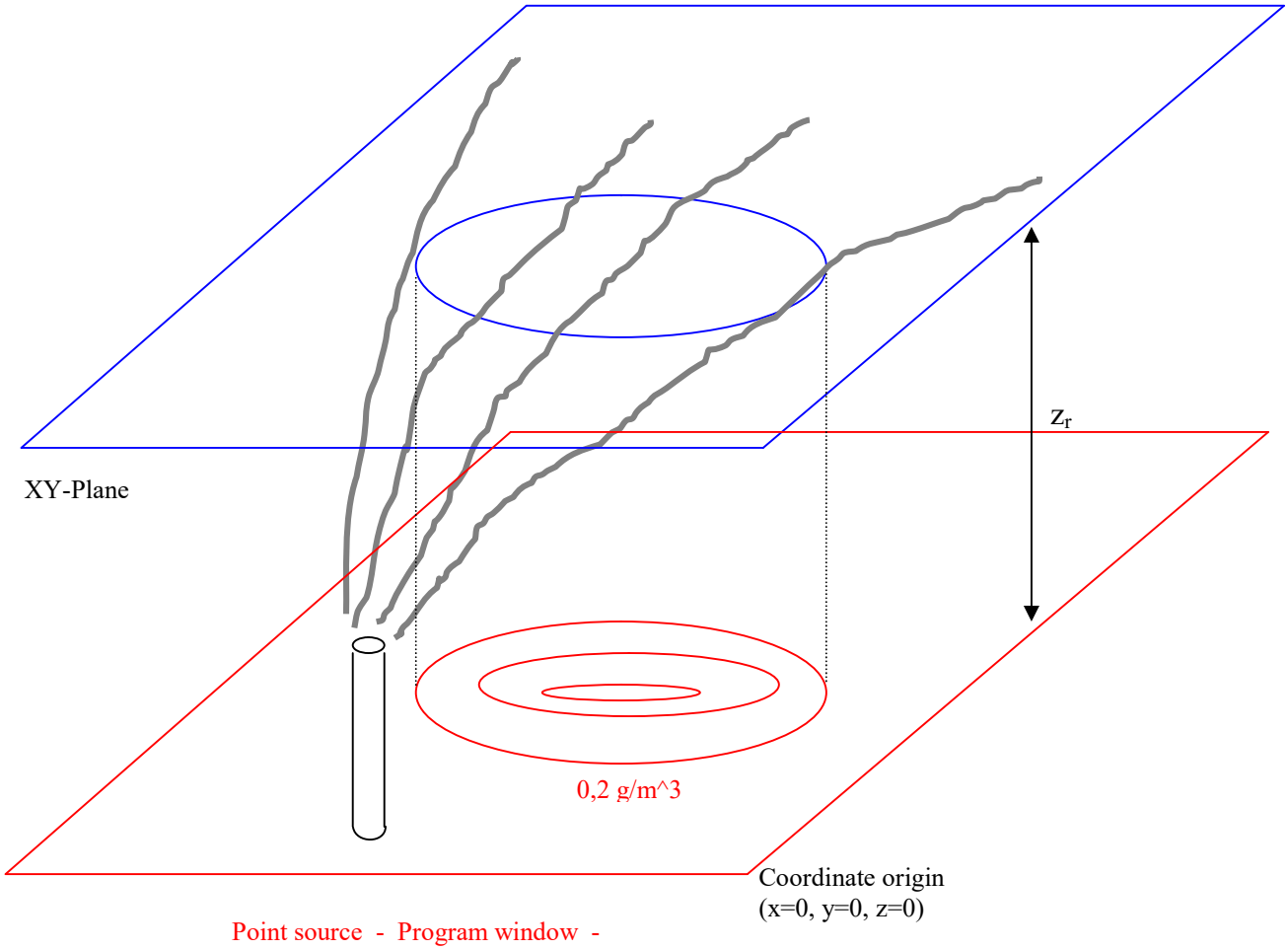
XY-Plane (parallel to land surface):

In such a case, the program window is a XY-plane (parallel to the land surface). A pollutant point source (stack) is represented by a small square.

In the Status bar at the bottom, we have X,Y and Z coordinate values in meters and data on our environmental system. Point the mouse where you want in the program window and the X,Y and Z values will be shown in the status bar at the bottom. If you select XY-Plane, a grid appears.

On the left bottom corner, two different text boxes appear: The position of the XY-plane with respect to the land surface (XY-plane height) and the pollutant concentration value (micrograms per cubic meter, ug/m³). Point the mouse where you want in the program window and the concentration value will be shown in the text box. Remember that 1g/m³=1mg/L.

The pollutant concentrations will be calculated in a parallel plane to the land surface (XY-Plane). The plane height will be determined by the user (z_r).

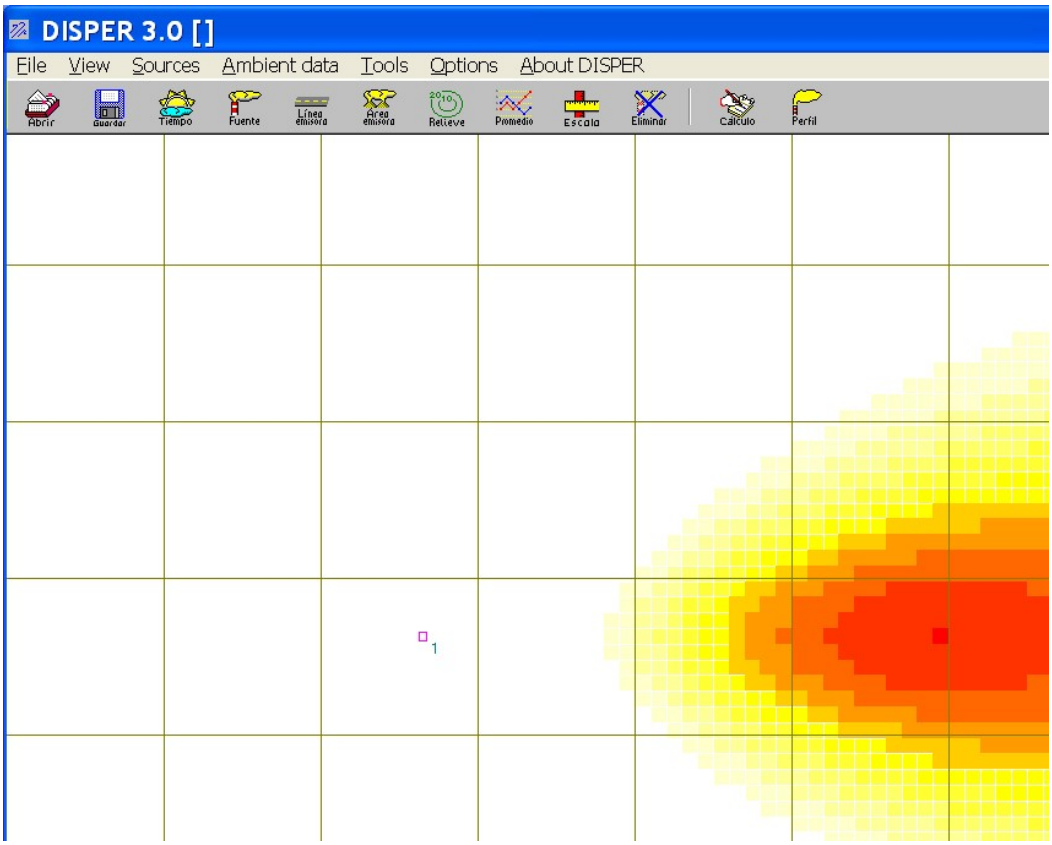


Point source - Program window - Plane representation

All the points of the XY-plane will be to a z_r height. The z_r value is chosen by the user before the calculation. We will be able to make many calculations considering different plane heights. The different plane heights will be determined by the user (z_r values). In this way, the physical form of the pollutant plume can be studied.

Example: Calculation in the XY-plane, zr=0 (height of the land surface). The red square represents a point source (position

of the pollutant stack). The red colour represents high pollutant concentrations.



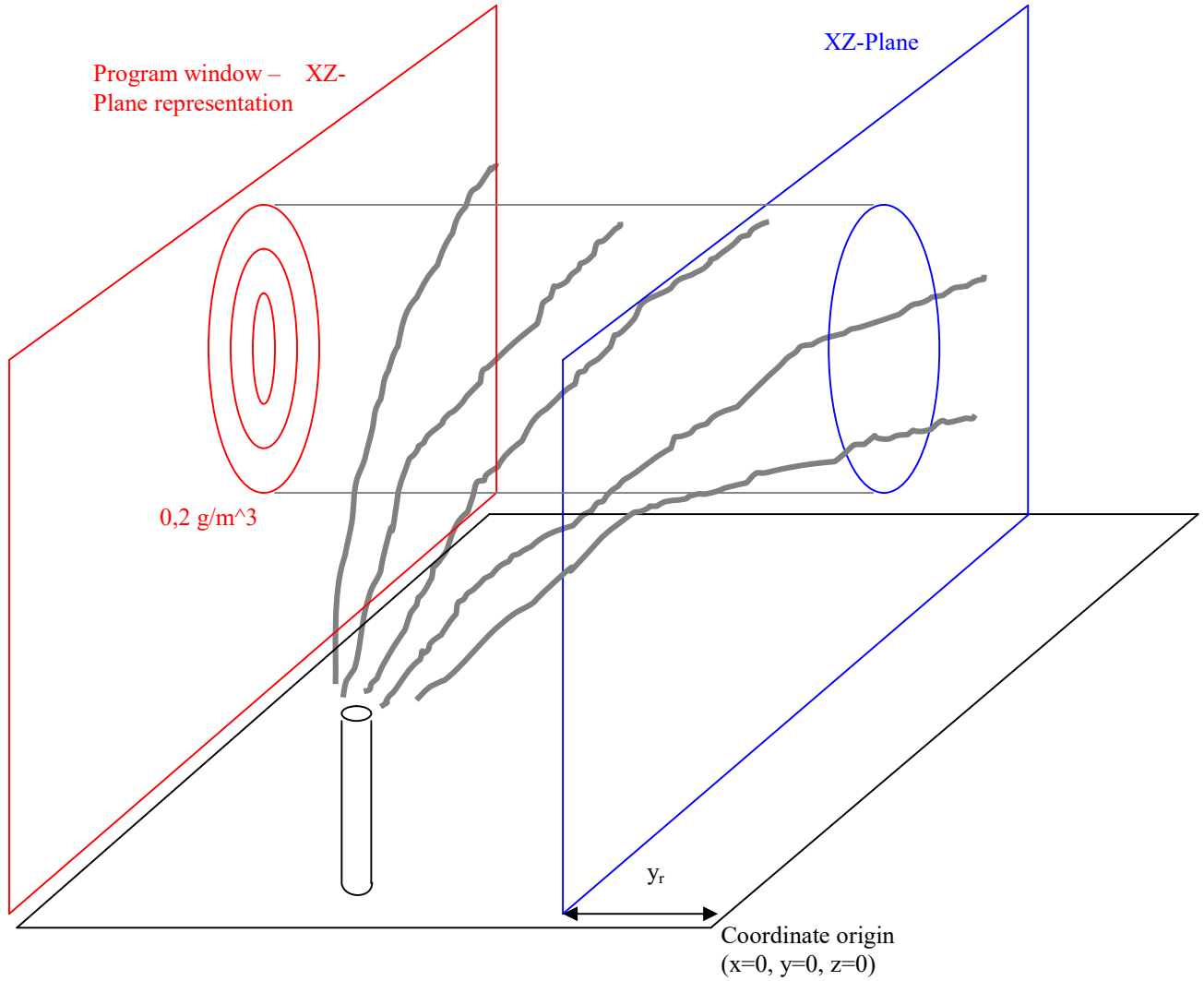
XZ-Plane (perpendicular to land surface):

In such a case, the program window is a XZ-plane (perpendicular to the land surface). A pollutant point source (stack) is represented by a small square.

In the Status bar at the bottom, we have X,Y and Z coordinate values in meters and data on our environmental system. Point the mouse where you want in the program window and the X,Y and Z values will be shown in the status bar at the bottom.

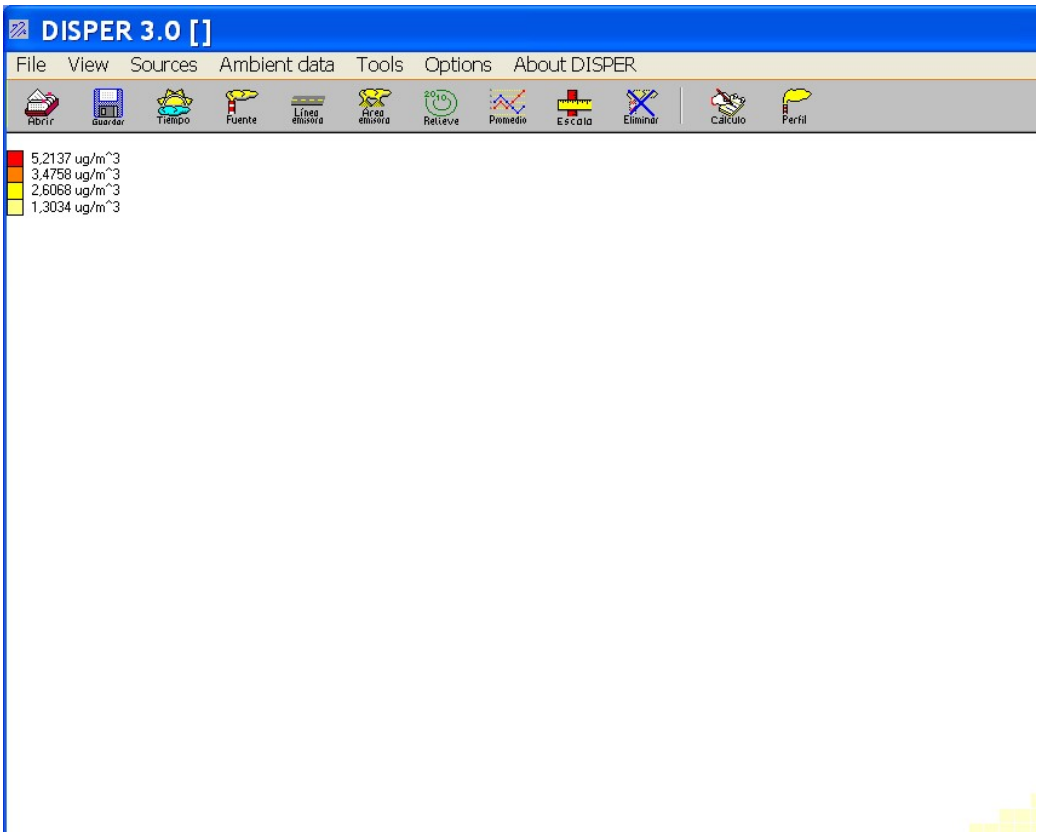
On the left bottom corner, a text box appears: the pollutant concentration value (micrograms per cubic meter, ug/m³). Point the mouse where you want in the program window and the concentration value will be shown in the text box. Remember that 1g/m³=1mg/L.

The pollutant concentrations will be calculated in a perpendicular plane to the land surface (XZ-Plane). The plane height will be determined by the user (y_r).

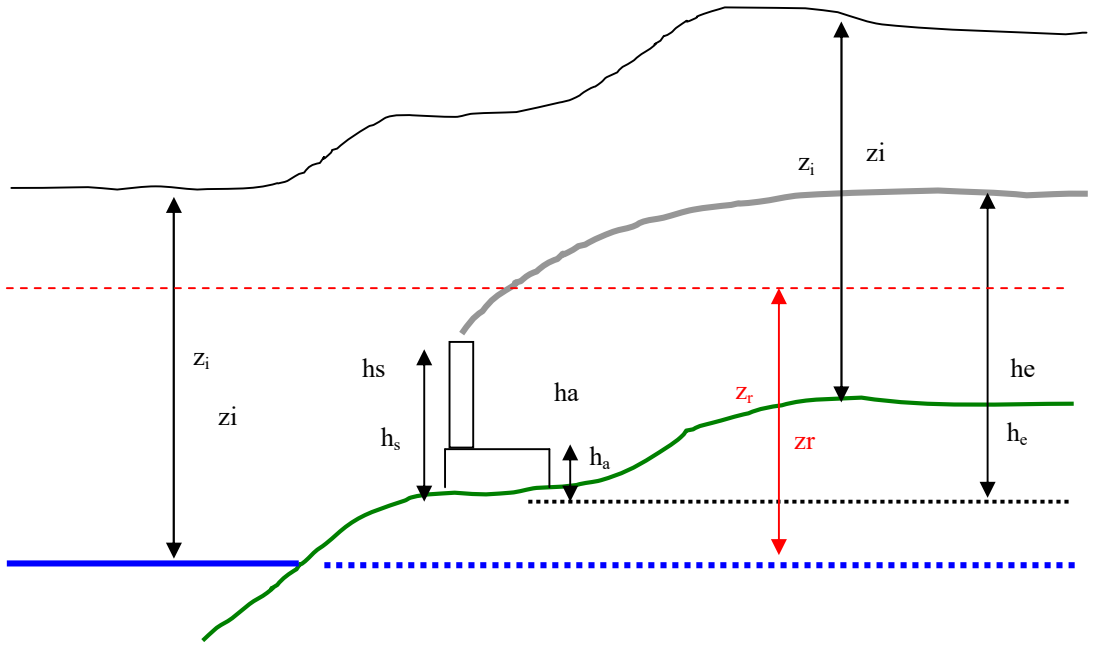


All the points of the XZ-Plane will be to a y_r height. The y_r value is chosen by the user before the calculation. We will be

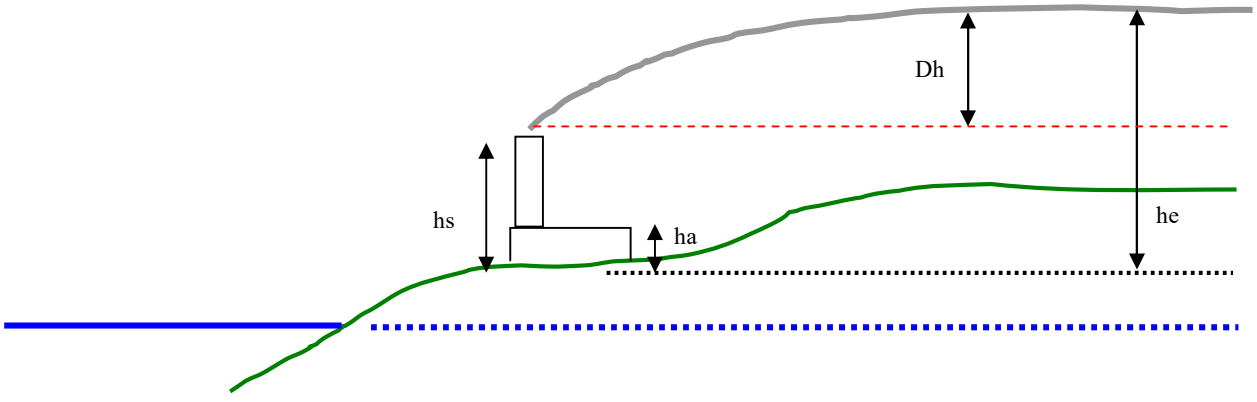
able to make many calculations considering different plane heights. The different plane heights will be determined by the user (y_r values). In this way, the physical form of the pollutant plume can be studied. Example: Calculation in the XZ-plane. The fuchsia strip represents a point source (position of the pollutant stack). The green line represents land surface. The red colour represents high pollutant concentrations.



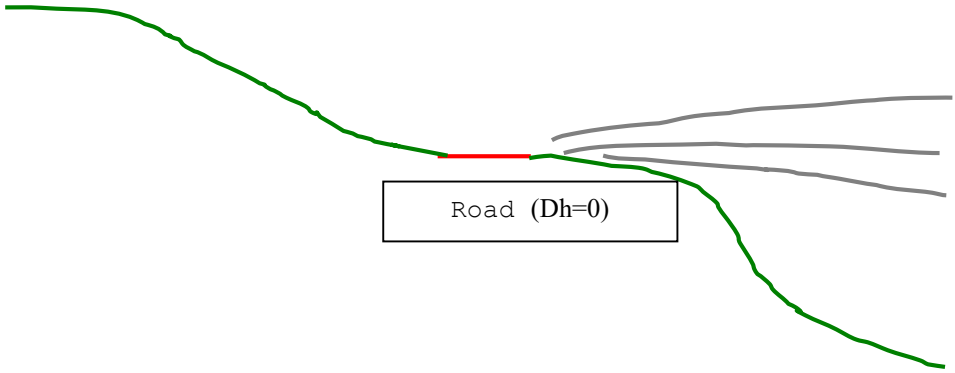
We will show you a typical calculation diagram: a Stack (point source) in elevated terrain.



zi=mixing height
hs=snack height
he=plume height
ha=anemometer height
zr=calculation plane height



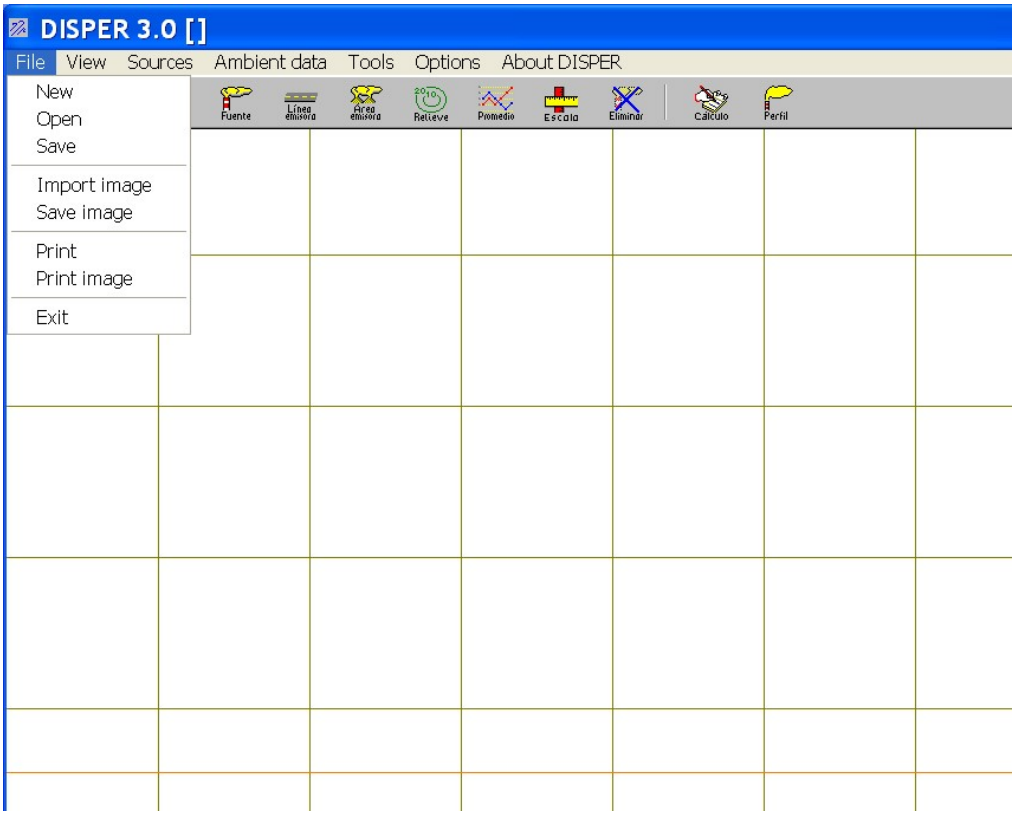
where Dh is the effective plume height.In the line and area source cases, we have that the effective plume height is zero (Dh=0). For example:



7.1 Menu Bar

Display the commands you use to build your simulation. When you choose one of the menus, the program displays a pull-down list of available commands. The program window has a basic tool bar under the Menu bar. The tool bar provides quick access to commonly used commands in the program. You click a button on the toolbar once to carry out the action represented by that button.

For example, when you choose **File** in the Menu bar, the program displays:



7.1.1 File

The File Menu contains the tools you use to open, close and save new and existing files, and import and export graphics. The File Menu lists: **New**, **Open**, **Save**, **Import Picture**, **Export Picture**, **Print**, **Print Picture** and **Exit**.

New.- This command is to begin a new simulation, deleting all that has been made previously.

Save the work with the Save command before clicking the New command. The program doesn't allow to open two files at the same time. This way, we can optimize the available memory and the calculation speed.

Open.- This command is to open an existing file. The program files exist as separate files with **.sim** filename extension.

Save the current work with the Save command before clicking the Open command. The program doesn't allow to open two files at the same time.

Save.- This command is to save an existing result.

The process of saving a file is carried out proportionally to the size in which the elements are drawn in the screen. Then, the saved file will depend on the screen format that we are using (for example, 1280x1024,...). If we try to read a file, saved in another different computer, we will have problems to open it.

Import Picture.- With this command you will be able to import images and pictures (previously saved BMP files). These images will be background pictures and images for your program window. You can display an image by double-clicking the filename of a bitmap (BMP).

Many programs and computer applications (AutoCad, 3d Studio, ArcView,...) export BMP files. You will be able to load pictures and images generated by these programs.

The displayed image size will depend on the size that had when it was saved. If it is necessary, modify the picture size before loading the image (for example, you can use windows Paint, Adobe Photoshop,…). You will be able to load BMP maps generated by AutoCad.

Bitmaps and scanned maps must be loaded into memory and then adapted to the program scale (we will make use of the **Scale** command). The X-Axis width (meters) in the program window can be easily changed to be able to compare both images (simulation results and background maps). Then, the X-Axis width (in meters) of the imported map and the X-Axis width (in meters) of the program window match together. The imported images are not stored physically in the simulation process. Terrain elevations (represented on the imported map) don't interact in the simulation process. We haven't the possibility

to zoom an imported map with the **Zoom** command. This command only acts in the calculation process. If it is necessary, zoom the map before loading the image.

Export Picture.- With this command you will be able to export images and pictures (BMP files). These images will contain the background picture and the simulation results.

Many programs, computer applications and word processors (AutoCad, 3d Studio, ArcView, MS Word,...) import BMP files. You will be able to load images generated by CASTOR-AIR.

Print.- The users' printer drivers and printers impact print quality. With this command you can send graphics and text (of the simulation results) to a printer. This command provides the best printing quality across a variety of printers because Windows translate text and graphics from the device-independent drawing space to the Printer object to best match the resolution and abilities of the printer. However, the background pictures cannot be printed.

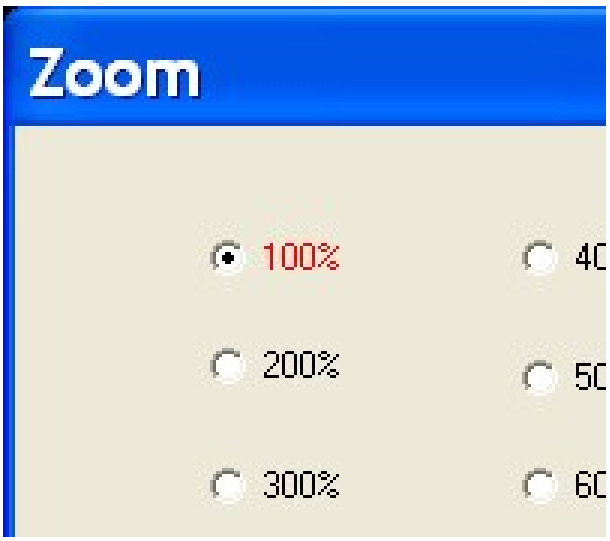
Print image.- This command send a pixel-by-pixel image of the program window to the printer. To print with **Print image** command, you must first display that information on the program window and then print with this command. This command is by far the easiest way to print from your application. Because it may send information to the printer at the resolution of the user's screen (typically 96 dots per inch), results can be disappointing on printers with much higher resolutions (typically 300 dots per inch for laser printers).

Exit.- The **Exit** command allows you to exit directly from the application.

7.1.2 View

The View Menu contains the tools you use to view your computer screen. The File Menu lists: **Zoom**, **Black background**, **White background**, **Draw grid lines**, **Eliminate grid lines**, **Draw picture**, **Eliminate picture**, **XY View** and **XZ View**.

Zoom.- We have the possibility to zoom a part of the program window with the **Zoom** command. However, we won't be able to enlarge background pictures with this command. If it is necessary, zoom the map before loading the background image. This command only acts in the calculation process. This way, we can place a point source in a side of the computer screen and we can calculate the concentrations in another different detailed region.



To activate the **Zoom** command, eliminate the background picture first.

Black background.- The Black background command allows you to have a black background colour in your screen.

White background.- The White background command allows you to have a white background colour in your screen.

Draw grid lines.- If you select **Draw grid lines** command, the grid appears.

Eliminate grid lines.- If you select **Eliminate grid lines** command, the grid disappears.

Draw picture.- With this command you will be able to see background images and pictures (previously loaded BMP files).

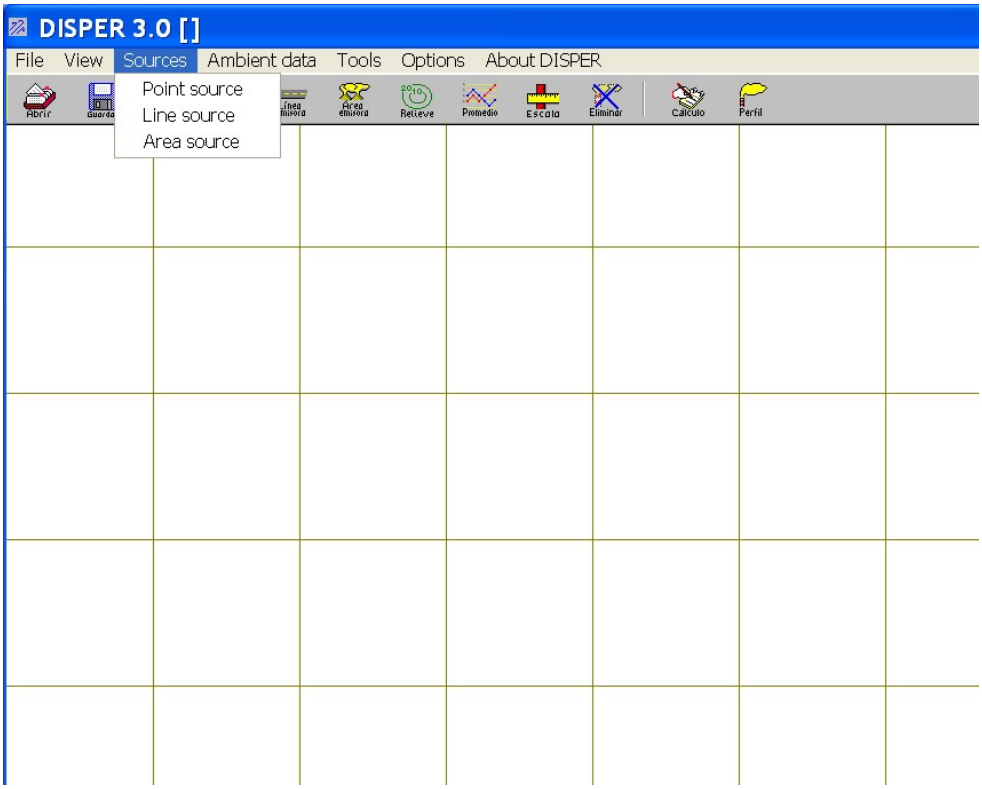
Eliminate picture.- With this command you will eliminate background images and pictures (previously loaded BMP files).

XY View.- With this command, you can draw using a plane that is parallel to the land surface (XY).

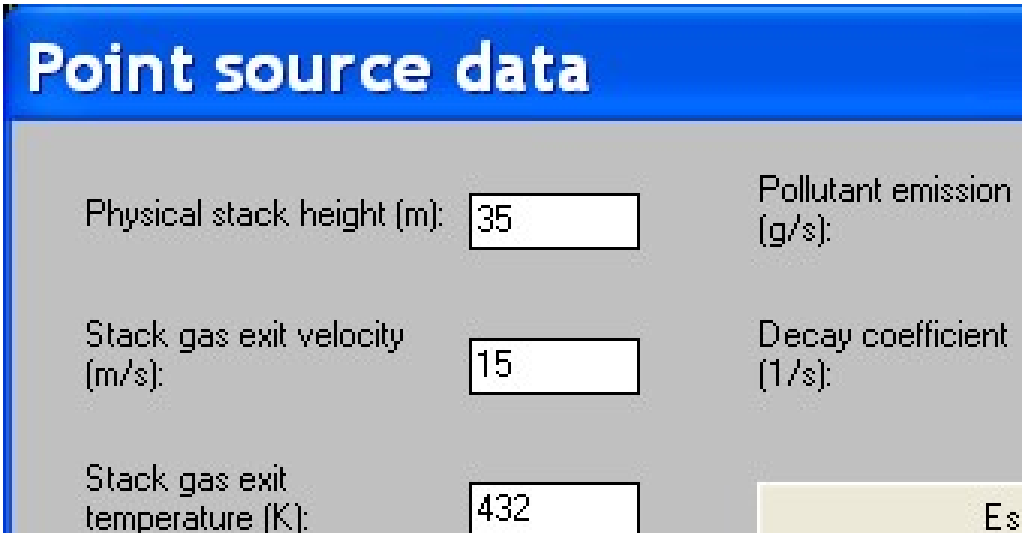
XZ View.- With this command, you can draw using a plane that is perpendicular to the land surface (XZ).

7.1.3 Source

The **Point source** Menu lists the possible pollutant sources: the point source, line source and area source.



Point source.- This is a pollutant point source. The stack size is small if we compare it with the size of the area in which we are simulating (point source). If you click this button, the next dialog box is shown:



The necessary data is:

Physical stack height (m): This is the physical stack height in meters.

Stack gas exit velocity v_s (m/s): This is the stack gas exit velocity. It can be around 15 m/s.

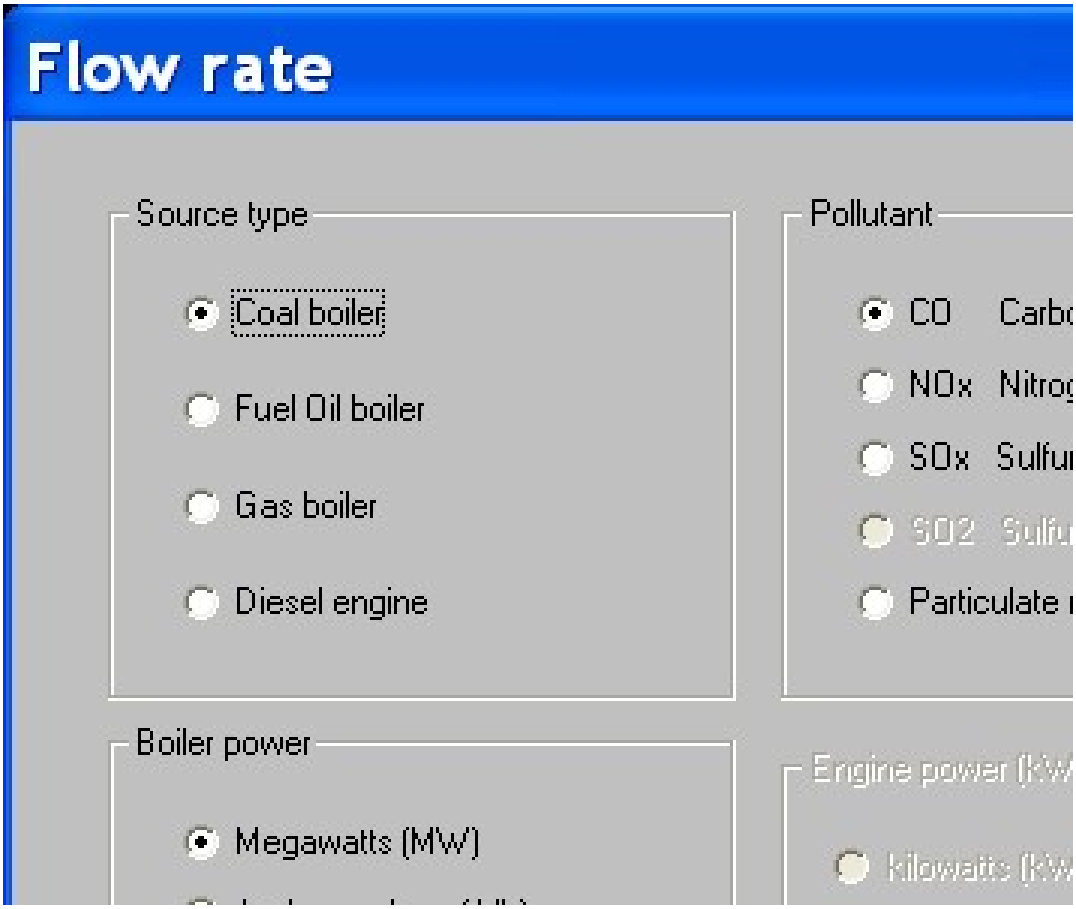
Stack gas exit temperature (K): The discharge concentration of the material of interest (pollutant or tracer) is defined as the excess concentration above any ambient concentration of that same material. $1g/m^3$=1ppm in air.

Stack inside diameter (m): This is the stack inside diameter.

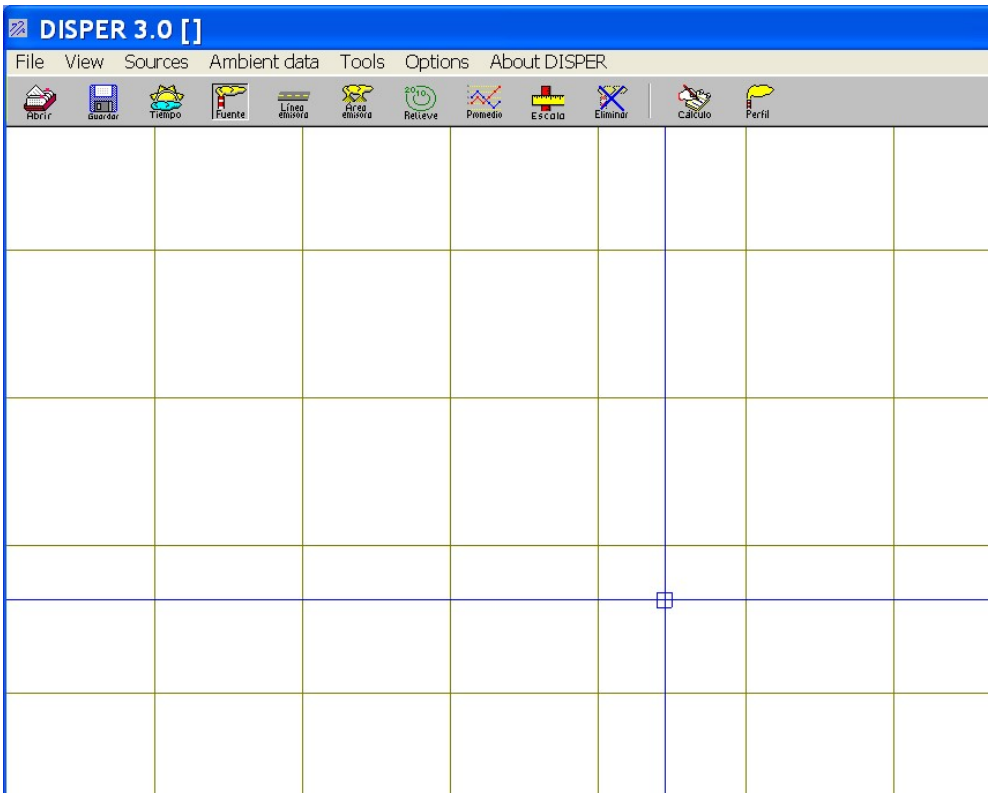
Pollutant emission rate (g/s): This is the pollutant emission rate.

Decay coefficient (1/s): This coefficient considers the half life of the pollutant if this disappears by means of chemical reactions (non-conservative pollutant).

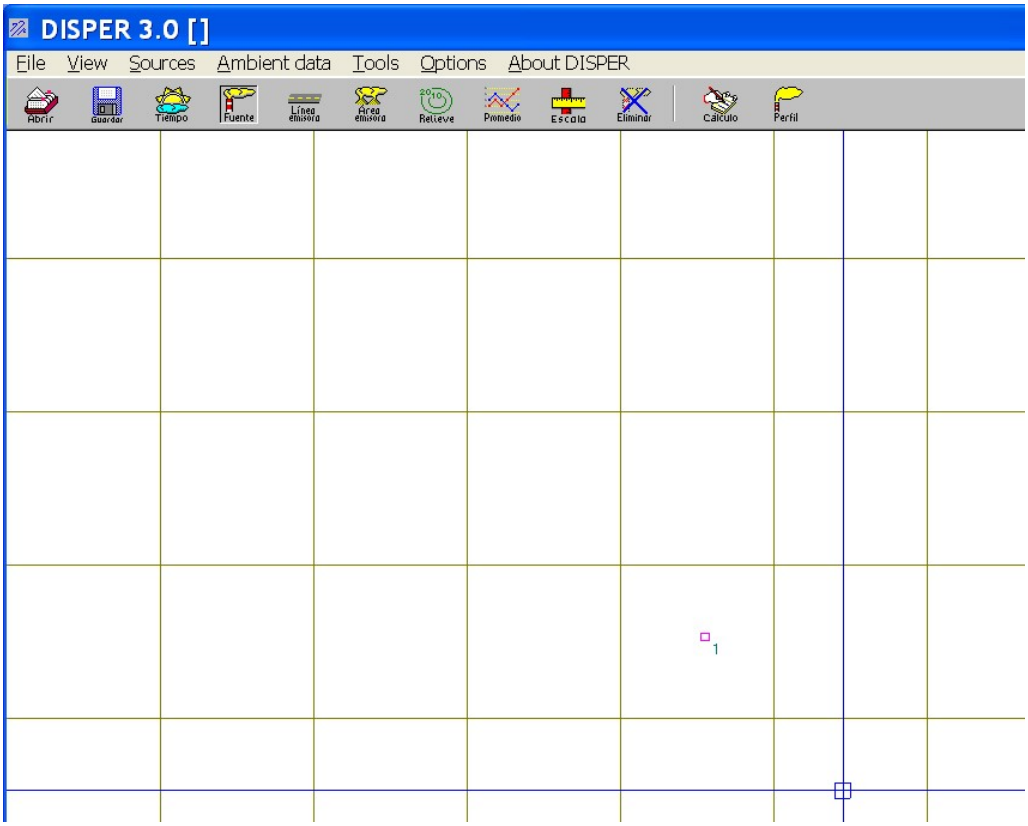
Estimate flow rate: With this button, you can estimate the pollutant flow rate if it is unknown. If you know the rate, you don't need to use this command. You can write it directly in the point source window. If you click this button, the next dialog box is shown:



If you click the OK button, the next program window is shown

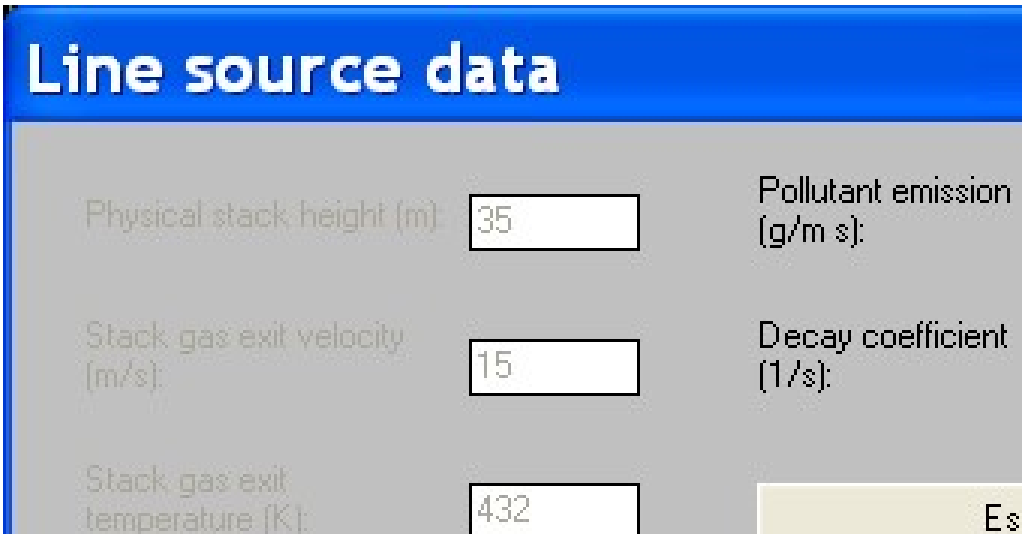


Two blue axis points the place where we can fix the stack position. After clicking the program window, you draw the stack.



The small fuchsia square shows the stack location. We can draw all the gas stacks that we want (up to 1,000). To change the point source data, we can click the stack location in the program window. Then, the point source dialogbox is again displayed. We are not able to put two gas stacks in the same location. The older is eliminated automatically.

Line source.- This is a pollutant line source. The line width is small if we compare it with the size of the area in which we are simulating (line source). If you click this button, the next dialog box is shown:

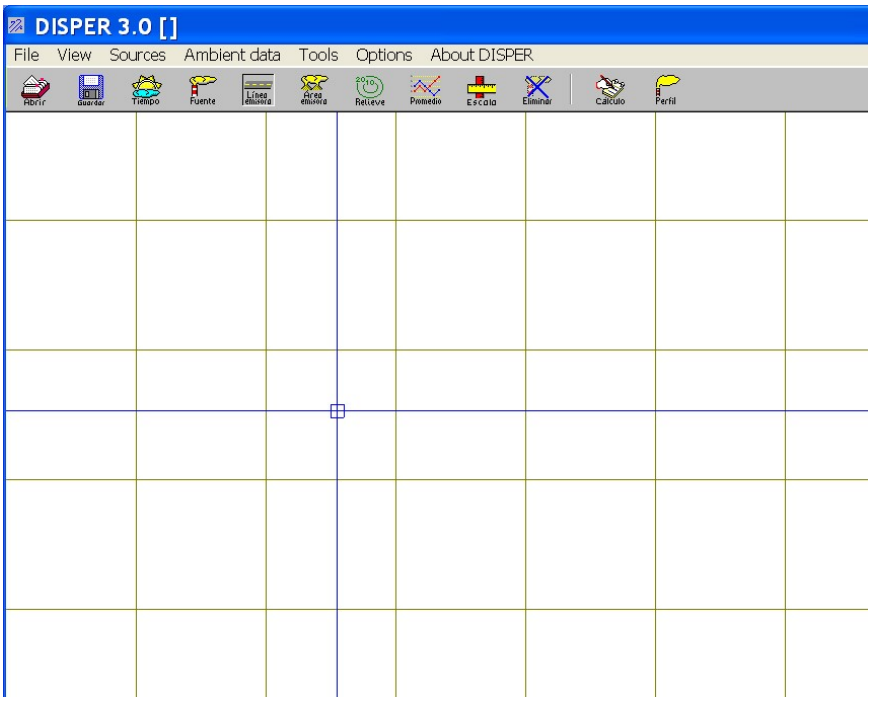


Here, only some data can be modified. The necessary data is:

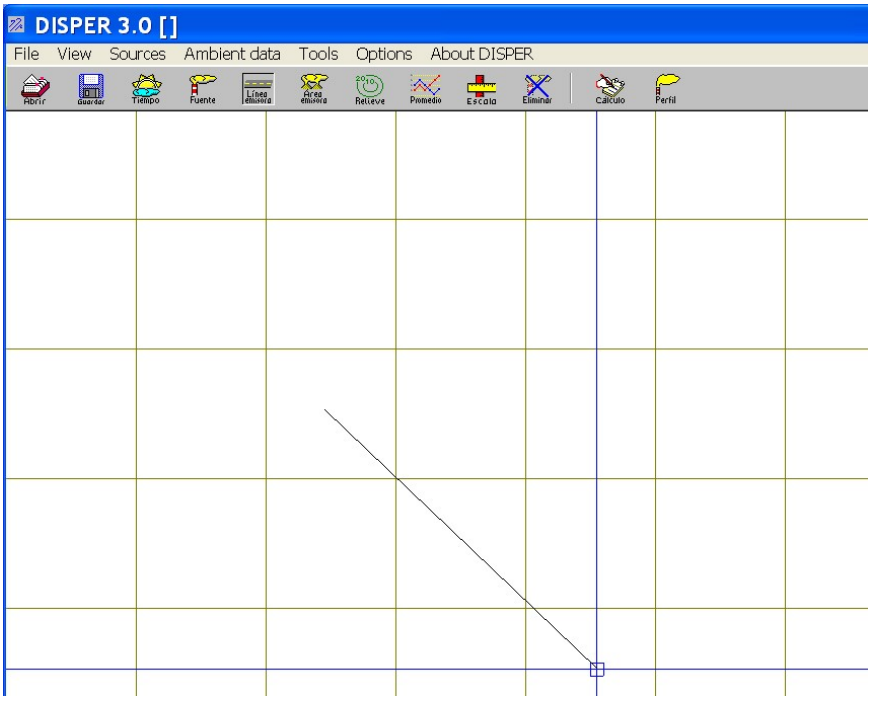
Pollutant emission rate (g/m s): This is the pollutant emission rate.

Decay coefficient (1/s): This coefficient considers the half life of the pollutant if this disappears by means of chemical reactions (non-conservative pollutant).

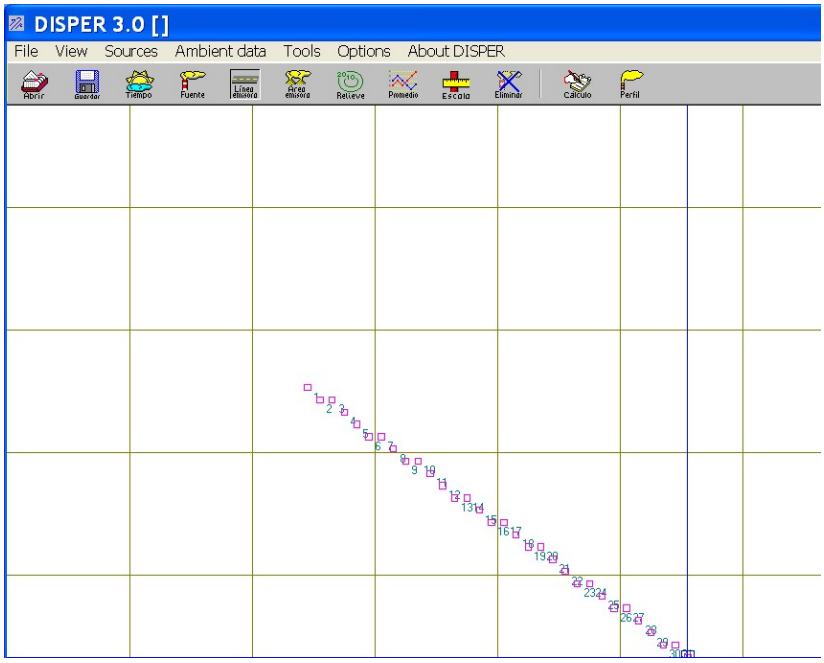
If you click the OK button, the next program window is shown



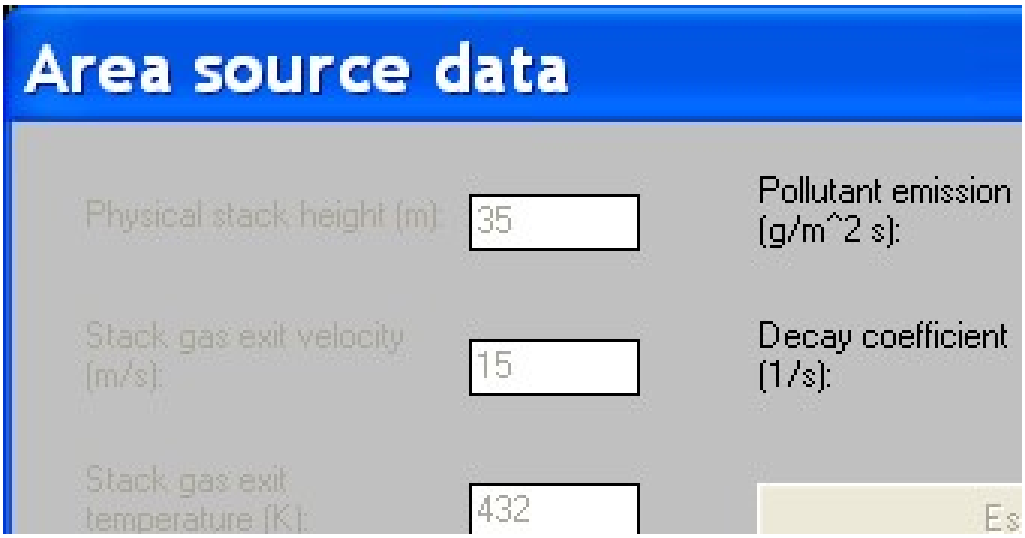
If you click the computer screen and move the mouse, a straight line is shown



If you click again on the computer screen, a line source is drawn



Area source.- This is a pollutant area source. The area width is small if we compare it with the size of the area in which we are simulating (area source). If you click this button, the next dialog box is shown:

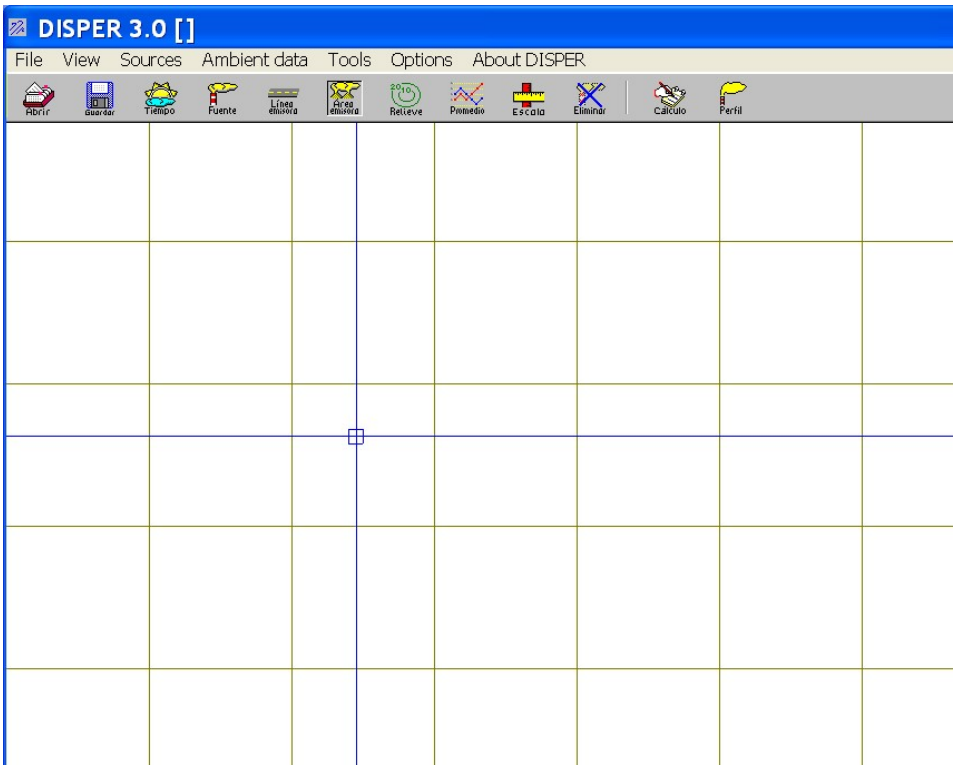


Here, only some data can be modified. The necessary data is:

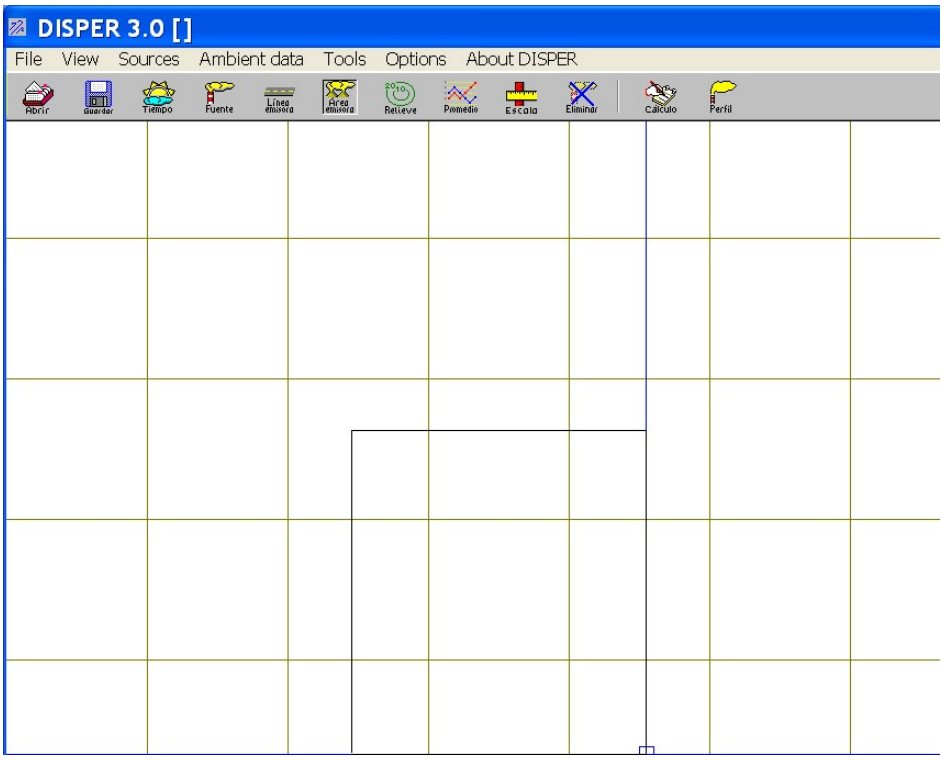
Pollutant emission rate (g/m^2 s): This is the pollutant emission rate per unit area and second.

Decay coefficient (1/s): This coefficient considers the half life of the pollutant if this disappears by means of chemical reactions (non-conservative pollutant).

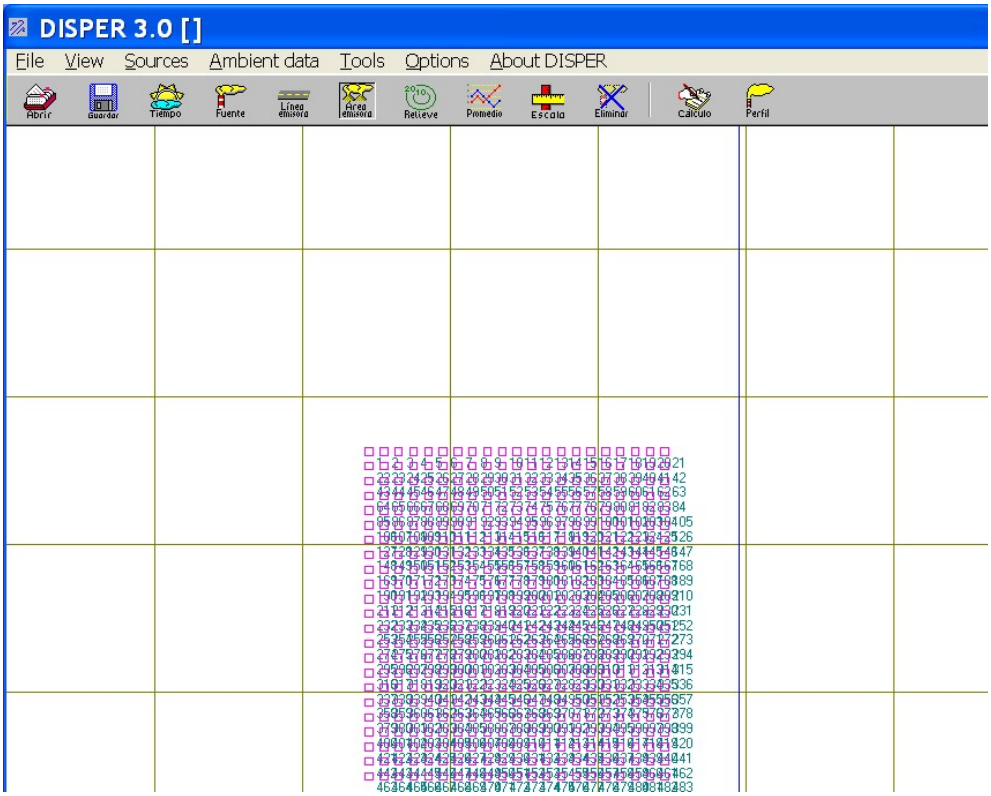
If you click the OK button, the next program window is shown



If you click the computer screen and move the mouse, a square is shown:



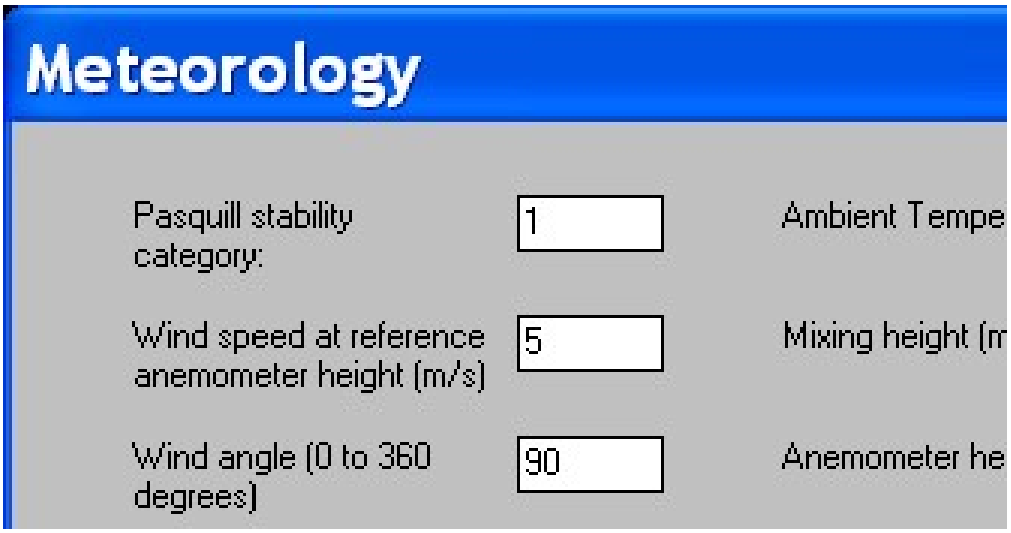
And if you click again on the computer screen, an area source is drawn:



7.1.4 Ambient data

Ambient conditions are defined by the land and atmospheric conditions in the vicinity of the pollutant emission. This Menu lists: **Meteorology** and **Topographic lines**.

Meteorology.- CASTOR-AIR analyses, as all mixing zone evaluations, are usually carried out under the assumption of steady-state ambient conditions. If you click this command, the next dialog box is shown:



The necessary data in the **Meteorology command** is:

Pasquill stability): Classification scheme that describes the degree of atmospheric turbulence. Categories range from extremely unstable (A=1) to extremely stable (F=6). Unstable conditions promote the rapid dispersion of atmospheric contaminants and result in lower air concentrations compared with stable conditions.

Wind speed at reference anemometer height (m/s): The measurement of wind speeds is usually done using a cup anemometer. The cup anemometer has a vertical axis. The number of revolutions per minute is registered

electronically.

Wind angle (0 to 360 degrees): It is the horizontal angle of wind measured clockwise from the North (at the window top).

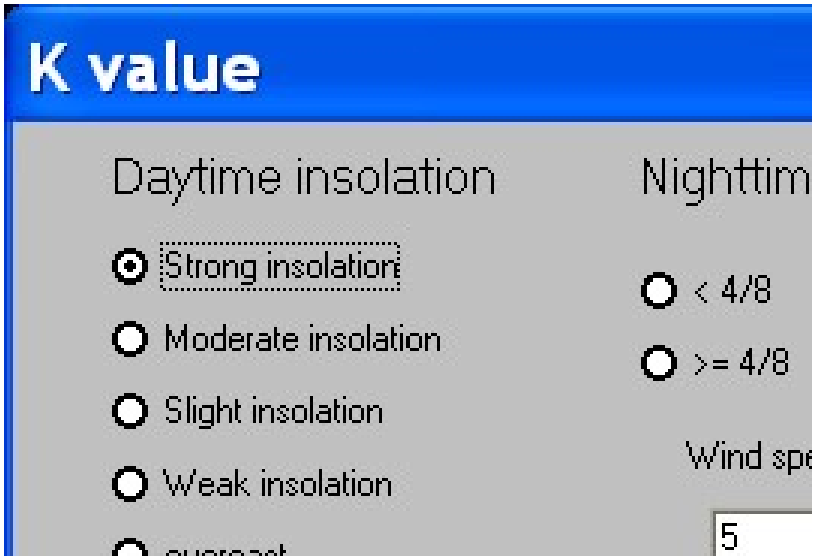
Ambient temperature (K): The temperature of the medium surrounding an object. This is the air temperature at stack location.

Mixing height (m): Mixing Height is used by meteorologists to quantify the vertical height of mixing in the atmosphere. It is the height at which vertical mixing takes place. There is a smaller volume which the pollutant can be dispersed. There is a seasonal variation of mixing height. For Summer daylight hours maximum mixing height can be a few thousand feet where as for Winter it can be a few hundred feet. It is lowest at night and increases during the day.

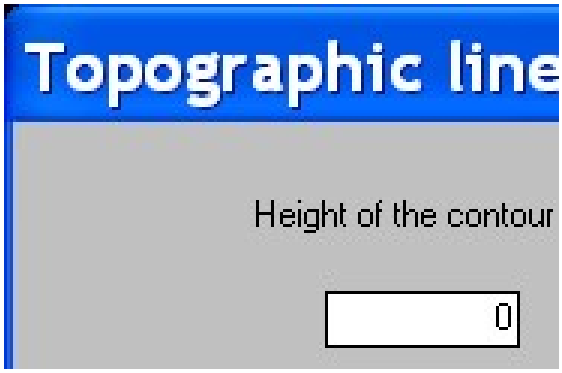
Anemometer height (m): This is the ambient temperature at stack location.

RURAL/URBAN option: This is the RURAL/URBAN terrain options.

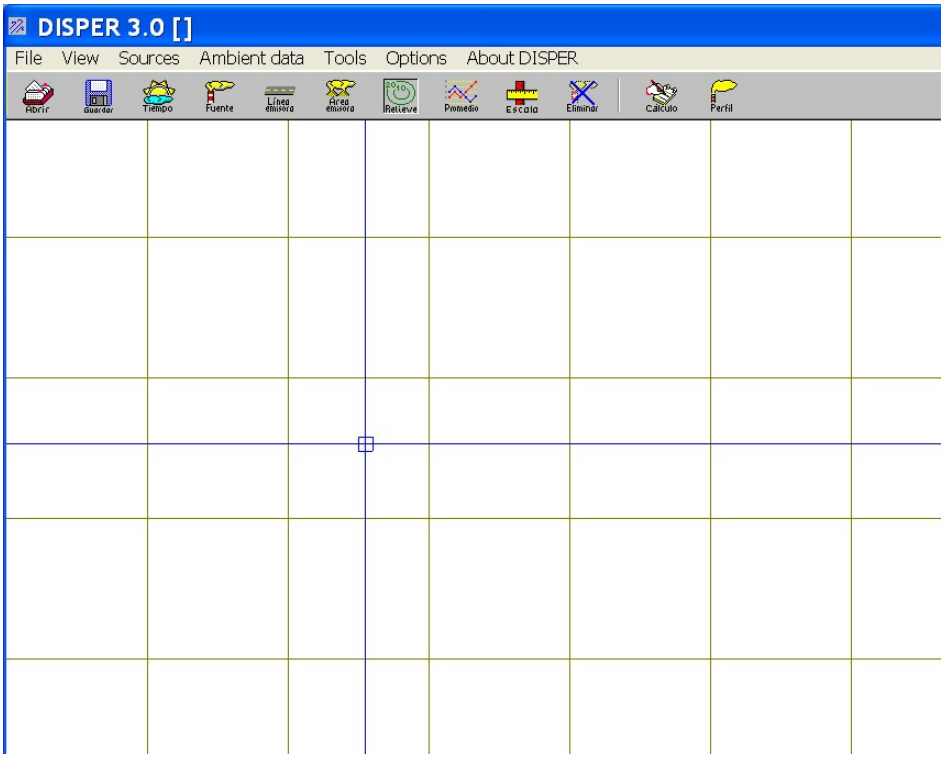
Obtain K value: With this button, you can estimate the Pasquill stability category if it is unknown. If you know the K value, you don't need to use this command. You can write it directly in the Meteorology window. If you click this button, the next dialog box is shown:



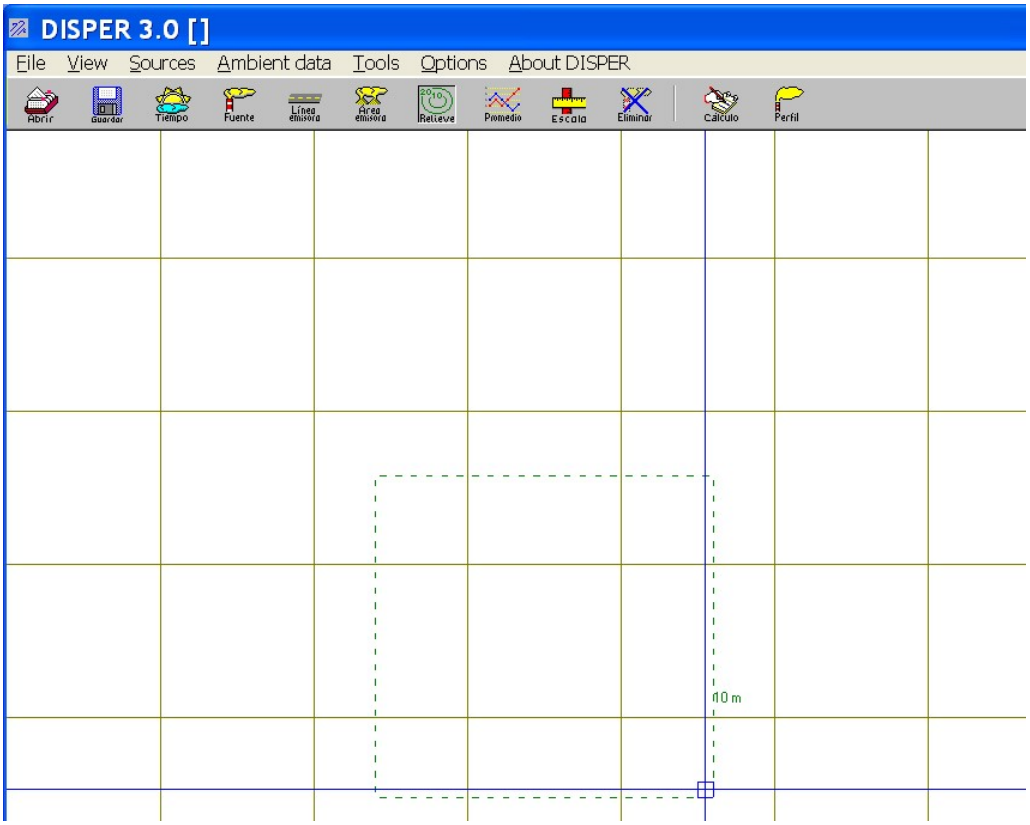
Topographic lines.- This command is to draw topographical lines. If you click this command, the next dialog box is shown:



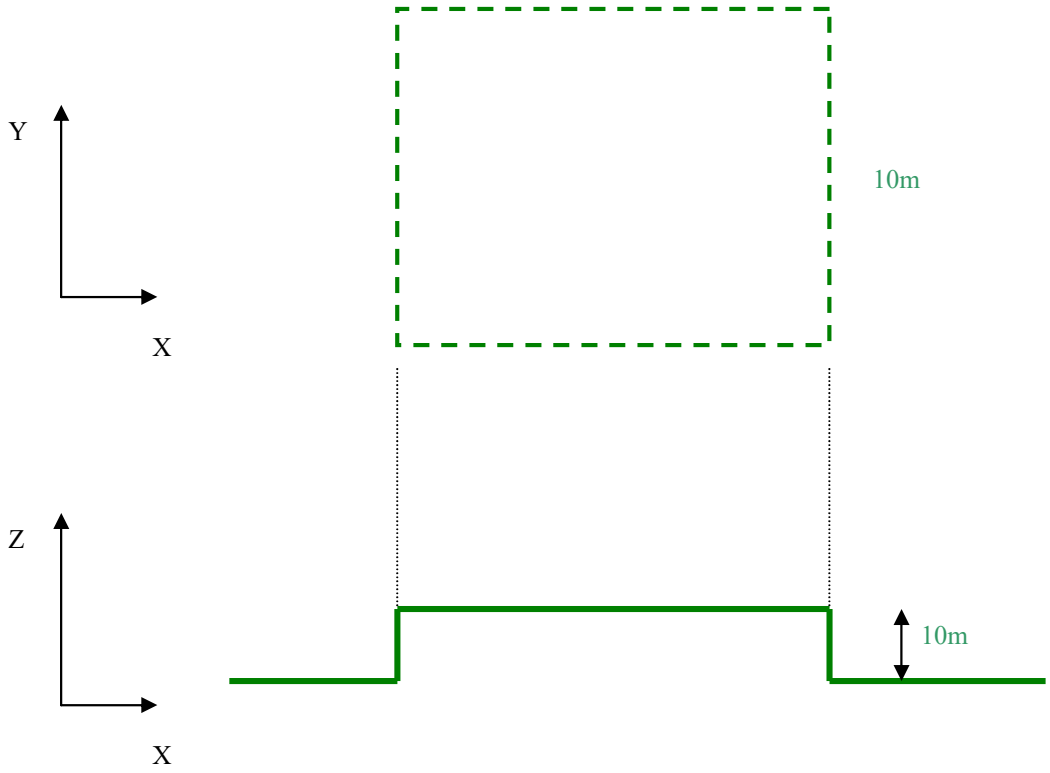
The height of the contour line can be written in the textbox. If you click the Accept button, the next computer screen is shown:



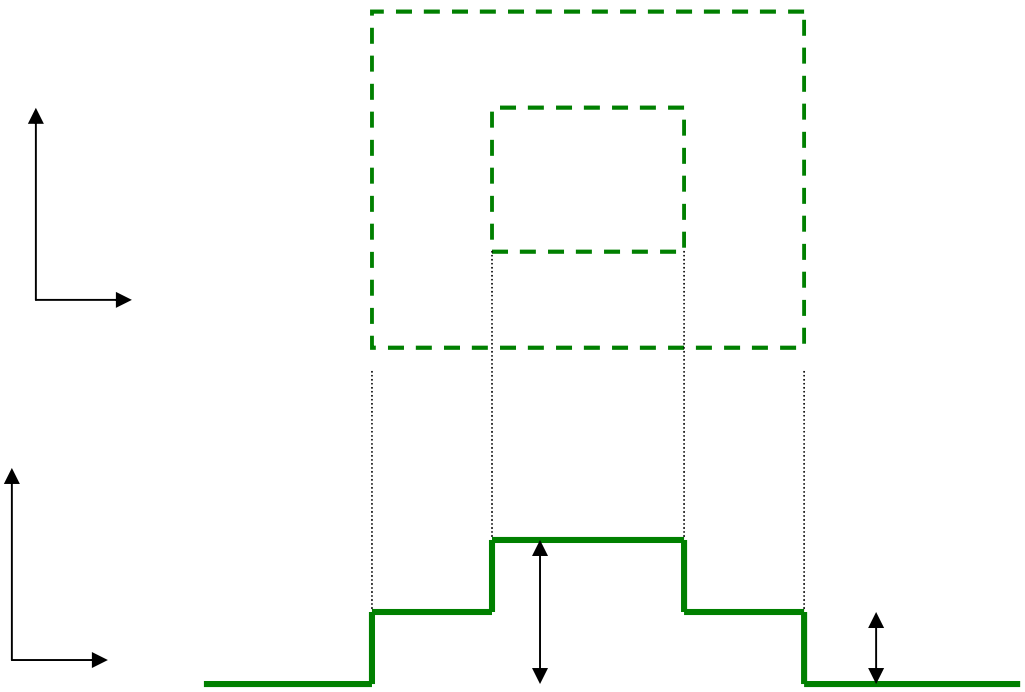
Then, and if you click the computer screen and move the mouse (mouse down), a square is shown and when you mouse up (the height of the contour line is different to zero):



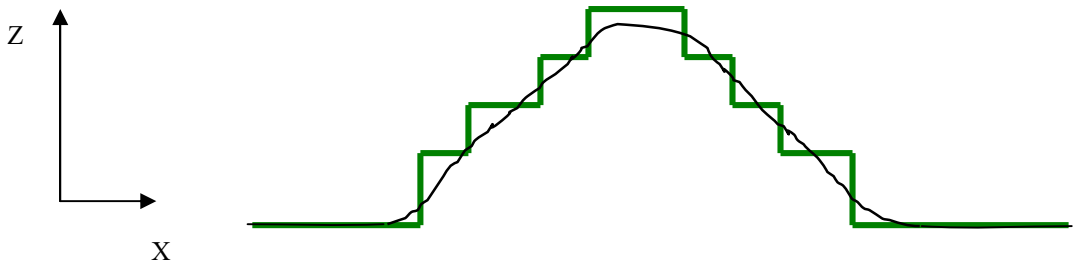
The area inside this contour has a 10m height. A rectangle elevation could be represented by the program in the next way:



To draw a small mountain, we can use a lot of small rectangles.

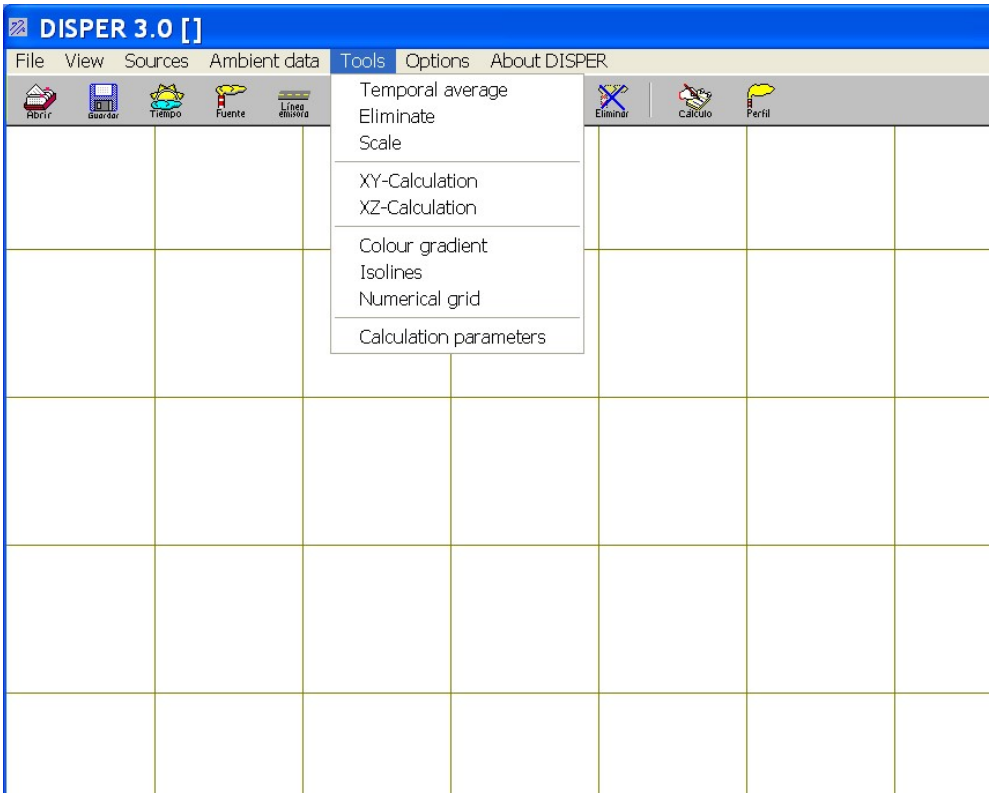


A mountain could be represented by the program in the next way:



7.1.5 Tools

The Tools Menu contains the tools you use to process your data. The File Menu lists: **Temporal average**, **Delete**, **Axis scale**, **XY-Calculation**, **XZ-Calculation**, **Colour gradient**, **Isolines**, **Numerical grid** and **Calculation parameters**. When you choose **Tools** in the Menu bar, the program displays:

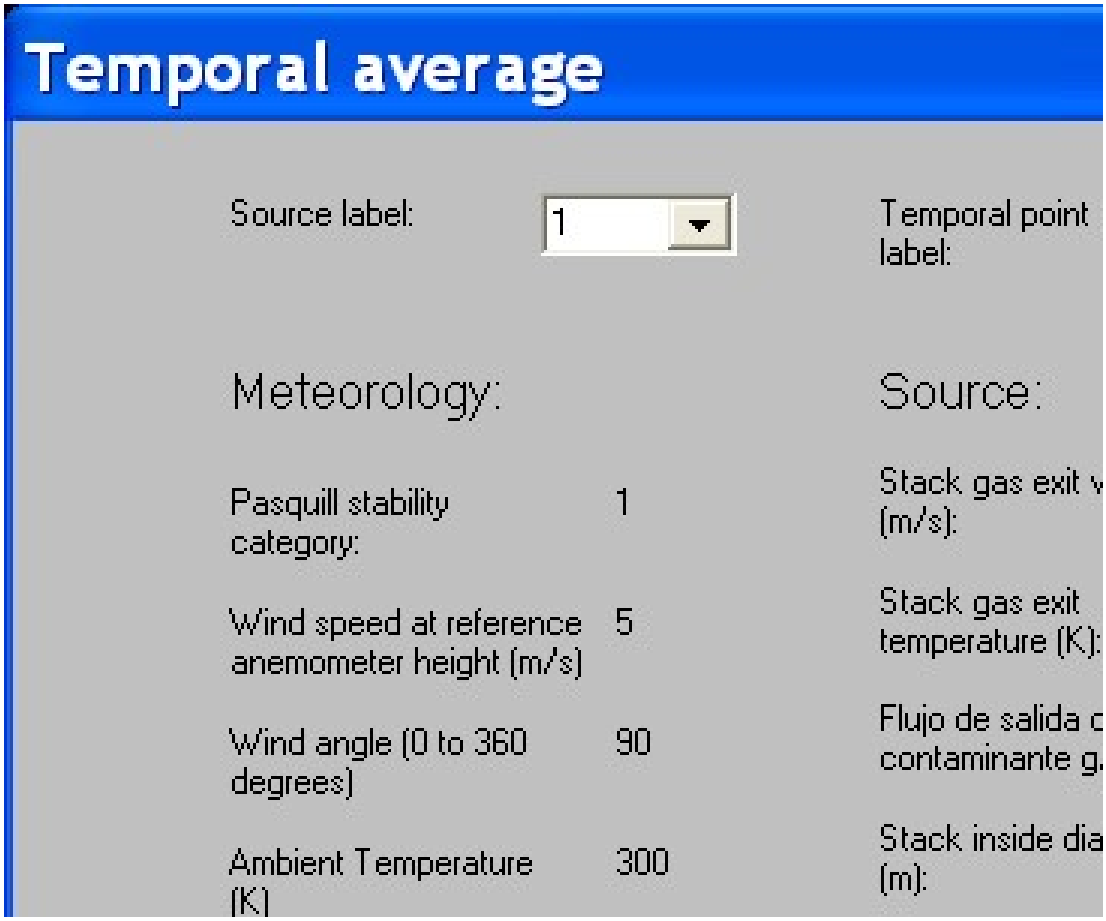


Temporal average.- Some discharge data can vary with time (velocity of the wind, pollutant rate,...). Taking this into account, the program can do temporal averages in the calculation. In the CASTOR-AIR software, these data are allowed to vary with time. If you click this command, the next dialog box is shown:

We can write in the text box the number of temporal points per average. To be able to make an average, we will take more than a temporal point.

The temporary points are elements of an average and we will be able to relate them with any temporary instant. That is to say, if we have data of winds for every hour of one day (a total of 24) and we want to make an average of the pollution in one day, we will be able to make a temporal average with 24 temporal points to calculate the daily average.

Each temporary point that we average represents the data in a hour of time. If we have monthly data, and we want to make an annual average, we will be able to average with 12 temporary points (the twelve months). Then, and if you click the OK button, the next dialog box is shown:

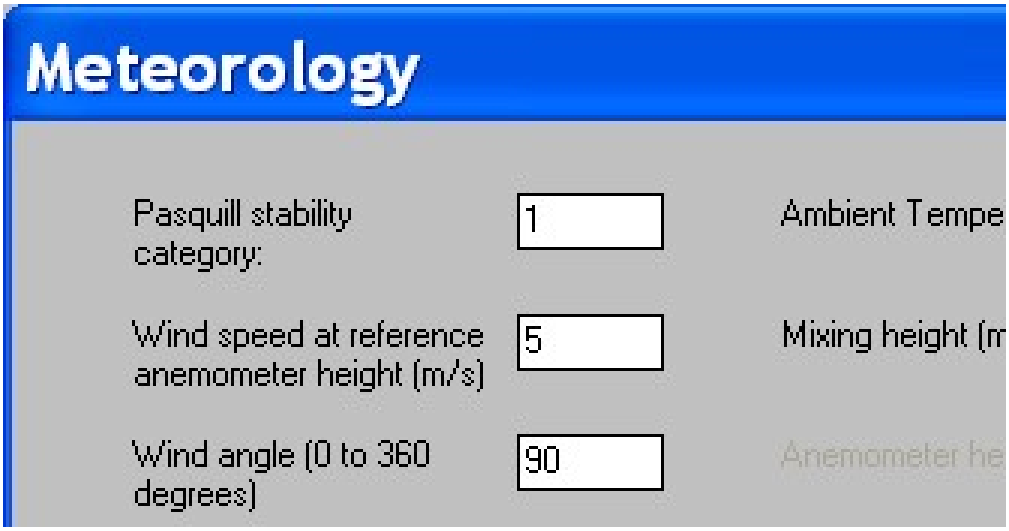


The window allows to visualize the data to make the average. It also allows to modify the data or to change them. We have two groups of data that can vary in time: Meteorology and Source data.

At the top of the dialog box, two different text boxes appear: source label and temporal point label. We can click both arrows to change these values and to visualize the data.

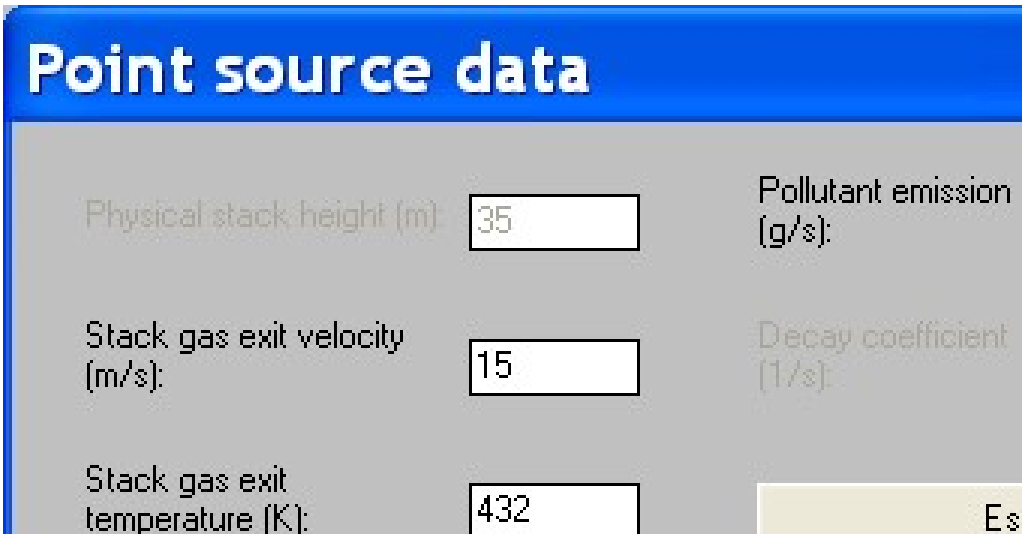
Every time that you enable a new average, the software allocates to all temporal points the same quantities. These quantities coincide with the values that we had in the **Meteorology** and **Source** dialogboxes before enabling an average.

To modify the ambient and emission data in the temporal average, we can click **Meteorology** and **Source** buttons in the dialogbox. Then, and if you click the **Meteorology** button, the next dialog box is shown:



Some data of the dialog box cannot be modified: the anemometer height and the RURAl/URBAN terrain option can not be modified. There is not interest in varying this data in time. To modify these data, we will have before to disable the temporal average and to open the source and Meteorology dialogboxes in the **source Menu** and in the **ambient data Menu**, respectively. To disable the temporary average, we will have to click the **Temporal average** command and to write **1** in the textbox of the **Number of temporal points**.

If you click the **source** button in the **Temporal average** dialogbox, the next dialog box is shown:

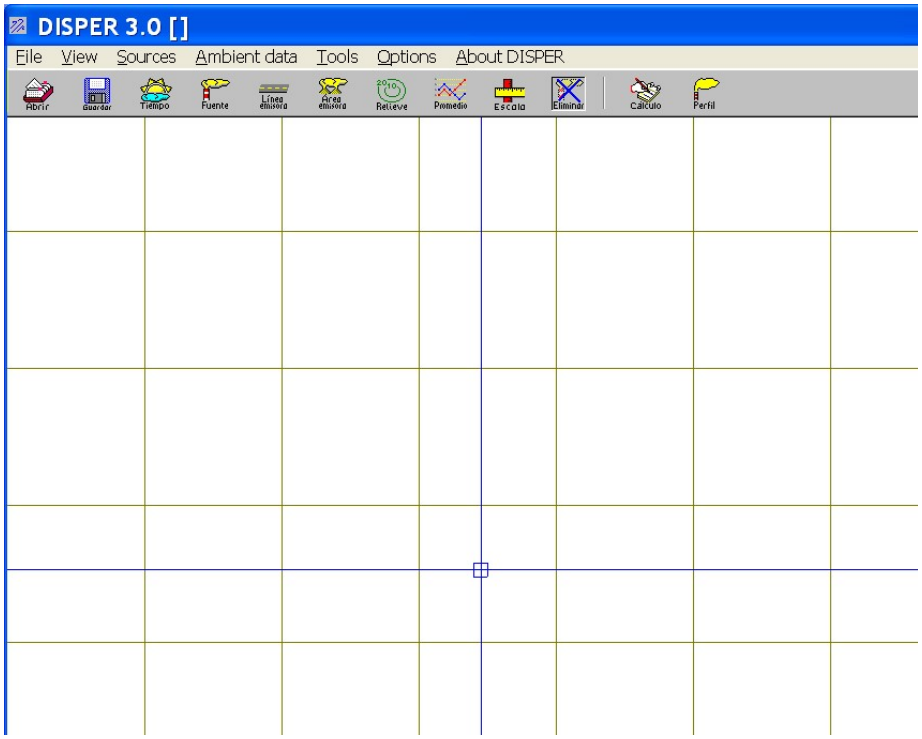


Some data of the dialog box cannot be modified: the physical stack height, the stack inside diameter and the decay coefficient. There is not interest in varying this data in time To modify these data, we will have before to disable the temporal average and to open the source and Meteorology dialogboxes in the **source Menu** and in the **ambient data Menu**, respectively. To disable the temporary average, we will have to click the **Temporal average** command and to write **1** in the textbox of the **Number of temporal points**.

Before running the calculation it is convenient to check the data that we have in the average.

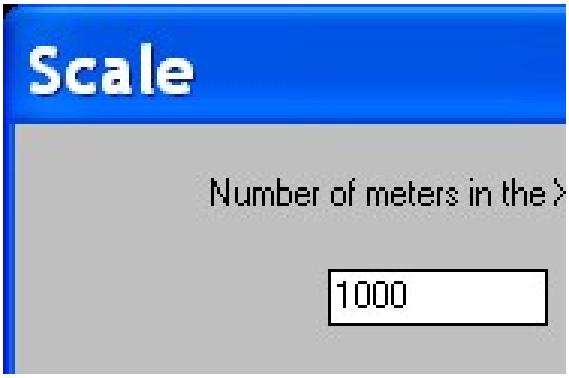
If we enable an average with more than a temporal point, and if later we increase the number of temporal points, it is necessary to be careful since there are data that can have null value. The ideal procedure is to define well, and from the beginning, the number of temporal points before writing the values for the average. If we want to modify an activated average it can be more comfortable to delete the activated average and then to define one new. To delete a temporal average, we will have to click the **Temporal average** command and to write **1** in the textbox of the **Number of temporal points**.

Delete.- This command is used to delete pollutant sources that we don't want in the simulation. If you click the **Delete** button, the next program window is shown:



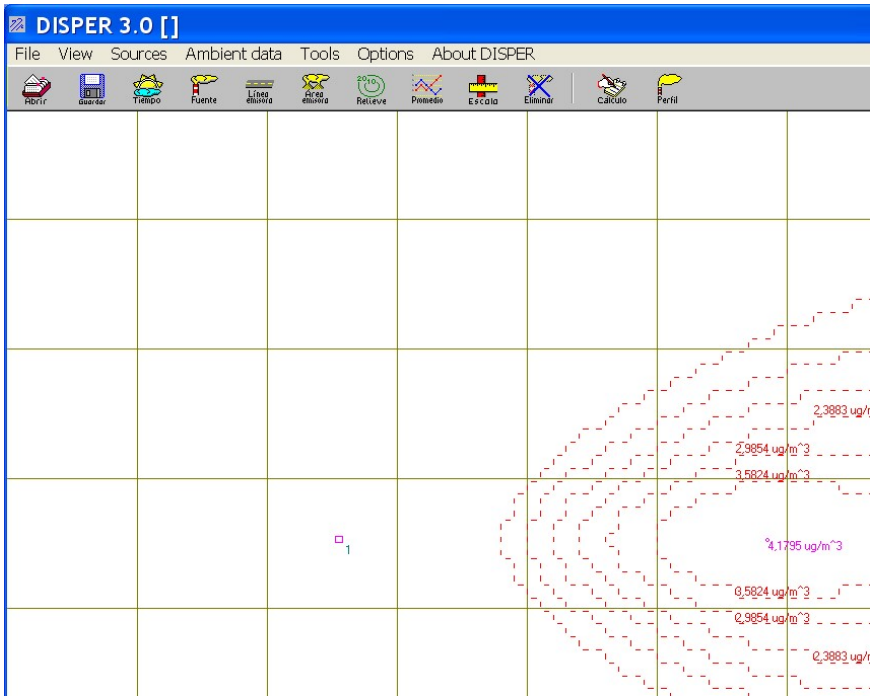
Clicking on these points we will delete them of the screen and of the calculation.

Scale.- With this command, we will decide the work area size in the simulation process. It is an important tool because with their good use we will be able to interpret and to extract interesting data of the numeric simulation. The scale is defined according to the width in meters that we want to associate to the X-Axis of our program window. If you click the **Scale** button, the next program window is shown:

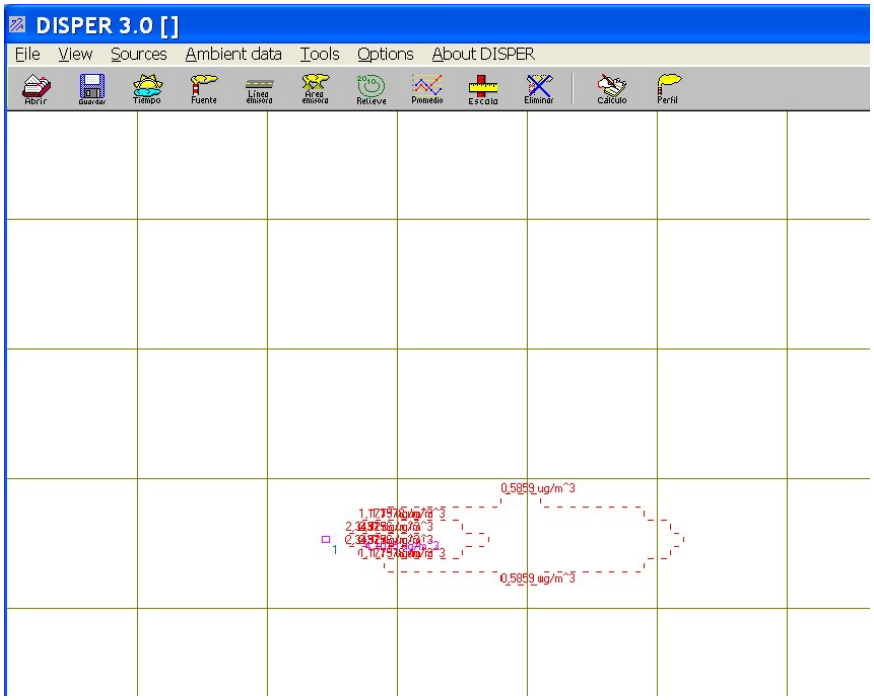


In this window we will be able to choose the number of meters that we want to have in the X-Axis. When we have the value written in the textbox, we will make click with the mouse on Accept button and this value will be modified and the previous window will disappear. If we click the Cancel button it closes the window without modifying the value. This command will be used before using the calculation command, since this parameter should be perfectly defined before making the simulation. When we use this command the program, we clean the whole screen of the computer and we lose all the elements of the simulation placed previously. If we don't want to lose the information obtained until the moment we will use the Save command before executing the Scale command.

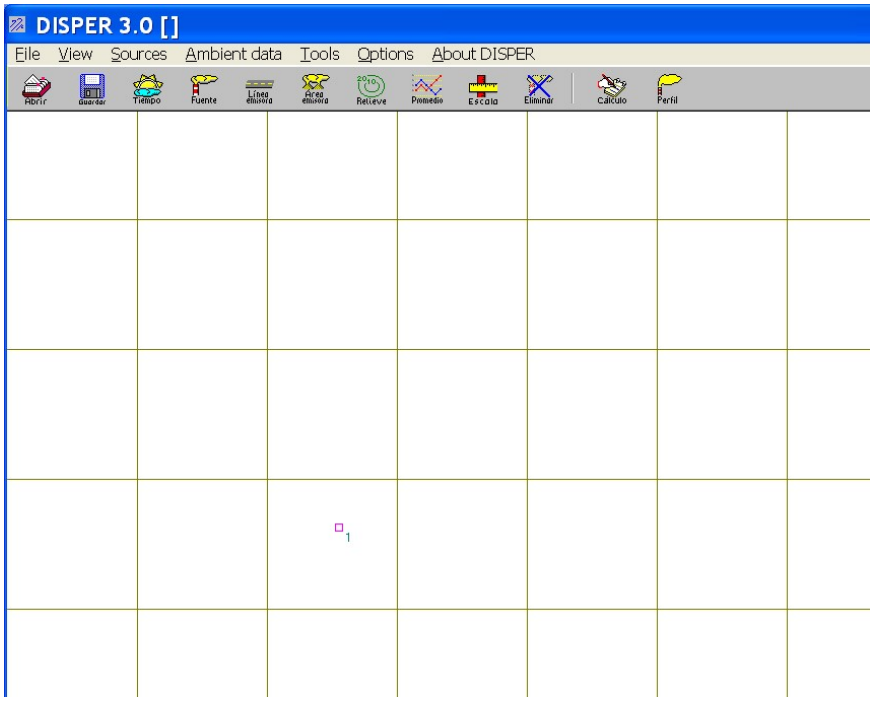
In certain situations, it can be interesting to have a high number of meters in the X-Axis for a better visualization. To illustrate the use of this command, we will carry out the same simulation varying the scale. We will use three different scales. Here, the width of the X-Axis is 1,000 m.



Here, the width of the X-Axis is 10,000 m.

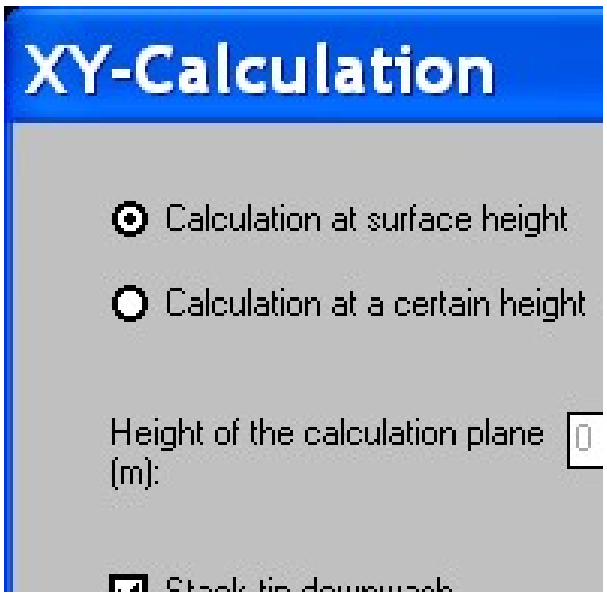


Here, the width of the X-Axis is 100 m.



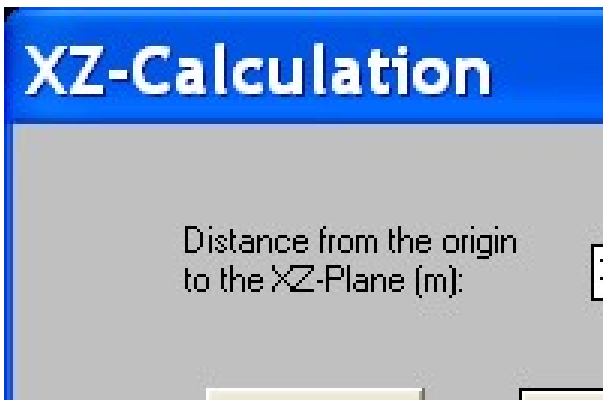
As we can see, when the X-Axis is 1,000 m, it is when we have a clearer representation, where it is shown the value of the maximum point and the concentration lines clearly.

XY-Calculation and XZ-Calculation.- The calculation commands run the necessary algorithm to carry out the numeric simulation. We will run the command after having fixed the necessary data for the simulation, that is to say, the sources, the ambient data, the scale,... If we change any initial data (as the position of the source, velocity of the wind,...), we will need to run the command again so that this is reflected in the result. We will be able to choose between XY-Calculation and XZ-Calculation commands to obtain different pollution maps. If we make click on **XY-Calculation** command, we open the following window :



In this window we will be able to choose if we want to carry out the calculation in the land surface or to a certain height (two options). In the first option, the calculation of the pollutant concentrations will be carried out at surface height. If we choose the option for the calculation to a certain height, we will write in the textbox the plane height in which we will obtain the results (0m for the surface of the sea).

If we make click on **XZ-Calculation** command, we open the following window :



In this window we will be able to write the distance to the origin (inferior left point of the screen) of the XZ-plane that is perpendicular to the land surface. On this plane we will carry out the XZ-Calculation.

The program works in the following way: while it calculates, the machine centers all the capacity of the CPU in the calculation, stopping the other tasks of Windows. If we want to stop a tedious calculation, we will be able to make it making use of the keys CTRL+ALT+DEL.

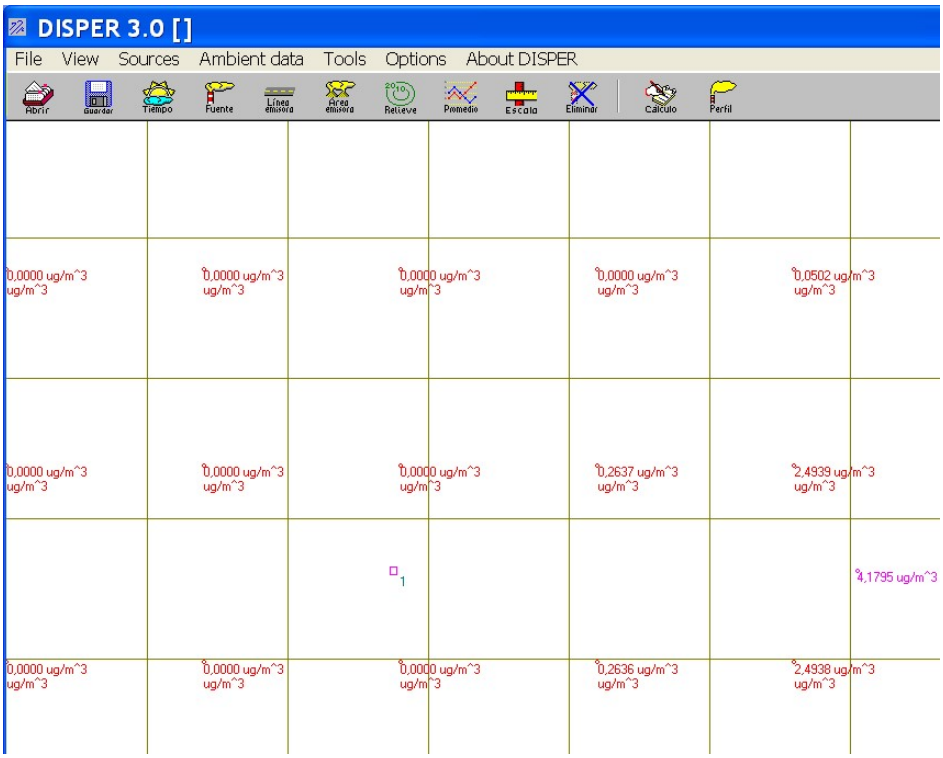
Note about this command.- Near the source, we can find diferences between both XY-calculation and XZ-calculation commads. The application uses a numerical grid for valuing an exponential function. The small differences between adjacent points, when the grid is implemented, can cause different concentration results due to the exponential behaviour near the source. Far away from the source, these differences can be neglected.

Colour gradient.- This command is to draw maps of pollution making use of a colour gradient. It is specially useful when the variation of the concentration of pollutants is very strong in a very short distance. The program takes the maximum value of the concentration and it assigns to the maximum the red colour. Then, the program assigns the different colours to the grade of pollution in a qualitative way. We will be able to obtain the exact values locating the arrow of the mouse on any point and looking at the inferior right textbox of the program.

Isolines.- This command is of effect contrary to the previous one. We will use this command with the purpose of obtaining the isolines again. This way we will be able to change representation easily making use of these last two commands.

Numerical grid.- This command allows us another alternative representation of the calculated concentrations. It establishes a numerical grid throughout the calculation screen. It is specially useful if we load topographical planes, because with the other representations there are many

images in the screen. If you click the **Numerical grid** button, the next program window is shown:

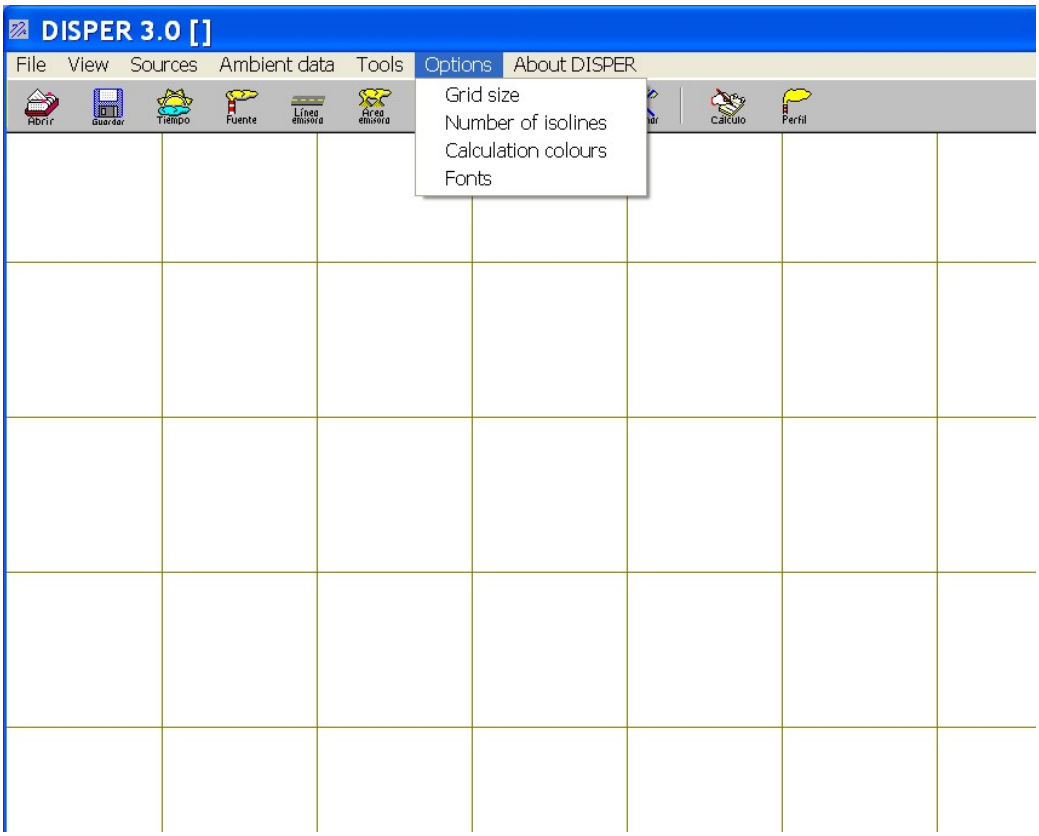


Calculation parameters.- This command will show us the parameters that we have assigned before carrying out the calculation. It is convenient their use with the purpose of verifying that we have written the parameters correctly. Once finish the calculation, the command shows us, also, the value of the maximum concentration and its position.

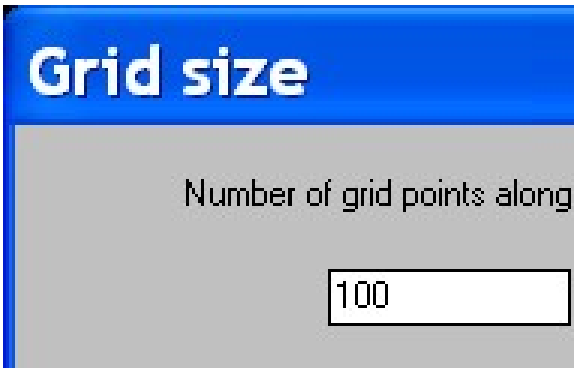
7.1.6 Options

The Options Menu includes all the elements for the numeric configuration of the simulations. We will use these commands before using the calculation command because these parameters should be perfectly defined before running the

simulation. The Options Menu lists: **Grid size**, **Number of Isolines**, **Calculation colours**, **Fonts**, **Calculation model** and **Odor units**. When you choose **Options** in the Menu bar, the program displays:



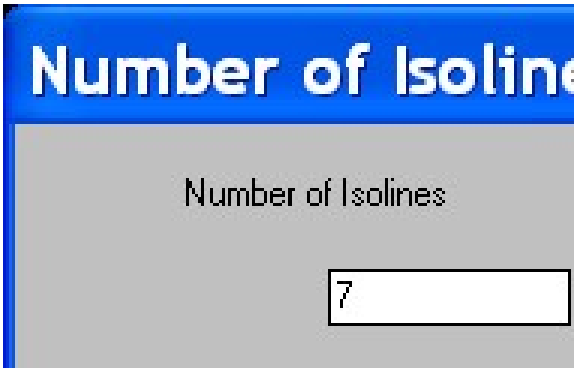
Grid size.- The grid size is an important parameter in the configuration of the system. We will decide the number of calculation points in the grid that we will take to make the simulation. As we increase the number of points, the computer will take much more time in carrying out the calculation but the result will be much more exact. If you click the **Grid size** command, the next program window is shown:



In this window we will be able to choose the number of grid points (calculation points) that we want to have in the X-Axis. The number of points to calculate will increase quadratically with the number of grid points along the X-Axis N, that is to say, it will increase as N^2.

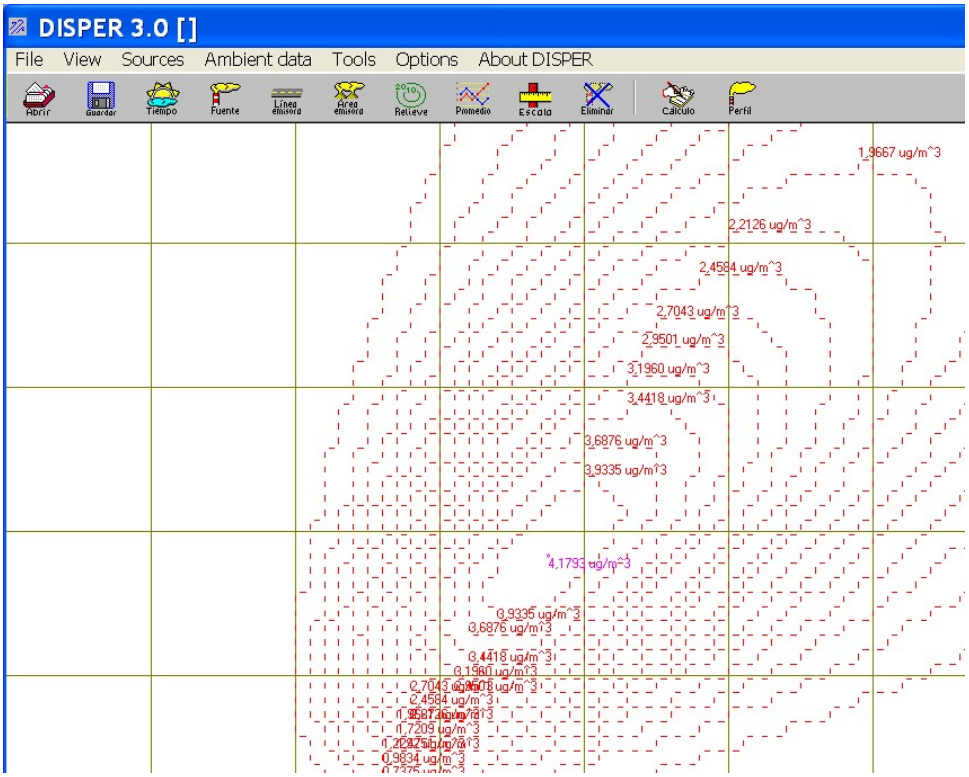
To increase the number of grid points produces that the program needs much more RAM-memory. If we take such a high number of grid points that it overcomes the available memory of the PC, the computer will be blocked.

Number of isolines.- This command is an auxiliary tool for making the maps of pollutant concentration. We will decide the number of isolines in the screen that we will take to make the representation. In certain situations, it can be interesting to have a high number of isolines for a better visualization. We will use this command before using the calculation command because this parameter should be perfectly defined before running the simulation. If you click the **Number of isolines** button, the next program window is shown:

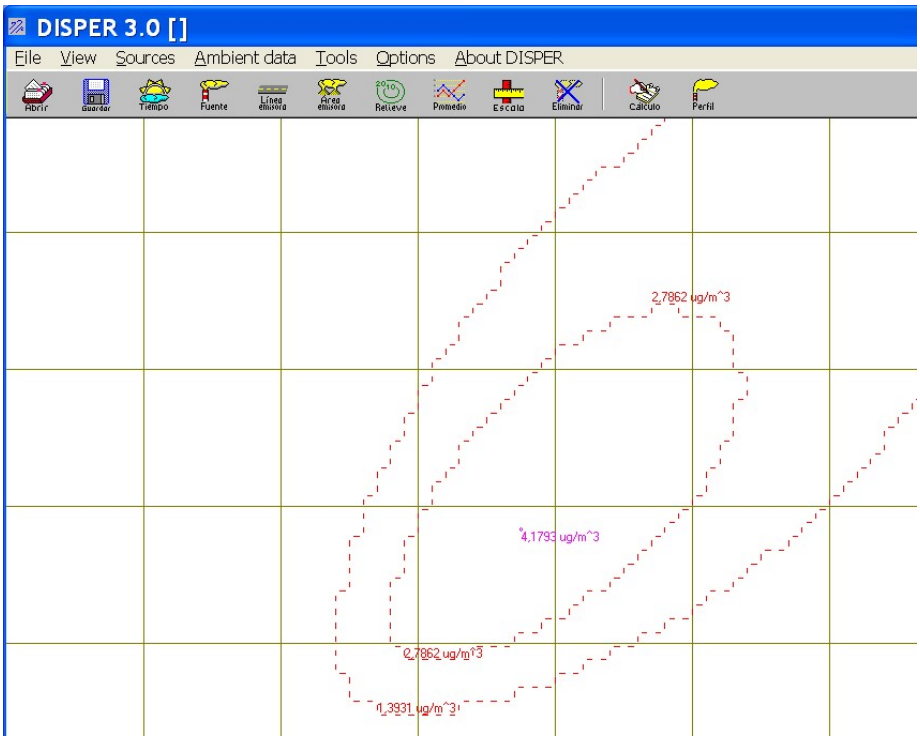


In this window we will be able to choose the number of isolines that we want to have in our computer screen. To calculate the lines, the program also considers to the maximum point as a line.

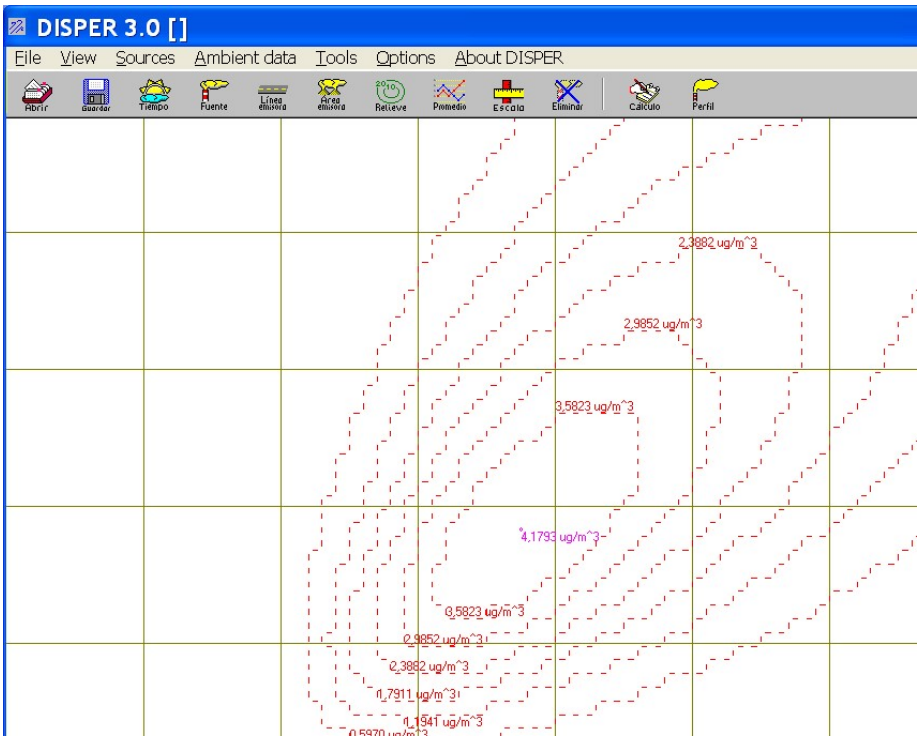
To illustrate the use of this command, we will carry out the same simulation varying the number of isolines. We will use three different number of isolines. Here, the number of isolines is 17.



Here, the number of isolines is 3.

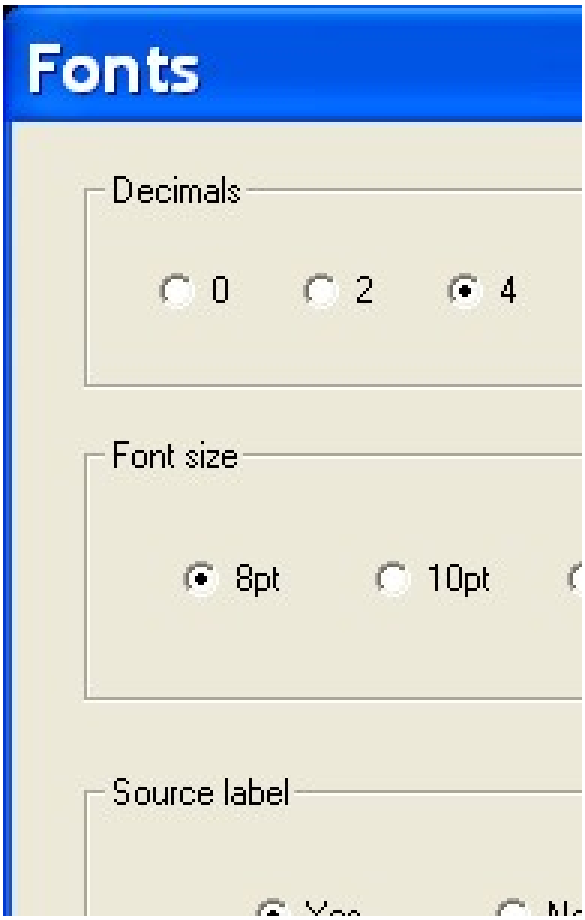


Here, the number of isolines is 7.



Calculation colours.- By means of this command, we will be able to change the colors of the isolines, of the maximum point and of the point sources.

Fonts.- This command is an auxiliary tool for making the maps of pollutant concentration. In this command we have three different options. We can choose: number of decimal places, font size and source label (Yes/No).



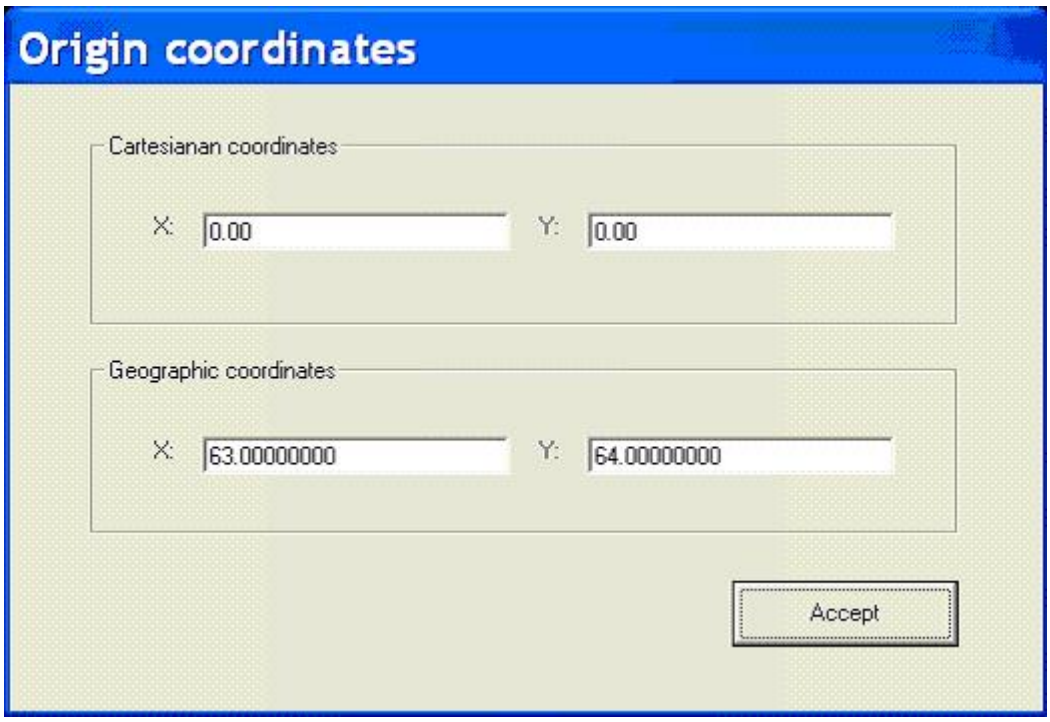
Calculation model.- This command is an auxiliary tool for changing the calculation model.

Odor units.- This command is an auxiliary tool for using odor units.

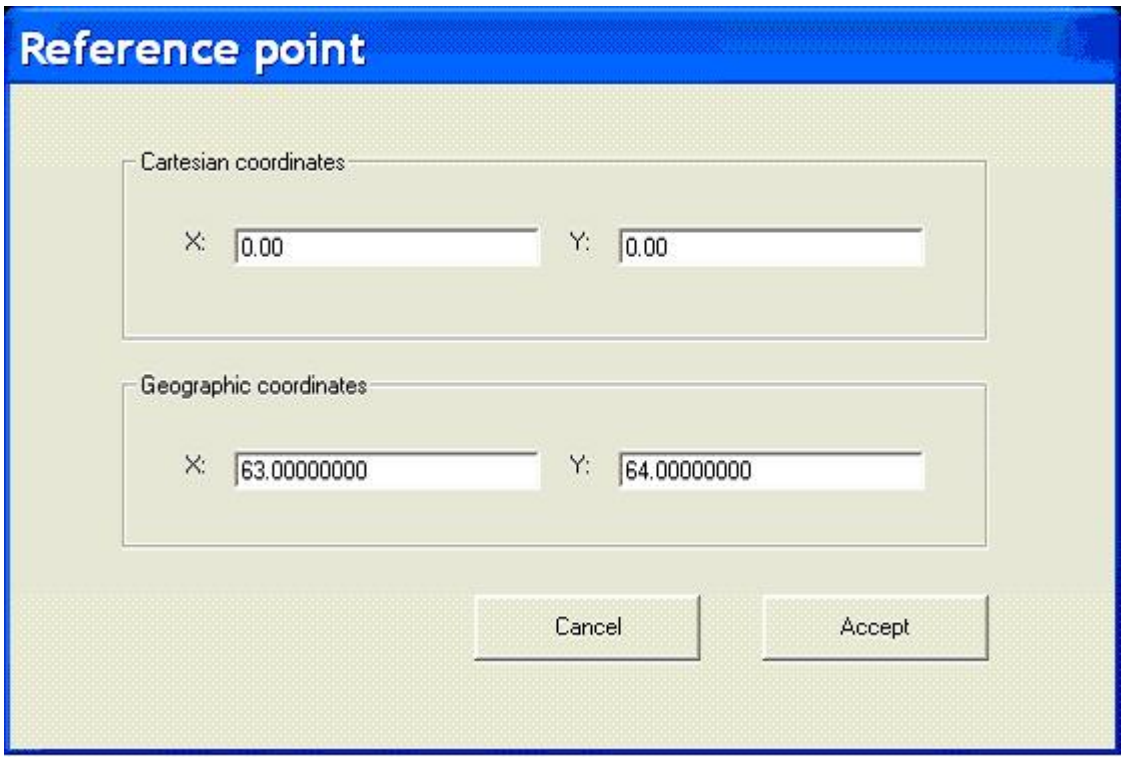
7.1.7 GIS

In this option it can be found all necessary to work with geographical information system.

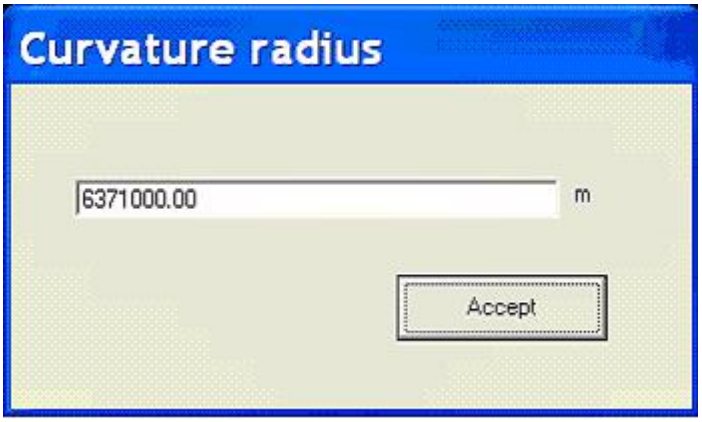
Coordinates of the origin.- With this command we can choose the value for the origin of coordinates. It is initially in the left bottom corner of the program window. It is possible to work with geographic and Cartesian coordinates.



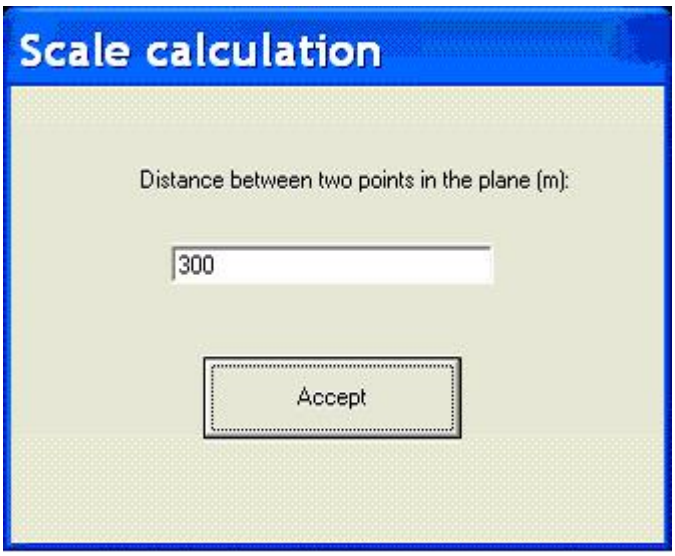
Reference points.- With this command we can decide the coordinate values of a point, that we previously know, in the map in order to have a referenced system. It is possible to work with geographical and Cartesian coordinates. After that, it will be possible to export the results to a GIS system.



Radius of curvature.- By means of this command, you can choose a value for the Earth radius. This radius can be slightly modified to adjust the reference system with the available data. The program considers the Earth as a perfect sphere with an exact radius. We know that this is not exactly true. This option is to correct this kind of effects.



Scale calculation.- With this command it is possible to estimate the map scale that corresponds to a background image, that has trees previously imported by the user. It is necessary to know the distance between to different points in the map. After introducing the distance data, you can click consecutively both points, and the scale will be automatically calculated.



Export maximum, concentrations,….- These are to export the different elements of the programs (isolines, source positions,…) to Microsoft EXCEL csv file. To import without problems with Arcview we have used the english format system for the numbers. For example, one euro and 30 cents is 1.30 euros (NOT 1,30!) in the english format.
If you are using the spanish format, for example, when you open the exported file with EXCEL you obtain "al numbers in the same box". In such a case, the best way is to change your number format in your computer. It is very easy. Just go to WINDOWS >> START >> CONTROL PANEL >> REGIONAL CONFIGURATION and look for english format before opening with your EXCEL program.

7.1.8 3D

The 3D commands are for a qualitative representation, not quantitative. The system generates random points to help you to obtain a 3D view of the pollution process. The pollution concentration value that appears in the screen is an orientative value. In the 3D options you can modify the number of random points and other parameters.

The 3D window is an extension of the 2D XY window. The X coordinate, Y coordinate and concentration value that appear on the bottom of the screen correspond to the XY plane view. The calculated XY data will be deleted after a 3D calculation. The PRINT command only prints the XY view. To print in 3D, you need to use the PRINT IMAGE command. Or you can save a BMP file and print such a file with an another standard program (windows PAINT, ...).

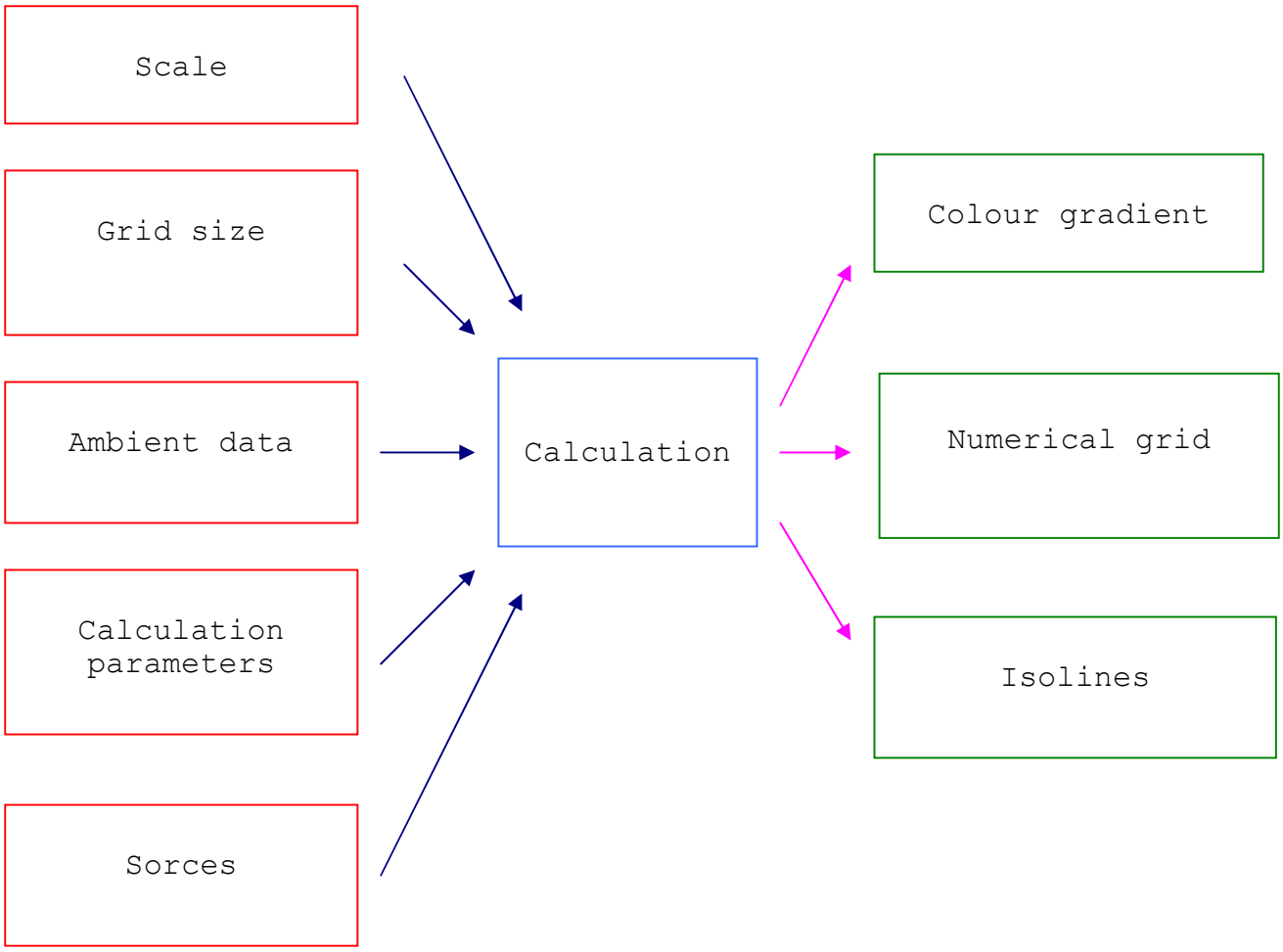
7.2 Icon bar

The menu bar display the commands you use to build your simulation. When you choose one of the menus, the program displays a pull-down list of available commands. The program window has a basic icon bar under the Menu bar. The icon bar provides quick access to commonly used commands in the program. You click a button on the icon bar once to carry out the action represented by that button.

8. Application structure

In this section, the general structure of the application will be shown. The Options Menu includes all the elements for the numeric configuration of the simulations. We will use these commands before using the calculation command because these parameters should be perfectly defined before running the simulation.

If we change any initial data (as the position of the source, velocity of the wind,...), we will need to run the command again so that this is reflected in the result. We will be able to choose between XY-Calculation and XZ-Calculation commands to obtain different pollution maps.



Colour gradient, Isolines and Numerical grid commands should be applied after running the calculation.

9. Mathematical algorithms

Symbols

Symbol / Definition

A = Linear decay term for vertical dispersion in Schulman-Scire downwash (dimensionless)
A_e= Effective area for open pit emissions (dimensionless)
D = Exponential decay term for Gaussian plume equation (dimensionless)
D_B= Brownian diffusivity (cm/s)
D_r= Relative pit depth (dimensionless)
d_e= Effective pit depth (m)
d_p= Particle diameter for particulate emissions (µm)
d_s= Stack inside diameter (m)
F_b= Buoyancy flux parameter (m^4/s^3)
F_d= Dry deposition flux (g/m^2)
F_m= Momentum flux parameter (m^4/s^2)
F_Q= Plume depletion factor for dry deposition (dimensionless)
F_T= Terrain adjustment factor (dimensionless)
F_w= Wet deposition flux (g/m^2)
f= Frequency of occurrence of a wind speed and stability category combination (dimensionless)
g= Acceleration due to gravity (9.80616 m/s^2)
h_b= Building height (m)
h_e= Plume (or effective stack) height (m)
h_s= Physical stack height (m)
h_{ter}= Height of terrain above stack base (m)
h_s= Release height modified for stack-tip downwash (m)
h_w= Crosswind projected width of building adjacent to a stack (m)
k= von Karman constant (= 0.4)
L= Monin-Obukhov length (m)
L_y= Initial plume length for Schulman-Scire downwash sources with enhanced lateral plume spread (m)
L_b= Lesser of the building height and crosswind projected building width (m)
_= Alongwind length of open pit source (m)
P(x,y)= Profile adjustment factor (dimensionless)
p= Wind speed power law profile exponent (dimensionless)
Q_A= Area Source pollutant emission rate (g/s)
Q_e= Effective emission rate for effective area source for an open pit source (g/s)
Q_i= Adjusted emission rate for particle size category for open pit emissions (g/s)
Q_s= Pollutant emission rate (g/s)
Q_t= Total amount of pollutant emitted during time period t (g)
R= Precipitation rate (mm/hr)
R_o= Initial plume radius for Schulman-Scire downwash sources (m)
R(z,z_d)= Atmospheric resistance to vertical transport (s/cm)
r= Radial distance range in a polar receptor network (m)
r_a= Atmospheric resistance (s/cm)
r_d= Deposition layer resistance (s/cm)
s= Stability parameter = FUNC {g {{¶ theta}/¶z } over {T_a}}
S= Smoothing term for smoothing across adjacent sectors in the Long Term model (dimensionless)
S_{CF}= Splip correction factor (dimensionless)
Sc= Schmidt number = FUNC { upsilon /D_B } (dimensionless)
St= Stokes number (dimensionless)

T_a= Ambient temperature (K)
T_s= Stack gas exit temperature (K)
u_{ref}= Wind speed measured at reference anemometer height (m/s)
u_s= Wind speed adjusted to release height (m/s)
u_*= Surface friction velocity (m/s)
V= Vertical term of the Gaussian plume equation (dimensionless)
V_d= Vertical term with dry deposition of the Gaussian plume equation (dimensionless)
v_d= Particle deposition velocity (cm/s)
v_g= Gravitational settling velocity for particles (cm/s)
v_s= Stack gas exit velocity (m/s)
X= X-coordinate in a Cartesian grid receptor network (m)
x_o= Length of side of square area source (m)
Y= Y-coordinate in a Cartesian grid receptor network (m)
q= Direction in a polar receptor network (degrees)
x= Downwind distance from source to receptor (m)
x_y= Lateral virtual point source distance (m)
x_z= Vertical virtual point source distance (m)
x_f= Downwind distance to final plume rise (m)
x^*= Downwind distance at which turbulence dominates entrainment (m)
y= Crosswind distance from source to receptor (m)
z= Receptor/terrain height above mean sea level (m)
z_d= Dry deposition reference height (m)
z_r= Receptor height above ground level (i.e. flagpole) (m)
z_{ref}= Reference height for wind speed power law (m)
z_s= Stack base elevation above mean sea level (m)
z_i= Mixing height (m)
z_0= Surface roughness height (m)
ß= Entrainment coefficient used in buoyant rise for Schulman-Scire downwash sources = 0.6
$ß_j$= Jet entrainment coefficient used in gradual momentum plume rise calculations FUNC {~=~{1 over 3} + {{u_s} over {v_s}}}
Dh= Plume rise (m)
dq/dz= Potential temperature gradient with height (K/m)
L= Precipitation scavenging ratio (s^{-1})
l= Precipitation rate coefficient $(s\text{-}mm/hr)^{-1}$
pi = 3.14159
Gamma= Decay coefficient = $0.693/T_{1/2}$ (s^{-1})
y_H= Stability adjustment factor (dimensionless)
f= Fraction of mass in a particular settling velocity category for particulates (dimensionless)
rho= Particle density (g/cm^3)
rho_{AIR}= Density of air (g/cm^3)
sig_y= Horizontal (lateral) dispersion parameter (m)
sig_{yo}= Initial horizontal dispersion parameter for virtual point source (m)
sig_{ye}= Effective lateral dispersion parameter including effects of buoyancy-induced dispersion (m)
sig_z= Vertical dispersion parameter (m)
sig_{zo}= Initial vertical dispersion parameter for virtual point source (m)
sig_{ze}=Effective vertical dispersion parameter including effects of buoyancy-induced dispersion (m)
U=Viscosity of air = 0.15 cm^2/s
µ=Absolute viscosity of air = 1.81 x 10^{-4} g/cm/s
C=Concentration ($µg/m^3$)
c_d=Concentration with dry deposition effects ($µg/m^3$)

The mathematical model that the software uses provides options to model emissions from a wide range of sources that might be present at industrial areas and urban areas. The basis of the model is the straight-line, steady-state Gaussian plume equation, which is used to model simple point source emissions from stacks, roads, storage piles and conveyor belts. Emission sources are categorized into three basic types of sources: point sources, line sources and area sources. The algorithms used to model each of these source types are described in detail in the following sections.

The DISPER dispersion model accepts meteorological data records to define the conditions for plume rise and transport. The model estimates the concentration value for each source and receptor combination and calculates user-selected averages.

9.1 Point source emissions

The model uses a steady-state Gaussian plume equation to model emissions from point sources, such as stacks.

9.1.1 The Gaussian Equation

The model for stacks uses the steady-state Gaussian plume equation for a continuous elevated source. For each source, the origin of the stack coordinate system is placed at the ground surface at the base of the stack. The x axis is positive in the downwind direction, the y axis is crosswind (normal) to the x axis and the z axis extends vertically. The fixed receptor locations are converted to each source's coordinate system. The hourly concentrations calculated for each source at each receptor are summed to obtain the total concentration produced at each receptor by the combined source emissions.

For a Gaussian plume, the hourly concentration at downwind distance x (meters) and crosswind distance y (meters) is given by:

$$c = (Q\ K\ V\ D/2\ pi\ u_s\ sig_y\ sig_z)\ exp[-0.5(y/sig_y)^2] \quad (1)$$

where:

Q= pollutant emission rate (mass per unit time)

K= a scaling coefficient to convert calculated concentrations to desired units (default value of 1 x 10^6 for Q in g/s and concentration in µg/m^3)

V= vertical term (See Section 1.1.6)

D= decay term (See Section 1.1.7)

sig_y,sig_z= standard deviation of lateral and vertical concentration distribution (m) (See Section 1.1.5)

u_s= mean wind speed (m/s) at release height (See Section 1.1.3)

9.1.2 Downwind and Crosswind Distances

The model uses a Cartesian receptor network. All receptor points are converted to Cartesian (X,Y) coordinates prior to performing the dispersion calculations. In the Cartesian coordinate system, the X axis is positive to the east of the user-specified origin and the Y axis is positive to the north. The user must define the location of each source with respect to the origin of the grid using Cartesian coordinates. If the X and Y coordinates of the source are X(S) and Y(S), the downwind distance x to the receptor, along the direction of plume travel, is given by:

$$x=-[X(R)-X(S)]\sin(WD)-[Y(R)-Y(S)]\cos(WD) \quad (2)$$

where WD is the direction from which the wind is blowing. The downwind distance is used in calculating the distance-dependent plume rise and the dispersion parameters. The crosswind distance y to the receptor from the plume centerline is given by:

$$y=-[X(R)-X(S)]\cos(WD)-[Y(R)-Y(S)]\sin(WD) \quad (3)$$

9.1.3 Wind Speed Profile

The wind power law is used to adjust the observed wind speed, u_{ref}, from a reference measurement height, z_{ref}, to the stack or release height, h_s. The stack height wind speed, u_s, is used in the Gaussian plume equation. The power law equation is of the form:

$$u_s = u_{ref}(h_s/z_{ref})^p \qquad (4)$$

where p is the wind profile exponent. Values of p may be provided by the user as a function of stability category and wind speed class. Default values are as follows:

Stability Category	*Rural Exponent*	*Urban Exponent*
A	*0.07*	*0.15*
B	*0.07*	*0.15*
C	*0.10*	*0.20*
D	*0.15*	*0.25*
E	*0.35*	*0.30*
F	*0.55*	*0.30*

The stack height wind speed, u_s, is not allowed to be less than 1.0 m/s.

9.1.4 Plume Rise Formulas

The plume height is used in the calculation of the Vertical Term. The distance dependent momentum plume rise equations are used to determine if the plume is affected by the wake region for building downwash calculations.

Stack-tip Downwash.

In order to consider stack-tip downwash, modification of the physical stack height is performed. The modified physical stack height h_s is found from:

$$h_s' = h_s + 2d_s[(v_s/u_s) - 1.5] \quad \text{for} \quad v_s < 1.5u_s \qquad (5$$

or

$$h_s' = h_s \quad \text{for} \quad v_s > o = 1.5u_s \qquad (6)$$

where h_s is physical stack height (m), v_s is stack gas exit velocity (m/s), and d_s is stack top diameter (m). If stack tip downwash is not considered, $h_s' = h_s$ in the following equations.

Buoyancy and Momentum Fluxes.

For most plume rise situations, the value of the Briggs buoyancy flux parameter, F_b (m^4/s^3), is needed

$$F_b = g v_s d_s^2 (DT/4T_s) \qquad (7)$$

where $DT = T_s - T_a$, T_s is stack gas temperature (K), and T_a is ambient air temperature (K).

For determining plume rise, the momentum flux parameter, F_m (m^4/s^2), is calculated based on the following formula:

$$F_m = g v_s^2 d_s^2 (T_a/4T_s) \qquad (8)$$

Unstable or Neutral - Crossover Between Momentum and Buoyancy.

For cases with stack gas temperature greater than or equal to ambient temperature, it must be determined whether the plume rise is dominated by momentum or buoyancy. The crossover temperature difference, $(DT)_c$, is determined as follows:

for $F_b < 55$,

$$(DT)_c = 0.0297\ T_s (v_s/d_s^2)^{1/3} \qquad (9)$$

and for $F_b >= 55$,

$$(DT)_c = 0.00575\ T_s (v_s^2/d_s)^{1/3} \qquad (10)$$

If DT, exceeds or equals $(DT)_c$, plume rise is assumed to be buoyancy dominated, otherwise plume rise is assumed to be momentum dominated.

Unstable or Neutral - Buoyancy Rise.

For situations where DT exceeds $(DT)_c$ as determined above, buoyancy is assumed to dominate. The distance to final rise, x_f, is assumed to be $3.5x^*$, where x^* is the distance at which atmospheric turbulence begins to dominate entrainment. The value of x_f is calculated as follows:

for $F_b < 55$:

$$x_f = 49 F_b^{5/8} \qquad (11)$$

and for F_b >= 55:

$$x_f = 119 F_b^{2/5} \qquad (12)$$

The final effective plume height, h_e (m), is determined as

for F_b < 55:

$$h_e = h_s + (21.425\ F_b^{3/4} / u_s) \qquad (13)$$

and for F_b = 55:

$$h_e = h_s + (38.71\ F_b^{3/5} / u_s) \qquad (14)$$

Unstable or Neutral - Momentum Rise.

For situations where the stack gas temperature is less than or equal to the ambient air temperature, the assumption is made that the plume rise is dominated by momentum. If DT is less than $(DT)_c$, the assumption is also made that the plume rise is dominated by momentum. The plume height is calculated as:

$$h_e = h_s + 3 d_s (v_s / u_s) \qquad (15)$$

Briggs suggests that this equation is most applicable when v_s/u_s is greater than 4.

Stability Parameter.

For stable situations, the stability parameter, s, is calculated:

$$s = g[(dT/dz)/T_a] \qquad (16)$$

As a default approximation, for stability class E (or 5) dT/dz is taken as 0.020 K/m, and for class F (or 6), dT/dz is taken as 0.035 K/m.

Stable - Crossover Between Momentum and Buoyancy.

For cases with stack gas temperature greater than or equal to ambient temperature, it must be determined whether the plume rise is dominated by momentum or buoyancy. The $(DT)_c$ is determined and solving for DT, as follows:

$$(DT)_c = 0.019582\ T_s\ v_s\ s^{1/2} \qquad (17)$$

If the difference between DT exceeds or equals $(DT)_c$, plume rise is assumed to be buoyancy dominated, otherwise plume rise is assumed to be momentum dominated.

Stable - Buoyancy Rise.

For situations where DT exceeds $(DT)_c$ as determined above, buoyancy is assumed to dominate. The distance x_f is determined by

$$x_f = 2.0715\ u_s\ s^{-1/2} \qquad (18)$$

The plume height, h_e, is determined by

$$h_e = h_s + 2.6\ [F_b/(u_s s)]^{1/3} \qquad (19)$$

Stable - Momentum Rise.

Where the stack gas temperature is less than or equal to the ambient air temperature, the assumption is made that the plume rise is dominated by momentum. Then,

$$h_e = h_s + 1.5[F_m/(u_s s^{1/2})]^{1/3} \qquad (20)$$

The equation for unstable-neutral momentum rise is also evaluated. The lower result of these two equations is used as the resulting plume height.

All Conditions - Distance Less Than Distance to Final Rise.

Where gradual rise is to be estimated for unstable, neutral, or stable conditions, if the distance downwind from source to receptor, x, is less than the distance to final rise:

$$h_e = h_s + 1.60\ [(F_b\ x^2)^{1/3}/u_s] \qquad (21)$$

This height will be used only for buoyancy dominated conditions; should it exceed the final rise for the appropriate condition. For momentum dominated conditions, the following equations are used to calculate a distance dependent momentum plume rise:

a) unstable conditions:

$$h_e=h_s+[3F_m x/(bet_j^2 u_s^2)]^{1/3} \qquad (22)$$

where x is the downwind distance, with a maximum value x_{max}:

$$x_{max}=4d_s(v_s+3u_s)/(v_s u_s) \quad \text{for } F_b=0 \qquad (23)$$

$$x_{max}=49\ F_b^{5/8} \quad \text{for } 0 < F_b < 55\ m^2s^3 \qquad (24)$$

$$x_{max}=119\ F_b^{2/5} \quad \text{for } F_b > 55\ m^2s^3 \qquad (25)$$

b) stable conditions:

$$h_e=h_s+(3F_m)^{1/3}\{\sin[x\ s^{1/2}/u_s]\}^{1/3}[bet_j^2 u_s s^{1/2}]^{-1/3} \qquad (26)$$

where x is the downwind distance, with a maximum value x_{max}:

$$x_{max}=0.5\ pi\ u_s/s^{1/2} \qquad (27)$$

The jet entrainment coefficient, bet_j, is given by,

$$bet_j=(1/3)+(u_s/v_s) \qquad (28)$$

If the distance-dependent momentum rise exceeds the final rise for the appropriate condition, then the final rise is substituted instead.

9.1.5 The Dispersion Parameters

Point Source Dispersion Parameters:

Equations that approximately fit the Pasquill-Gifford curves are used to calculate sig_y and sig_z (in meters) for the rural mode. The equations used to calculate sig_y are of the form:

$$sig_y=465.11628 \times \tan(TH) \quad (29)$$

where:

$$TH=0.017453293[c - d \ln(x)] \quad (30)$$

In both Equations the downwind distance x is in kilometers. The equation used to calculate sig_z is of the form:

$$sig_z=ax^b \quad (31)$$

where the downwind distance x is in kilometers and sig_z is in meters.

Procedures Used to Account for Buoyancy-Induced Dispersion.

The method of Pasquill is used to account for the initial dispersion of plumes. With this method, the effective vertical dispersion s_{ze} is calculated as follows:

$$sig_{ze}=[sig_z^2 +(Dh/3.5)]^{1/2} \quad (32)$$

where sig_z is the vertical dispersion due to ambient turbulence and Dh is the plume rise due to momentum or buoyancy. The lateral plume spread is:

$$sig_{ye}=[sig_y^2 +(Dh/3.5)]^{1/2} \quad (33)$$

where sig_y is the lateral dispersion due to ambient turbulence. It should be noted that Dh is the distance-dependent plume rise if the receptor is located between the source and the distance to final rise, and final plume rise if the receptor is located beyond the distance to final rise.

9.1.6 The Vertical Term

The Vertical Term (V) accounts for the vertical distribution of the Gaussian plume. It includes the effects of source elevation, receptor elevation and plume rise. In addition to the plume height, receptor height and mixing height, the computation of the Vertical Term requires the vertical dispersion parameter (sig_z). The Vertical Term without deposition effects is then given by:

$$V= \exp\{-0.5\ [(z_r-h_e)/\ sig_z]^2\}+\exp\{-0.5\ [(z_r+h_e)/\ sig_z]^2\}+$$
$$+\{\exp[-0.5\ (H_1/sig_z)^2]+\exp[-0.5\ (H_2/sig_z)^2]\}_{i=1,2,...}+$$
$$+\{\exp[-0.5\ (H_3/sig_z)^2]+\exp[-0.5\ (H_4/sig_z)^2]\}_{i=1,2,...} \quad (34)$$

where:

$h_e = h_s + Dh$

$H_1 = z_r - (2iz_i - h_e)$

$H_2 = z_r + (2iz_i - h_e)$

$H_3 = z_r - (2iz_i + h_e)$

$H_4 = z_r + (2iz_i + h_e)$

z_r = receptor height above ground (flagpole) (m)

z_i = mixing height (m)

The infinite series term in Equation {} accounts for the effects of the restriction on vertical plume growth at the top of the mixing layer. This equation assumes that the mixing height in rural and urban areas is known for all stability categories.

The model make the following assumption about plume behavior in elevated simple terrain (terrain that exceeds the stack base elevation but is below the release height):

- The plume axis remains at the plume stabilization height as it passes over elevated or depressed terrain.
- The mixing height is terrain following.

- The wind speed is a function of height above sea level.

Thus, a modified plume stabilization height h_e_ is substituted for the effective stack height h_e in the Vertical Term given by Equation (1-50). For example, the effective plume stabilization height at the point x, y is given by:

$$h'_e = h_e + z_s - z_{(x,y)} \qquad (35)$$

where:

z_s= height above mean sea level of the base of the stack (m)

$z_{(x,y)}$= height above mean sea level of terrain at the receptor location (x,y) (m)

It should also be noted that, the ISC models truncate terrain at stack height as follows: if the terrain height z - z_s exceeds the source release height, the elevation of the receptor is automatically chopped off at the physical release height. The user is cautioned that concentrations at these complex terrain receptors are subject to considerable uncertainty.

9.1.7 The Decay Term (D)

The Decay Term is a simple method of accounting for pollutant removal by physical or chemical processes. It is of the form:

$$D = \exp(-\text{psi}\ x/u_s) \quad \text{for psi} > 0 \qquad (36)$$

$$D = 0 \quad \text{for psi} = 0 \qquad (37)$$

where:

psi= the decay coefficient (s^{-1}) (a value of zero means decay is not considered)

x= downwind distance (m)

For example, if $T_{1/2}$ is the pollutant half life in seconds, the user can obtain y from the relationship:

psi=0.693/$T_{1/2}$ **(38)**

The default value for psi is zero. That is, decay is not considered in the model calculations unless y is specified. However, a decay half life of 4 hours (y = 0.0000481 s^{-1}) corresponds to SO_2 when modeled.

9.2 Non-point source emissions

The CASTOR-AIR model include algorithms to model line and area sources, in addition to point sources. These non-point source options of the model are used to simulate the effects of emissions from a wide variety (conveyor belts, rail lines, area sources,…). The area source model is used to simulate the effects of fugitive emissions from sources such as storage piles and slag dumps.

In this application, the area and line sources (non-point sources) are represented by small many intervals (point sources). The program simulates the non-point sources solving each one of the defined intervals and calculating the total concentration. A great number of point sources simulates the geometry of these non-point sources.

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