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IMDIS
A Teaching Tool for Air Pollution Dispersion Modeling

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IMDIS Operating Manual

Foreword

Predicting air pollution dispersion in a region is a paramount topic usually integrated in Air Pollution Control Engineering courses. As a former professor of a similar course at the University of Minho, I have shared this interest with the author of this book. Romualdo Salcedo, Professor at the University of Porto, has preceded me as an invited teacher of the Biological Engineering undergraduate programme at UMinho and enthusiastically introduced me to several aspects of Air Pollution Control Engineering (and optimization) with the emphasis on Air Pollution Modeling (APM).

The teaching of air dispersion modelling has changed significantly in recent years, in large part due to new regulations and the availability of dedicated software tools. This book intends to serve as a reference to follow-up on a better comprehension of air pollution modeling with the aid of hands-on user-friendly software, highlighting the main advantages (but also disadvantages) of using Gaussian dispersion as the main drive to teach this subject. Throughout the book, author Romualdo Salcedo guides readers with an interactive multisource dispersion estimation tool, helping them understand how air dispersion models work.

IMDIS – A Teaching Tool for Air Pollution Dispersion Modeling begins with a background section that enables readers to quickly enter on APM subject. Next, the book offers sections on air dispersion model highlights and model evaluation, including:

- Calibration of dispersion models with site observed data and the usefulness of the model for uncorrelated sites.
- Comparison with analytical solutions and short-term models (CEMAPS and PTMAX) using examples from the literature.
- Extensive comparison with experimental data (five stacks emitting SO_2 from a petrochemical complex; one stack emitting SO_2 and fine particulates from a pulp and paper unit) and long-term models (Texas Climatological Model).
- Estimation of maximum concentration and critical conditions through a powerful global non-linear optimizer. This capability derives from the author knowledge and more than 35 year experience on numerical optimization that resulted in the development of powerful search algorithms for the global optimum for constrained non-linear continuous (NLP) and mixed-integer (MINLP) problems.
- The IMDIS (Interactive Multisource Dispersion) companion software, a graphical menu-driven computer program, is provided with the corresponding open free code. Independent modules exist for meteorological data, dispersion coefficients and sources. The book includes a detailed Operating Manual containing the program structure, the user interface guide and the fundamentals and examples of APM calculations. Readers can work with these examples to perform their own calculations.

With its comprehensive coverage, IMDIS – A Teaching Tool for Air Pollution Dispersion Modeling is recommended for engineers and scientist who need to perform and evaluate environmental impact assessments. The book's many examples and systematic instructions, strengths very different from traditional books, also make it ideal as a textbook for educational applications in the fields of chemical, biological and environmental engineering and environmental sciences.

Eugénio Campos Ferreira, July 2019

Acknowledgements

This work is dedicated to all who try to make earth cleaner and more enjoyable to live in, a survival condition for next generations.

Introduction

Teaching Air Pollution Modeling (APM) is not an easy task. It involves knowledge on possible approaches to APM, grasping the essentials of complex atmospheric phenomena, and last but not least, teaching without discouraging science or engineering students from pursuing further advanced studies on the subject.

As responsible of the Faculty of Engineering of the University of Porto of an air pollution course from 2004 to 2019, 4th year of undergraduate studies, although this course has naturally changed its focus from APM to Air Pollution Control (with more manageable contents for engineering students, at least in principle), I think I understand why it is so 'difficult' to teach APM. This acknowledgement led me to write about this subject, and I firmly think this book may help teachers to transmit knowledge and skills to their students, who may then gain a better understanding of such phenomena.

This book intends to give both course instructors and undergraduate students a tool to follow-up on a better comprehension of APM with the aid of hands-on user-friendly software, highlighting the main advantages (but also disadvantages) of using Gaussian Dispersion as the main drive to teach this subject. The author believes that the disadvantages of Gaussian modeling are by far surpassed by the advantages, at least at an entry level to the subject.

IMDIS (*Interactive Multisource Dispersion*) software is provided with an open free code such that instructors/students are welcome to use but also to change it by adding more features. It is recommended that an original version of the program be securely kept.

The development of this software, based on a subroutines' structure originally built around *QuickBasic*® for the Macintosh computer platform, took about a period of ten years to develop. To make the software available to Windows' users, it was translated into *Visual Basic*®, being currently available either as source-code or as a compiled version for use under any *Windows*® computer, independently of the operating system under which the software was originally developed.

A distinguishing feature of *IMDIS* is the capability to find globally maximum concentrations under multisource/rose-wind conditions, either from real meteorological data or from potentially worst-case scenarios (critical conditions). The later seem to be especially relevant to the atomic energy industry [1].

This capability derives from the author knowledge and +35 year work on numerical optimization that resulted in the development of powerful search algorithms for the global optimization for constrained NLP and MINLP problems [2, 3]. While it may be argued that Gaussian dispersion models are simple representations of reality, it is also known, that on average, over relatively short times and distances from the emitting sources, they do give enough accurate results, and thus can serve as teaching tools for science and engineering students, as the underlying principles are easy to understand.

Background

A dispersion model is a mathematical expression of the effects of the atmosphere upon air pollutants. This includes the effects of advection (transport) and dispersion (including dilution by the wind and dispersal due to turbulence) and may also include considerations of plume rise, wind shear, and chemical and physical transformations (including removal mechanisms) [1].

Thus, air pollutant dispersion is a complex phenomenon that we try to capture by modeling the various physical and chemical phenomena, to extract some useful information on pollutant concentration levels. As with every mathematical description of real systems, the degree of complexity is variable, where more complex descriptions are usually much more *CPU* and data demanding, albeit usually more accurate.

Inputs to a model are typically meteorological, source data, and dispersion data. Model outputs are estimated pollutant concentrations superimposed on some background value, averaged over different time periods. These time periods will affect the dispersion data, by correcting the dispersion coefficients in some accepted way [36], so that short-term (hours to a day) or long-term (monthly to annual) predictions can be made.

Dispersion models are used to predict future concentrations, but should be calibrated at each site by correlation with observed data. How this calibration is made will in some way dictate the usefulness of the model for uncorrelated sites. This will be discussed further down the text.

Predictions of plume rise are also important to estimate effective points of release, and *IMDIS* incorporates various modeling equations, as plumes rise gradually to final height depending on atmospheric stability. Recognizing that wind-speed gradients are also dependent on atmospheric stability, even for flat terrains, *IMDIS* incorporates this feature for its predictions of pollutant concentrations.

Through powerful optimization code developed for constrained non-linear continuous (NLP) or mixed-integer (MINLP) programming problems, *IMDIS* can find the location and value of the predicted globally maximum concentration, for a multitude of different input data, without recursion to trial-and-error procedures [2, 3].

IMDIS cannot treat long-range transport or pollutant transformation, neither dispersion over complex terrain nor pollutant decay (except for an exponential loss of primary pollutants) and the reader should be aware that these topics may be relevant for the task at hand. Simulation of particulate concentrations are made by assuming non-reflective plumes at the ground and complete absorption of fine particulates by ground-level vegetation.

The learning curve for students should be smoother with Gaussian modeling than with a more complex approach, such as Eulerian/Lagrangian modeling. A brief discussion of Gaussian models available from EPA in their UNAMAP package can be found in [1]. For an appraisal of more advanced Eulerian/Lagrangian models, as well

as how they compare with Gaussian models, the reader is referred elsewhere [28, 29, 30, 31].

It is expected that students will benefit from using *IMDIS*, in parallel with acquiring theoretical concepts from the course instructor.

1 Model Highlights

The validity of Gaussian models and their basics are very well explored by Turner [6] and by a report from the European Process Safety Center [7].

Basically, pollutants are emitted from a stack of some physical height (H_s), the plume may be elevated to the so-called effective height of release (H_e) both by momentum and thermal buoyancies due to the gas velocity and temperature (usually above ambient). The pollutants are diluted due to wind transport in the x direction, and by turbulent diffusion (dispersion) in both the lateral (y) and vertical (z) directions (Figure 1).

This is a simplified image of what may happen, as dispersion might occur in the wind direction (x), and the plume may take quite different shapes depending on the atmosphere's stability.

Special models called *puff-models* may be used to include dispersion in the wind direction that may be a relevant phenomenon at low wind speeds. Also, wind direction may change with height due to friction from the ground, but this is hard to predict and further complicates matters, introducing further uncertainties in the predicted concentration values.
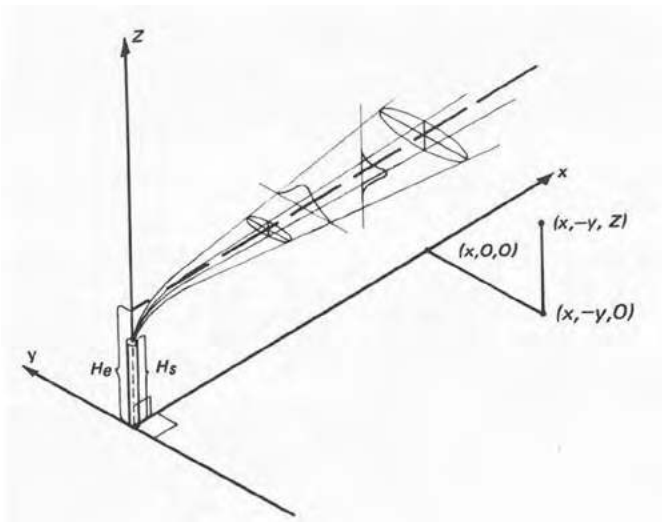

Figure 1 – Schematic representation of Gaussian dispersion [32].

IMDIS is a graphical menu-driven computer program that has been published before [4, 5], with the most relevant features as follows:

Independent modules exist for: Meteorological Data (i-*name.ros* files), Dispersion Coefficients (ii-*name.disper* files) and Sources (iii-*name.fon* files). These modules are case dependent and must be prepared by the teacher/student for each situation.

For sake of clarity, the number of equations that model atmospheric dispersion/ dilution is here kept to an absolute minimum, but the reader should be aware that IMDIS incorporates all necessary equations/relations within the limits of Gaussian modelling.

1.1 Meteorological Data

The meteorological module allows for up-to 6 stability classes, corresponding to A_F of the Pasquill-Gifford scheme, with a maximum of 16 sectors and 6 wind speeds per sector, with a minimum wind average speed of 1m/s allowed, as given in Table 1 [6, 8]. If mean speeds occur in any direction below 1m/s, their frequency of occurrence (x%) is simply discounted from the data, thus dictating that the model will only be applicable for (100-x)% of the measurements' time.

Table 1 – Atmospheric stability classes

Surface wind speed (at 10 m), m sec^{-1}	Day			Night	
	Incoming solar radiation			Thinly overcast or $\geqslant$4/8 low cloud	$\leqslant$3/8 Cloud
	Strong	Moderate	Slight		
$<$ 2	A	A-B	B		
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
$>$ 6	C	D	D	D	D

The effect of mixing height is considered, as well as user-defined stability-dependent wind profile power-law coefficients [6, 9], as per Eq. [1], where n varies with atmospheric stability.

$$\frac{U}{U1} = (H/z1)^n \tag{1}$$

The mixing height is an input, as this parameter is not evaluated by the model.

1.2 Dispersion Coefficients

Four different relations are built into *IMDIS* to estimate the horizontal and vertical dispersion coefficients (σ_y, σ_z), three for rural locations and small sampling times (3–10 min) [10–12] and one for urban locations and a larger sampling time (60 min) [33].

The UNAMAP 1-hr averaging time was adopted as default for both σ_y and σ_z, although the question remains if this is the correct value [36]. The user may alter the fitting parameters and sampling times, through a simple one-parameter equation (Eq. 2), up to 24h [9, 12, 36], but the functional dependence of the fitting formulas must remain unchanged. The parameter n in Eq. 2 may be stability dependent.

$$\frac{Cx}{Cp} = \left(\frac{tp}{tx.}\right)^n \tag{2}$$

1.3 Sources

The source module allows for a maximum of 50 point sources, including flares [12, 36]. Source altitudes are considered for the determination of relative heights between source-receptor pairs, and terrain adjustements are made, but stack heights (source altitude plus physical stack height) cannot be lower than receptors' altitudes. Thus, only moderate terrain corrections are allowed.

Eq. [3] gives the pollutant estimated concentration at ground level, according to the bi-Gaussian model, for a reflective source, viz., the pollutant upon reaching the ground is neither absorbed nor deposited.

$$\chi(x, y, z, H) = \frac{Q}{2\pi\sigma_y\sigma_z U} exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]$$
$$\left[exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right] + exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right] \tag{3}$$

In the model, fine particulates are considered to be completely absorbed upon reaching ground level, and reactive gases may be transformed in other chemical species due to chemical reactions during their transport. In this case, *IMDIS* incorporates a simple decay procedure to account for the disappearance of the primary pollutant.

If a lid exists at height above ground H_i that prevents pollution from dispersing upwards (an inversion lid), then the following applies (32):

$$\chi = \frac{Q}{(2\pi)^{\frac{1}{2}} U H_i \sigma_y} exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \tag{4}$$

Auxiliary computations are needed to perform the estimation of pollutant concentrations. These are: *Plume Rise*, *Wind Transport Speed* and *Receptor Definitions*.

Plume Rise is estimated by IMDIS using one of four different formulas: Holland [6], Briggs (either with or without information on plume enthalpy), as employed by Turner in the UNAMAP files [9], Davidson-Bryant [13] and Moses-Carson [14]. These

formulas can be overridden, if needed, if the actual plume rise can be estimated, for example from photographs or aircraft measurements. For stability classes *E* and F, the user can supply information relative to the potential temperature gradient ($d\theta/dz$), or else employ the defaults provided [12]. The heat release term from the stack may be known, in which case the required information will be prompted for both Briggs and Moses-Carson plume rise formulas.

The Wind Transport Speed affects both plume rise and pollutant concentrations. For plume rise, a wind integrated average from the physical stack height to the effective stack height is employed, obtained through an iterative process [10]. For dispersion estimates, two options are available: the wind velocity at the effective stack height [15], or an integrated average through the current plume vertical displacement [6, 9]. This last approach produces mean transport velocities that are both a function of atmospheric stability and distance downwind from the source. By specifying a flat wind profile, simulations can be done at stack tip, and this is usefull when comparing results with models that employ the wind speed at stack height as the wind transport velocity.

For a more detailed discussion of the meteorological variables relevant to pollutant dispersion, plume types as function of atmospheric stability and how they can be estimated, the reader should consult at least one of the following references [1, 6, 7, 9, 10, 14, 32, 37].

Apart from the input data, model outputs such as *Receptor Concentrations*, *Concentration Isopleths* and *Critical/Maximum Concentrations* must also be considered.

IMDIS employs bi-Gaussian dispersion with an added term to account for multiple reflections from a non-absorbing mixing height (see Eq. 3). Long-term averages (viz. >24h average), are estimated by assuming uniform transverse pollutant dispersion in each wind sector [6, 9, 12]. To avoid discontinuities between sector boundaries, a linear interpolation scheme is deployed between sector centerlines [9].

Up to 100 receptor coordinates can be input either through keyboard, mouse clicking or adjustable grid. In the last two cases, receptor coordinates are superimposed on the source mapping, which is totally scale-configurable with automatic re-drawing of the source/receptor sites. An important feature is the display of each source contribution to the computed concentration at each receptor.

Variable search areas can be chosen to draw concentration isopleths, with either high precision (every pixel) or lower precision (faster execution) schemes. By default, six isopleths are drawn from the maximum computed concentration down, but the user may afterwards choose any number of isopleths up to 15, for the same search area, without having to re-run the program. A sequential averaging scheme [9] is adopted for the estimation of short-term average isopleths (up to 24 hr sampling time) via sequential input of shorter-term estimates (1 hr) data. Running averages are not allowed as it is assumed that all the short-term data have the same time basis.

For the estimation of maximum concentration and critical conditions (worst-case scenarios), *IMDIS* employs a powerful global non-linear optimizer, that has been

shown to provide excellent results for constrained nonconvex non-linear programing (NLP) and for mixed-integer non-linear programming problems (MINLP) [2, 3, 16, 17, 18]. From the point of view of running *IMDIS*, the estimation of maximum concentration and its location should preceed the drawing of isopleths, so that the most relevant location of highest concentrations is readily discovered. The optimization framework works for any combination of source/dispersion/meteorological data. However, for a simple single source/wind direction, a simpler and faster univariate golden search algorithm may also be employed [19].

The user can choose the optimization region (search space) through graphical interaction with a mapping of the pollution sources, or otherwise employ the defaults provided. This is a region of circular area with a 20km radius centered at the origin $(x, y) = (0, 0)$.

For critical conditions, the critical wind speed is searched between the limits imposed by the stability validation based on surface winds [6], with an upper limit of 15m/s (Table 1). To ensure that the search for the critical wind is made in the downwind direction for all sources, a coordinate transformation as proposed [20] is implemented. This transformation relates the terrain coordinates (x, y) to the wind direction θ, to ensure that the search is performed only downstream (relative to the wind) of the active source. The advantage of using a global optimizer will become apparent for a 10-source problem proposed in [20], where comparison of results is made with the use of a non-linear unimodal search algorithm [19].

For short term estimates, validation of stability classes based on surface wind speed is optionally available [6]. Thus, the effect of stability class with the same windrose information is possible to assess, by creating a single stability (chosen at will), as all valid stabilities for those wind speeds will be automatically created as per the data from Table 1.

Simple removing processes characterized by a constant decay rate [21], and totally absorbed pollutants (such as fine particulates) are also treated by the model.

IMDIS is quite user-friendly, as the different file types (source, wind rose, dispersion) are automatically recognized by the corresponding sub-models. Also, error-trapping routines and automatic data checking were extensively developed and tested.

2 Model Evaluation

There are no universally accepted criteria for assessing model performance [1, 22].

Some criteria usually accepted are [11, 22, 23, 24]:

i.) Analysis of paired predicted and observed concentrations;
ii.) Analysis of paired predicted and analytical solutions, when available;
iii.) Inter-comparison between predictions from different models;
iv.) Ability to predict peak concentrations;
v.) Kolmogorov test for comparison of the unpaired cumulative frequency distributions;
vi.) Hanna's normalized bias and mean square error.

In the testing of *IMDIS*, the only criteria evaluated were the first four.

2.1 Comparison with Analytical Solutions and Short-term Models

Simple examples are available in the literature [6, 9, 25]. The objective of these tests was to establish the soundness of the various sub-models with emphasis on estimation of dispersion coefficients, plume rise, receptor concentrations and critical conditions, but also to eliminate possible sources of programming errors. The agreement between *IMDIS* and the analytical solutions is very good, both for receptor concentration actual maxima or critical conditions [25]. The main causes for the observed differences was on the dispersion estimates (σ_y, σ_z), where differences as small as 3% can produce much larger ($\approx$20%) differences in the computed concentrations.

IMDIS was next compared to single-source short-term programs, such as *CEMAPS* and *PTMAX* [26, 27]. The results from *IMDIS* agree within 5% with those from these two models. To estimate critical conditions, *PTMAX* employs an analytical scheme dependent on the dispersion coefficients' formulas, contrary to the numerical non-linear solvers of *IMDIS* that makes it of more general applicability.

Below we examine the model response to a multisource problem, in order to find the critical conditions and their sensitivity to sub-modules such as plume rise and dispersion formulas.

Example 1
In air pollution, it may be relevant to estimate the critical conditions for pollution levels, i.e., meteorological conditions that under one or more stacks may produce the worst possible situations. These are called critical conditions, and the unknowns to be found are the direction and average speed of the wind, as well as the coordinates of the critical concentration point and its value. The usefulness of this is not much on the values per se, but as an estimate of where pollution monitors should be placed.

Let us consider a 10-source test case given in [20], for the determination of the critical condition (wind speed and wind direction, maximum concentration location and value). Table I gives the source emission characteristics description and relative location.

The following 10 sources are at the same altitude (for simplicity, at zero altitude) with the following characteristics:

Table 2 – Emission sources characteristics for Example 1

Source no.	1	2	3	4	5	6	7	8	9	10
X (m)	-3000	−2600	-1100	1000	1000	2700	3000	-2000	0	1500
Y (m)	-2500	-300	-1700	-2500	2200	1000	-1600	2500	0	-1600
H (m)	183	183	160	160	152.4	152.4	121.9	121.9	91.4	91.4
D (m)	8	8	7.6	7.6	6.3	6.3	4.3	4.3	5	5
Q (g/s)	2883	2883	2391	2391	2174	2174	1174	1174	1304	1304
Ug (m/s)	19.25	19.25	17.69	17.69	23.40	23.40	27.13	27.13	22.29	22.29

X, Y – arbitrary terrain coordinates at altitude zero; H – physical stack height, D – physical stack diameter; Q – SO_2 emission rate; Ug – gas velocity from stack.

The search region for the decision vector $\{x, y, U, Q\}$, slightly changed from the original data [20], is as follows:

-50000 ≤ x ≤ 50000 m
-50000 ≤ y ≤ 50000 m
0 ≤ U ≤ 12.5 m/s
0 ≤ Θ ≤ 2π

For simplicity, ambient temperature at ground level and from gases released from stacks is as follows:

T_a = 288 K
T_g = 413 K

Solution:
IMDIS was run by creating the source file *WangLuus*.fon (Figure 2), using Holland's equation for all sources for estimating plume rise, and by creating a fictitious meteorological file with a single-sector and single wind speed, arbitrarily set at 0° N. This is a fictitious file that is needed to find the atmospheric stabilities compatible with

the possible wind speed variation from 1 to 12.5 m/s [20]. From Turner [6], this data is compatible with the occurrence of stabilities C and D (refer to Table 1).

Next, we choose the optimization to be done. As we are looking for the critical conditions for a ten source case, we bypass the *1-source/1-sector* dialog boxes (see Figure 3), but also the *(X, Y, Cmax)*, as we want to find the critical *U*. We are left with the *(U, X, Y, Cmax) – General* and with the *Search by Default*. This last option differs from the *(U, X, Y, Cmax) – General*, because the search region is by default defined by a circle with a fixed radius of 20km with center at the origin.

Figure 2 – Source data for example 1. All sources use Hollands's equation for plume rise.

Figure 3 shows the type of optimization to be done. As there is only a wind direction and speed, to be determined as causing the worst-case ground-level concentration, Figure 4a shows the results from the local golden search optimizer, and Figure 4b from the global SGA optimizer. For both optimizers, critical conditions are a function of atmospheric stability, but the global search algorithm gives higher critical concentrations for both stabilities. For stability D, the location of the critical point is heavily dependent on the algorithm. Thus, for difficult problems, only the global search algorithm should be employed to find the critical conditions.

The results obtained above may be refined by conducting a search over a smaller region than the one used (± 20 x 20 km). Also, different results might be obtained by using different plume rise formulas.
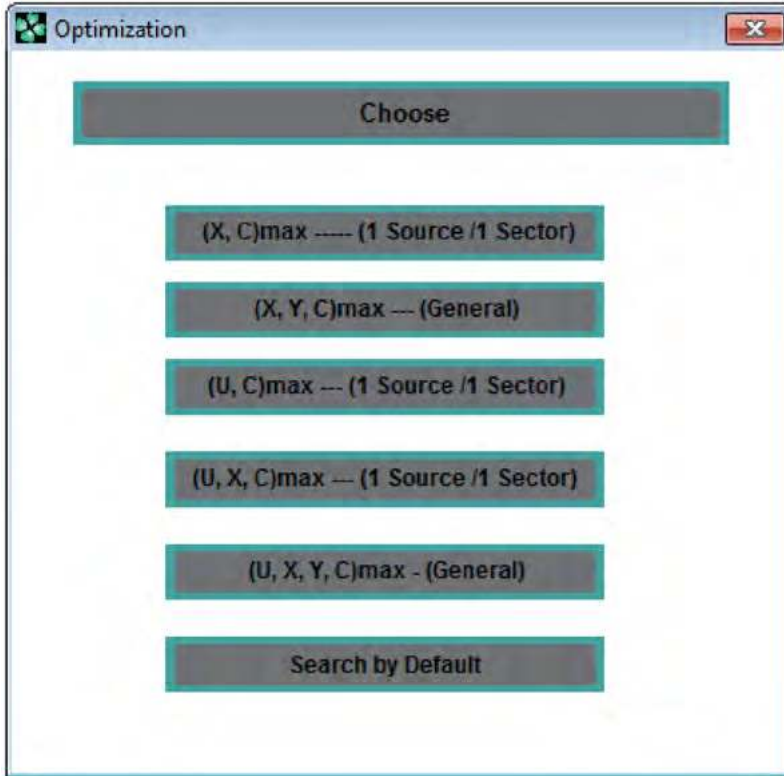
Figure 3 – Choosing the type of optimization to be done *(U, X, Y, C) – General* or *Search by Default.*

Figure 4a – Critical condition estimates from the Golden Section optimizer (Holland plume rise).

Next we can draw the corresponding isopleths, in the **isopleths submenu**. For example, for stability C, using the information provided in Figure 4a or 4b, as they are very similar, we obtain Figure 5a and a critical concentration of 2135.9 µg/m³, very close to the result reported by the SGA optimizer (Figure 4b).

Now we repeat the process with stability D, where the optimizers gave quite different results. Figs. 6a - 6b show the corresponding isopleths (five concentration intervals were chosen), where it is clear that this is indeed a difficult subject, that may

Figure 4b – Critical condition estimates from the SGA optimizer (Holland plume rise).
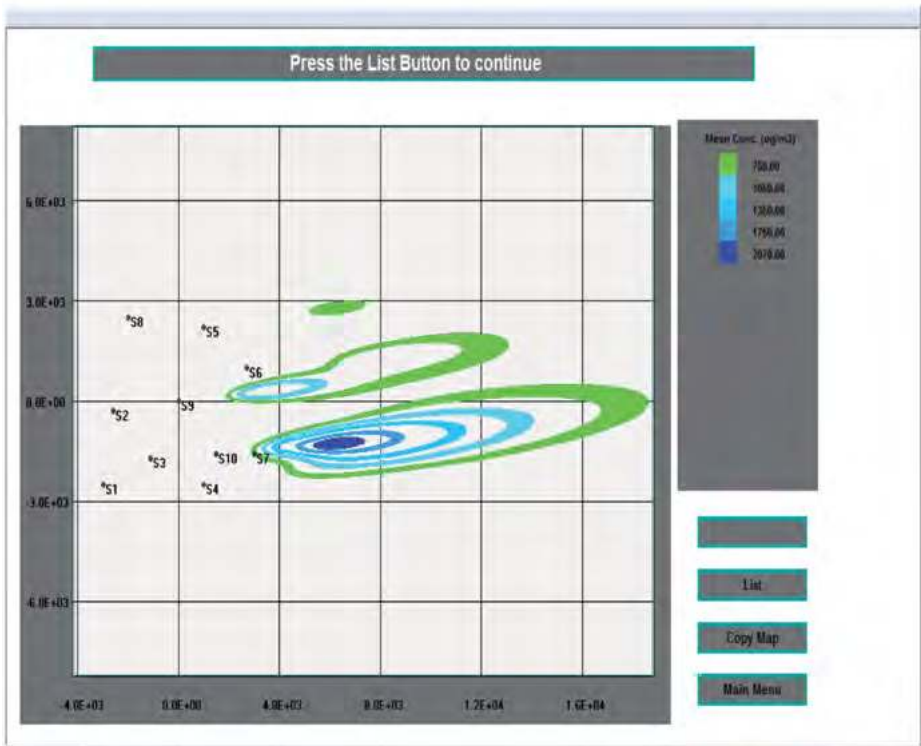
Figure 5a – Selected isopleths corresponding to stability C (data from Figs. 4a or 4b).

also be greatly influenced by the choice of the sub-modules, especially the dispersion sub-module.

With the data from the Golden Search optimizer, the critical concentration is found to be 1308.8 µg/m^3, larger than the value reported from this optimizer (Figure 4a), and the selected isopleths can be seen in Figure 6a.

With the data from SGA optimizer, the critical concentration is found to be 1433.5 µg/m^3, very similar to the value reported from this optimizer (Figure 4b), and the selected isopleths can be seen in Figure 6b.
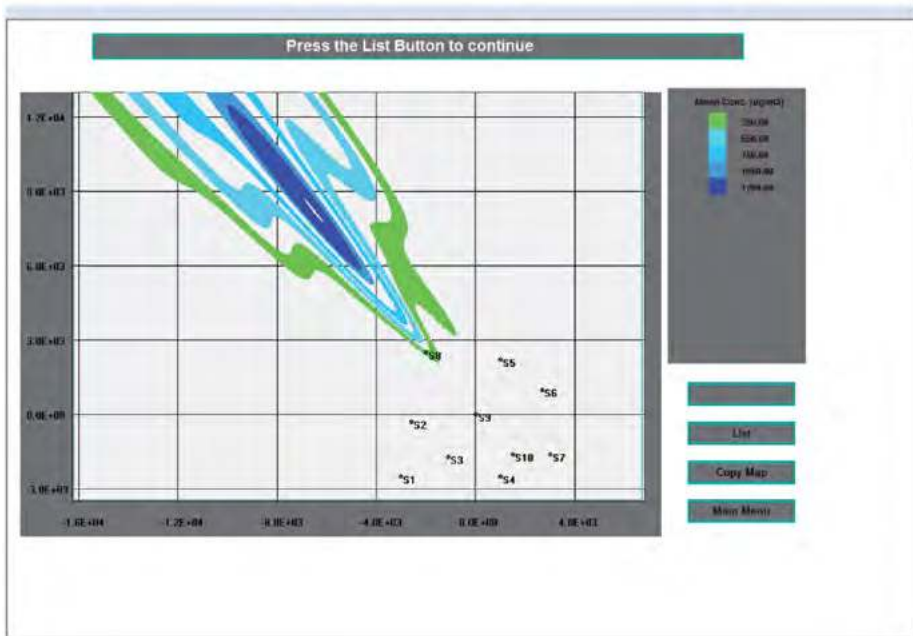
Figure 6a – Selected isopleths corresponding to stability D (data from Figure 4a).
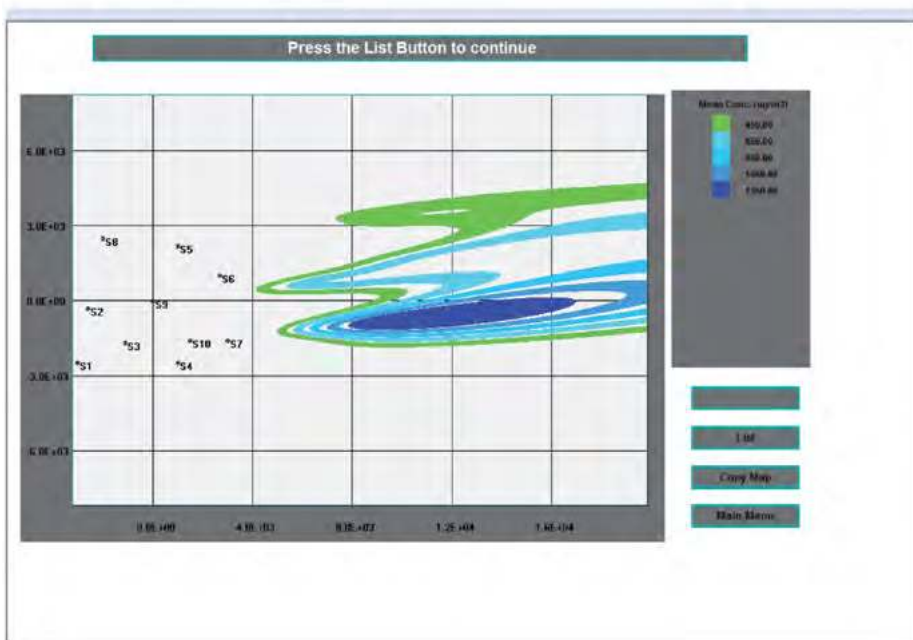
Figure 6b – Selected isopleths corresponding to stability D (data from Figure 4b).

Clearly, the exhaustive pixel-by-pixel search for the critical conditions is no better than using the global SGA optimizer.

Wang and Luus [20] have only considered stability D (neutral or adiabatic conditions), and have used an analytical approximation to the Pasquill-Gifford estimates of plume rise, but with a multiplicative correction factor of 0.8 for the concentration. The Pasquill-Gifford dispersion estimates are used by *IMDIS* as given by Turner [6], or by Green [11]. With the Green formulas, the critical condition for stability *D* is 3.4m/s@140°N, with maximum concentration of 952 μg/m^3, located at $x \approx$ –7000m and $y \approx$ 8416m. These compare reasonably with Wang and Luus' results of 964 μg/m^3 (= 771/0.8)@(x; y)=(−8040m; 9370m).

2.2 Comparison with Experimental Data and Long-term Models

The estimates from *IMDIS* should be compared with experimental data. Chuang [34] reports SF$_6$ (a tracer) concentration values for 29 receptors, for an oil burning power plant, for two consecutive hours with 15min sampling times, with prevailing stabilities being *C* and *D* with equal probability. The stack height was 70m.

IMDIS was used with both Holland and Briggs plume rise formulas, and the best correlation (r = 0.935) was obtained using Holland's equation, although with some scatter at very low concentration levels (<0.5 μg/m^3). The observed maximum concentration was measured at 3km from the plant, and IMDIS locates the maximum between 1 to 3 km from the plant, depending on atmospheric stability and plume rise formula.

Next, we compare IMDIS with a long-term model, the *TCM* (Texas Climatological Model) as used in [12] to predict seasonal SO$_2$ concentrations from a Portuguese petrochemical complex at Sines for a 4-year period (1979–1982). Here only the data from Winter of 1981 and Spring of 1982 were used, because complete data is only available for these periods.

The terrain surrounding the complex is relatively flat, and data is available at three sampling stations located at different altitudes (43, 103 and 196m). There are five stacks emitting SO$_2$ with physical stack heights from 120 to 234m, located at terrain altitudes of 29 to 43m. The frequency distributions of atmospheric stability for the 6 Pasquill-Gifford classes, together with the corresponding 6 wind speed classes and 16 sectors are also known. This information was obtained from a modified meteorological STAR program, the STARCAN program [12] that combines the wind frequencies observed at Sines with the atmospheric stabilities observed at Lisbon, ≈ 80km north of Sines.

Good correlations for Spring 1982 were obtained using Moses-Carson and Briggs plume rise formulas (respectively r^2 = 0.772 and r^2 = 0.764). However, *IMDIS* under-

predicts concentrations by about 3–4 µg/m³, a sign that the background may be significant [4, 5, 12].

IMDIS was compared to *TCM_STARCAN* and to *TCM_STAR*, and curiously a much better correlation was obtained using the meteorological data from Lisbon (r^2 = 0.877) than from Sines (r^2 = 0.320). Both *IMDIS* and *TCM* give poor predictions for Winter, using either the *STAR* or *STARCAN* stability data, presumably due to the lack of knowledge on vertical mixing heights [12].

Below we explore in more detail the 1982 Spring period, using *IMDIS*.

Example 2

Figure 7 shows the source data for Sines and Figure 8 shows the wind-rose frequency distributions. These can be obtained under Excel® using available software [35]. Stability frequencies are 73.4%(D), followed by 9.1%(E), 8.7%(C), 5.8%(F), 2.6%(B) and 0.4%(A).

Source Data

| Atm. Pressure | 1013 | mbar |
| Atm. Temperature | 293 | K |

Source No.	X (m)	Y (m)	H (m)	Alt (m)	Rate (g/s)	Th.En. (MW)	Vs (m/s)	D (m)	T (K)	dH (m)
1	0	0	234	41	432		3.85	5.9	513	
2	264	-202	120	43	281		20	3.8	1273	
3	-2444	2903	150	29	25.7		1.31	3.1	473	
4	-2444	2903	150	29	134.3		5.52	3.1	403	
5	-2444	2903	150	29	84.9		3.4	3.1	403	

Power Law Coefficients

Stab A	Stab B	Stab C	Stab D	Stab E	Stab F
0.1	0.15	0.2	0.25	0.25	0.3

Figure 7 – Source data for petrochemical complex at Sines [12].

Two different horizontal and vertical dispersion formulas were used, as they are appropriate for this case (conditions are neither urban neither with stack physical heights below 50m). These are given in Figs 9a–9b. Also, simulations were done with two formulas for plume rise, Holland and Briggs [6].

Maximum concentrations and isopleths were obtained for each combination of plume rise/dispersion formulas, for an altitude of 43m (the lowest altitude for a sampling station). First, maximum values of concentration and their locations were obtained using the optimization capabilities of *IMDIS*, as then we can correctly locate where we should draw the isopleths, a more demanding *CPU* task. A background value of 4µg/m³ was added to the initial conditions, as suggested [12].
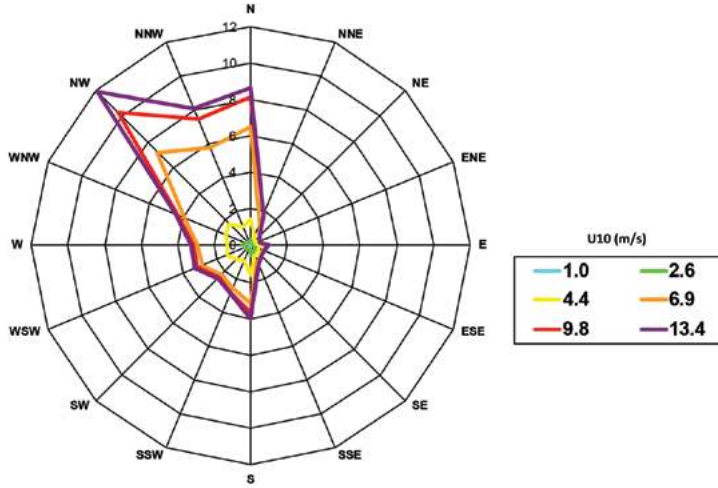
Figure 8 – Wind-rose overall weight-averaged frequency distribution.

SIGMAY EQUATION:		PASQUILL					
		Stab A	Stab B	Stab C	Stab D	Stab E	Stab F
	a	-0.023	-0.015	-0.012	-0.006	-0.006	-0.003
	b	0.35	0.248	0.175	0.108	0.088	0.054
SIGMAZ EQUATION:		PASQUILL					
		Stab A	Stab B	Stab C	Stab D	Stab E	Stab F
	a	0.88	-0.985	-1.186	-1.35	-3.357	-3.8
	b	-0.152	0.82	0.85	0.793	1.456	1.419
	c	0.147	0.017	0.005	0.002	-0.053	-0.055
Sampling Period	60 min						

Figure 9a – Pasquill parameters for σ_y and σ_z [6].

SIGMAY EQUATION:		GREEN					
		Stab A	Stab B	Stab C	Stab D	Stab E	Stab F
	a	0.927	0.37	0.283	0.707	1.07	1.17
	b	250	202	134	70.7	56.6	37
	c	0.189	0.162	0.134	0.135	0.137	0.134
SIGMAZ EQUATION:		GREEN					
		Stab A	Stab B	Stab C	Stab D	Stab E	Stab F
	a	0.927	0.37	0.283	0.707	1.07	1.17
	b	102	96.2	72.2	47.5	33.5	22
	c	-1.918	-0.101	0.102	0.465	0.624	0.7
Sampling Period	60 min						

Figure 9b – Green parameters for σ_y and σ_z [11].

Table 3 – Maximum conditions for Spring 1982, for Briggs/Holland plume rises and Green/Pasquill dispersion combinations, for the 43m altitude receptor

	Briggs		Holland	
	Green	Pasquill	Green	Pasquill
x (m)	-2443	4537	264	3598
y (m)	-0.095	-4537	-3024	-3536
C (µg/m3))	7.8	9.6	10.5	13.1
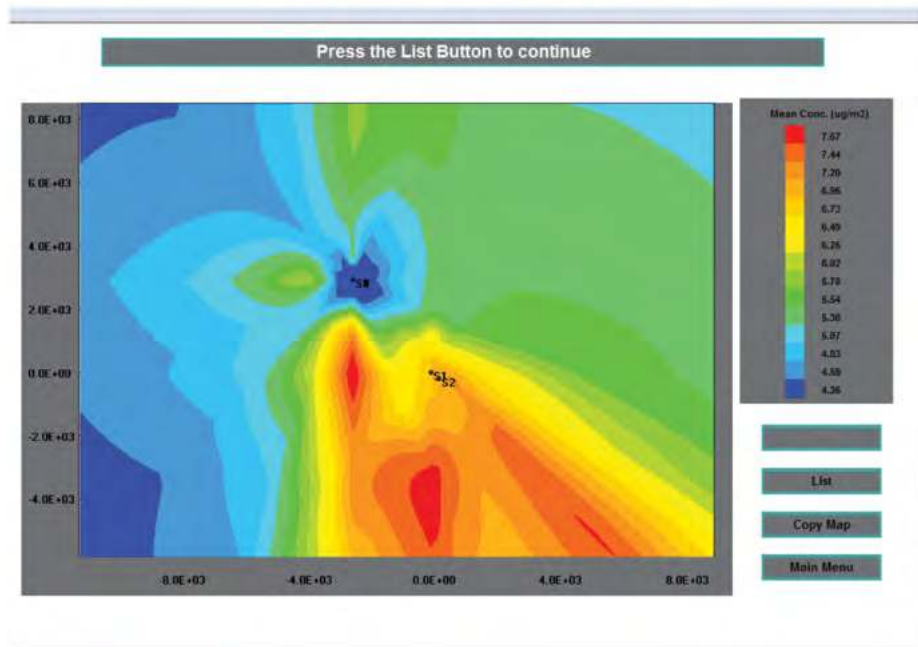
Figure 10a – Isopleths for Spring 1982 with Briggs plume rise and Green dispersion – 43m altitude recepto.

Table 3 shows the optimization results that served as guidelines for the isopleths location given in Figs. 10a–10d.

We can conclude that, in this case, Green dispersion coefficients predict lower concentrations than Pasquill's dispersion, and that Briggs plume rise formulas also predict lower concentrations than Holland's formula.

Next, we examine the situation for the 196m altitude receptor. Using the same reasoning as before, we first estimate the maximum concentration value and location, using the optimization capabilities of *IMDIS*. The results can be seen in Table 4. The corresponding isopleths can be seen in Figs. 11a–11d.
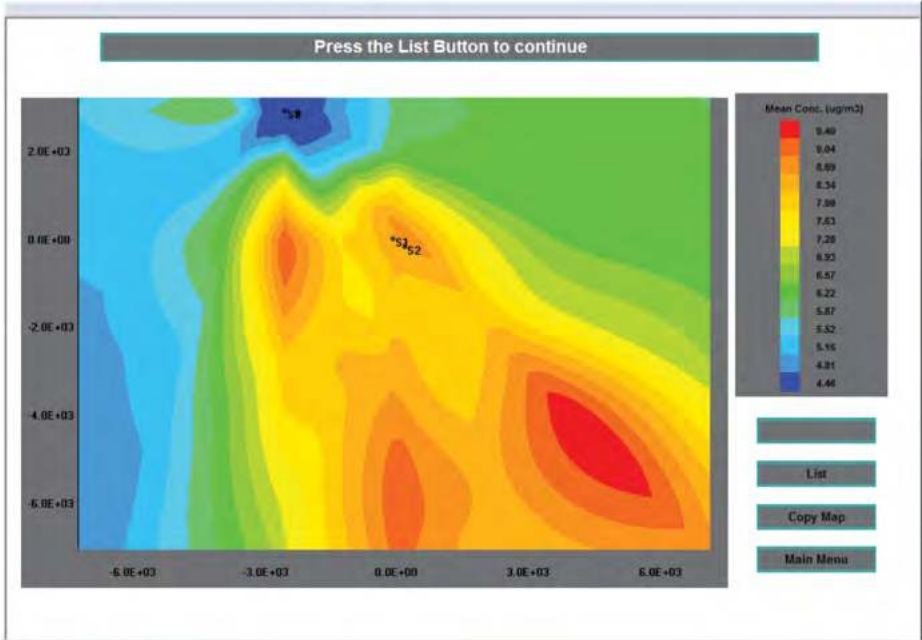
Figure 10b – Isopleths for Spring 1982 with Briggs plume rise and Pasquill dispersion – 43m altitude receptor.
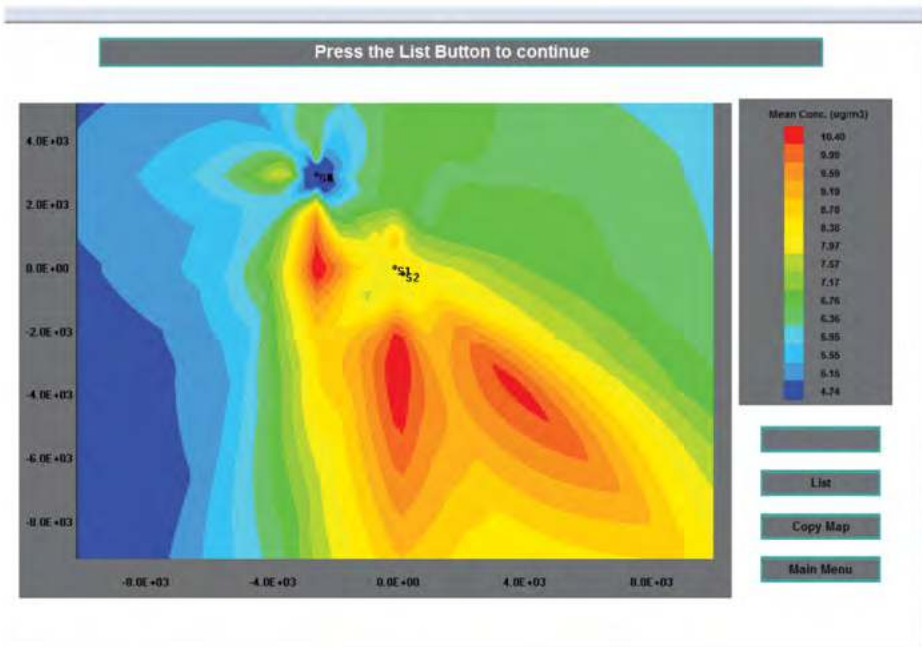
Figure 10c – Isopleths for Spring 1982 with Holland plume rise and Green dispersion – 43m altitude receptor.
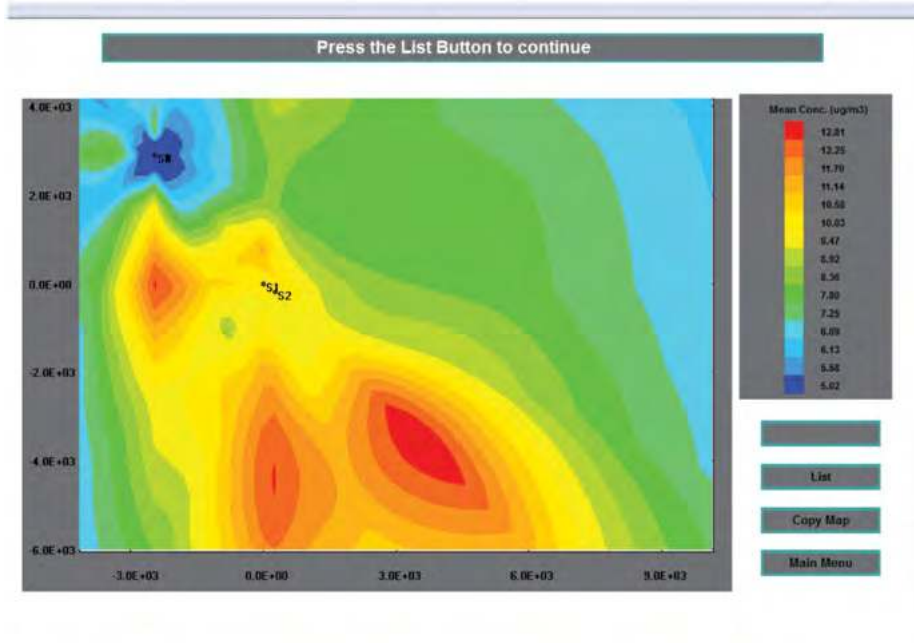
Figure 10d – Isopleths for Spring 1982 with Holland plume rise and Pasquill dispersion – 43m altitude receptor.

Table 4 – Maximum conditions for Spring 1982, for Briggs/Holland plume rises and Green/Pasquill dispersion combinations, for the 196m altitude receptor

	Briggs		**Holland**	
	Green	Pasquill	Green	Pasquill
x (m)	2813	2436	1657	1567
y (m)	-2813	-4436	-1657	-1567
C (µg/m3))	11.7	14.9	27.0	32.5

Again, we conclude that the Pasquill/Holland combination predict the highest concentrations.

These graphs can be easily redrawn with different values for the isopleths, as the numerical values corresponding to each pixel position (x, y, altitude, concentration) is kept in a file. For example, choosing the following 5 isopleths as per Figure 12, we get Figure 13.
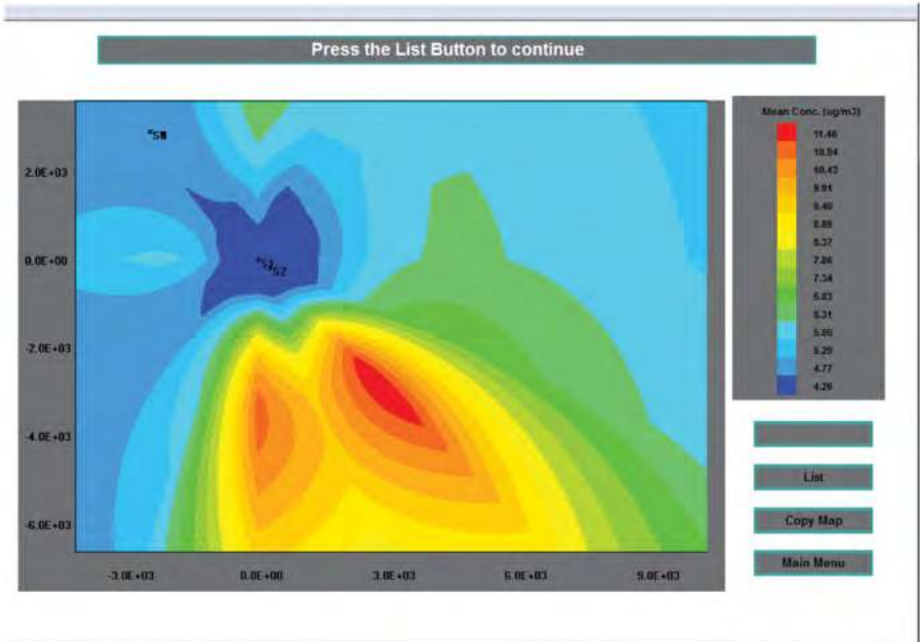
Figure 11a – Isopleths for Spring 1982 with Briggs plume rise and Green dispersion – 196m altitude receptor.
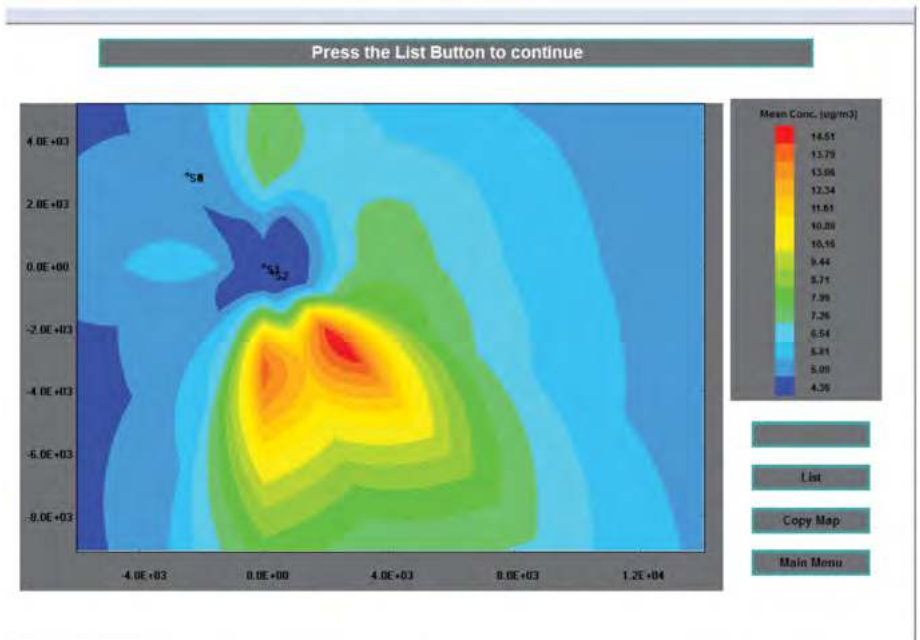
Figure 11b – Isopleths for Spring 1982 with Briggs plume rise and Pasquill dispersion – 196m altitude receptor.
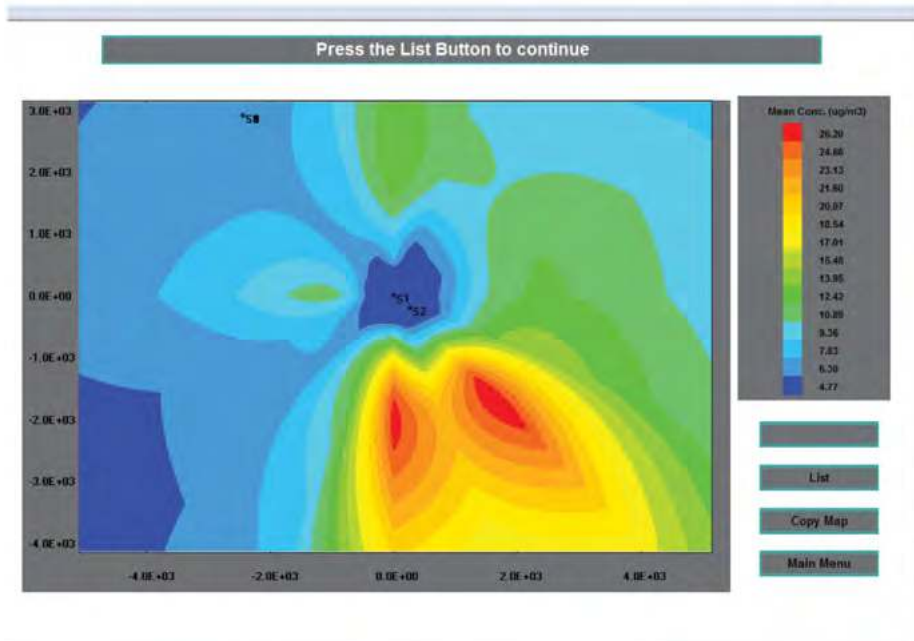
Figure 11c – Isopleths for Spring 1982 with Holland plume rise and Green dispersion – 196m altitude receptor.
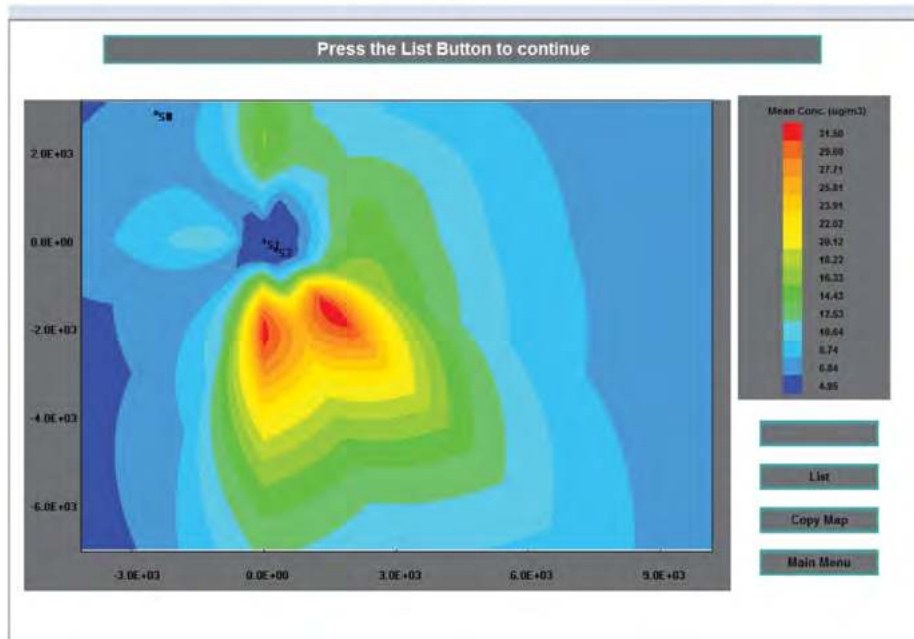
Figure 11d – Isopleths for Spring 1982 with Holland plume rise and Pasquill dispersion – 196m altitude receptor.

Figure 12 – Choosing isopleths for Spring 1982 with Holland plume rise and Pasquill dispersion – 196m altitude receptor (chosen by the user).

Figure 13 – Isopleths for Spring 1982 with Holland plume rise and Pasquill dispersion – 196m altitude receptor (chosen by the user as per Figure 12).

Example 3

It is instructive to run an example that compares gaseous and fine particulate emissions. We next study such an example, where wind-roses are available for every month of the year 1991, and both SO_2 and fine particulates are emitted from one single 93m stack, located at 30m altitude in the North of Portugal, in a pulp and paper industry. Particles are controlled by an electrostatic precipitator, so they should be quite fine (<5 μm). Figure 14 shows the source file, and Figure 15 the wind rose frequency distributions for each atmospheric stability [35]. Stability frequencies are 41.9%(D), followed by 32.1%(E+F), 16.3%(C), and 9.8%(B).

Source Data										

Atm. Pressure		1020	mbar							
Atm. Temperature		282.7	K							

Source	X	Y	H	Alt	Rate	Th.En.	Vs	D	T	dH
No.	(m)	(m)	(m)	(m)	(g/s)	(MW)	(m/s)	(m)	(K)	(m)
1	0	0	93	30	23		8	3.7	488.2	

Power Law Coefficients					
Stab A	Stab B	Stab C	Stab D	Stab E	Stab F
0.1	0.15	0.2	0.25	0.25	0.3

Figure 14 – Characteristics of the stack at a Portuguese Pulp & Paper unit.
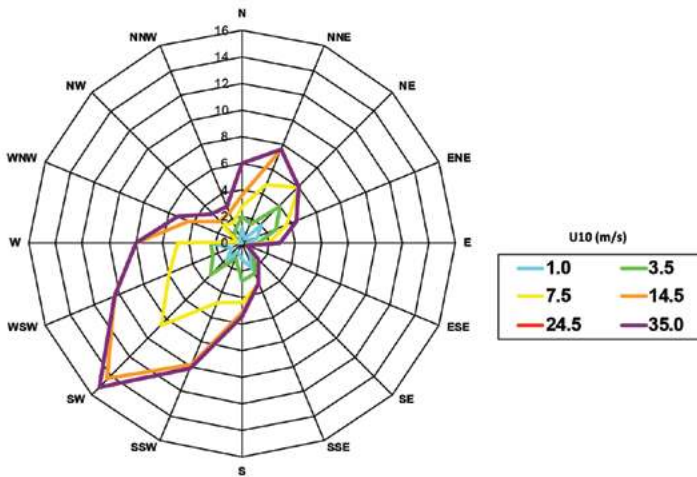
Figure 15 – Wind-rose overall weighted-average frequency distribution.

We choose the month of July, but any demonstration month will give similar conclusions. *IMDIS* was first run with the optimizers to give an estimate of the maximum concentrations, and this can be seen in Figure 16a for SO_2 and on Figure 17a for fine particles.

> **Final results for height 0 m**
>
> X : 1519.523 m   Y : 1519.523 m   Max. Conc. : 0.4 ug/m3
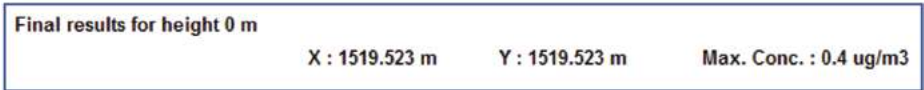
Figure 16a – Location and value of SO$_2$ maximum concentration (Viana do Castelo).
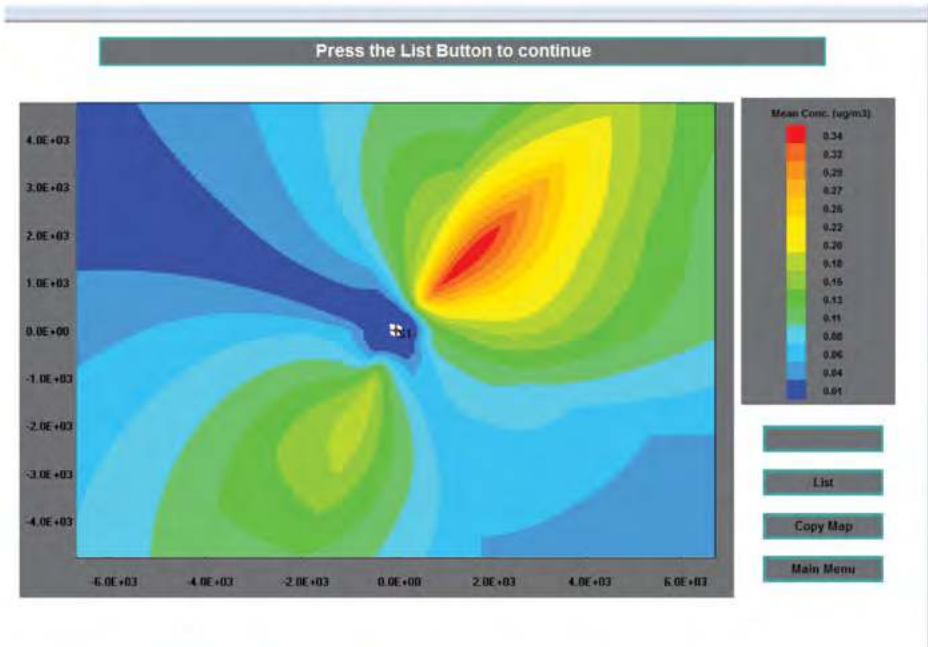
Figure 16b –SO$_2$ isopleths (Viana, Green dispersion coefficients, Briggs plume rise).

> **Final results for height 0 m**
>
> X : 1519.436 m   Y : 1519.436 m   Max. Conc. : 0.2 ug/m3

Figure 17a – Location and value of fine particulate maximum concentration (Viana do Castelo).

Figure 16b shows the corresponding isopleths for SO$_2$ and Fig. 17b, for particulates. Obviously, the location is the same but SO$_2$ concentrations are larger ($\approx$ 2x) because the ground was considered totally absorbing for particulates and totally reflective for SO$_2$.
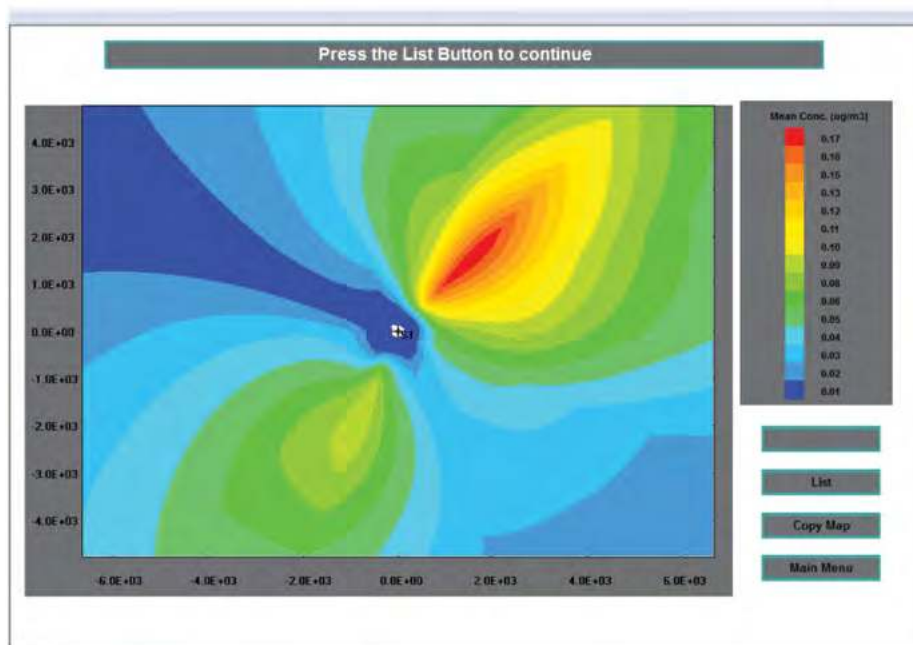
Figure 17b –Fine particle isopleths (Viana, Green dispersion coefficients, Briggs plume rise).

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IMDIS Operating Manual

Overview and Program Structure

IMDIS has been published before, but at a simplified level and on a restricted access basis [4, 5].

The existence of a main menu to link to all program activity is a trait that eases program execution even for novice users, allowing to simulate different approaches of the same scenario without the need to repeat data input.

The control of the information acquired in the data acquisition dialogs, in particular the numerical/alphanumeric nature of the parameters and physical limits, if any, of the various quantities involved; the storage of input data and results in text files, under different types, according to the type of information, such as wind-rose, dispersion, and emitting source(s); the display of the input data and the results by on-screen listing and outwards listing, through communication with printing devices, is another welcome feature that has been incorporated in the *IMDIS* package.

The numerical calculation subroutines are basically the original ones developed for the *Macintosh*® environment. The great change from earlier versions of the software is related to a much easier communication with the user, through a friendly *GUI*. The inclusion of colors to the graphical interface, the increase of the dimensions of the main window, the acquisition of data carried out interactively, sequentially and with instructions to more easily provide the user with the required information, provides a more functional, interactive and simpler communication interface. I believe this will greatly enhance the user experience.

Image 1 presents a generic flowchart of how *IMDIS* operates. The colored rectangular blocks represent the options in the main menu. Some of the main sub-menus are represented by the remaining rectangular blocks. It can also be seen how data storage and data output are processed.

A very usefull feature is the ability to correct wrong choices from the main menu by simply closing the respective window. The main menu and all files downloaded to memory will remain active and the correct choice of path can then be easily pursued.

To guide the user through somewhat complex menus, that may quickly become cumbersome, each sub-menu prompts for what data is expected to be answered, so that there are no ambiguities left.
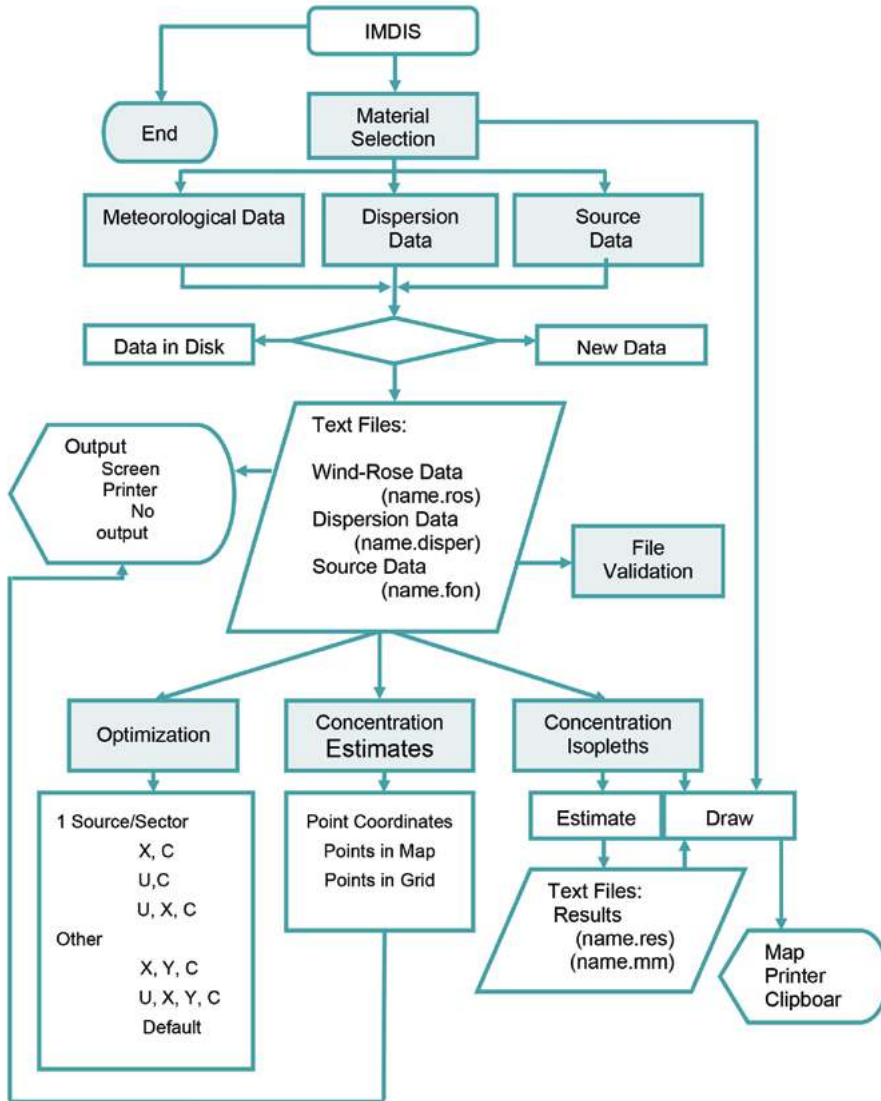
Image 1: Flowchart representing how *IMDIS* operates.

1 *IMDIS* – User Interface and Fundamentals

Once *IMDIS* is executed, the main interface of the program is presented. The main menu is on the left-hand side. All the necessary procedures for the creation and execution of the simulation are initiated in this menu.

Initially, the user has only access to the menus for materials selection, file validation and stopping the execution of the application.
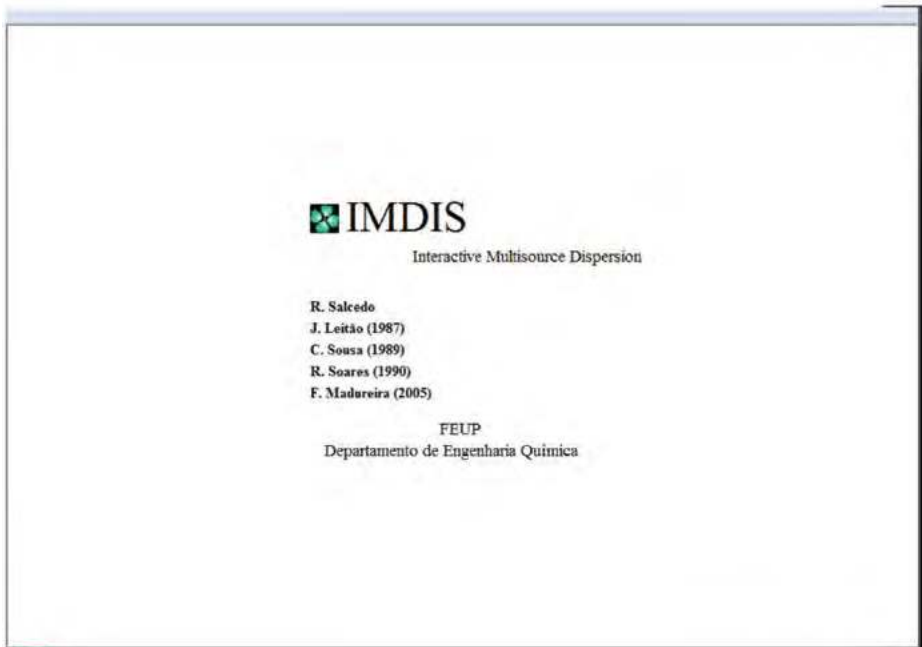
Image 2: *IMDIS* main interface.

1.1 Selection of Materials

1.1.1 Gases/Particles Menu

The first step in the creation of the required simulation consists of selecting the kind of materials released by the emission sources. By activating the Gases/Particles button in the main menu, a dialog box appears (**Image 3**) in the central area of the window where you can select one between gases and particles.

Depending on the selection, the information to be provided will be different. In the case of gaseous emissions, **Image 4** (image on the left-hand side), the inert/
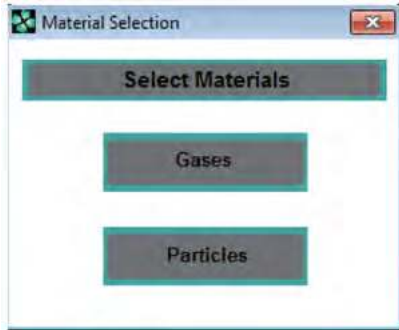
Image 3: Materials type selection.
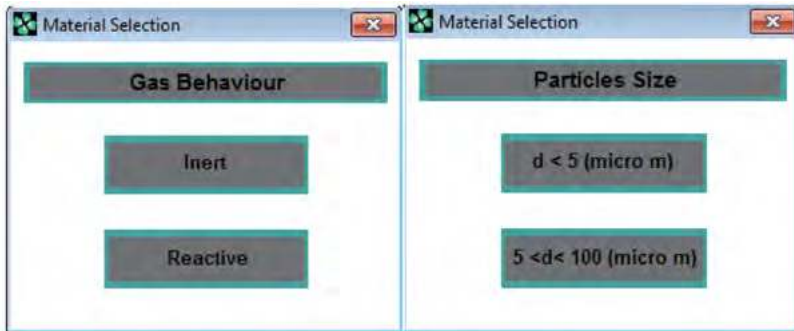
Image 4a and 4b: Characterization of the selected materials.

reactive behavior of the gases must be defined. In the case of particles (image on the right-hand side), the main characterization parameter is their dominant size. Particles within [5, 100]μm suffer sedimentation, while particles below 5 μm are treated as gases for transport, but are considered totally absorbed upon touching the ground.

The reactive gas option implies setting the half-life of the gas, viz. time necessary to decay pollutant concentration by 50%.

The selection of particles between 5 and 100μm requires setting their diameter and specific gravity. Regardless of the choice, it is helpful to define a background concentration, which corresponds to the atmospheric concentration of the material in question, and which is not released from the stack(s) under study. Unfortunately, many times this information is not available.

Thus,

- The option of dispersion simulation for particles between 5 and 100μm in diameter is included, by allowing these particles to sediment along the plume path; particles smaller than 5 μm are treated as non-reflective gases;
- The possibility to define a background concentration in order to consider the existence of a specific material (particle or gas in the atmosphere) which were not released from the stacks under study.

To avoid execution errors and provide physical consistency to the parameters introduced by the user, there are control subroutines which warn the user of inconsistencies and display messages at the top of the dialog box (see **Image 5**, text in white). This icon also shows instructions which aid communication and facilitate the use of the program.
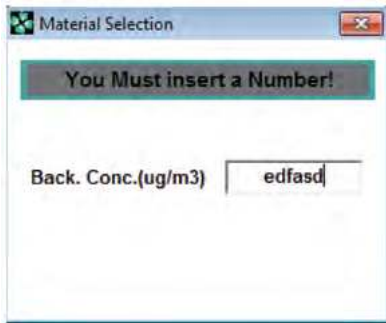
Image 5: Error messages.

Once the process of selecting and characterizing the materials is concluded, the dialog box is automatically closed, and all icons in the main menu become accessible.

1.2 Data Entry

The data needed for the creation of the simulation is organized in three separate sets.
- *Meteorological Data*, which provides all necessary information for the characterization of the meteorological conditions during the period under analysis;
- *Dispersion Data*, which contain the information about the dispersion coefficients;
- *Pollutant Emission Data*, which contain information directly related to the sources.

In order to define all data corresponding to each set, all of the three buttons in this section of the main menu have to be pressed in turn. The first window that appears when selecting any one of the three options is depicted in **Image 6**. As previously stated, data is stored in text files of different types for better organization and use of the information. For this reason, the possibility of loading information from existing files or creating new data is presented, if desired.

When opting to load the information from existing files, a predefined dialog is presented by the operating system, in which the user can locate and open the file for reading. To avoid confusions, the user can only see the type of file which can hold the data to be read. For instance, when loading meteorological data, only **ros** files are available, as can be seen in **Image 7**. If no file is selected, the dialog shown in **Image 6** remains visible to allow a new choice to be made. Once the file has been selected, the

Image 6: Mode selection of acquisition of information.
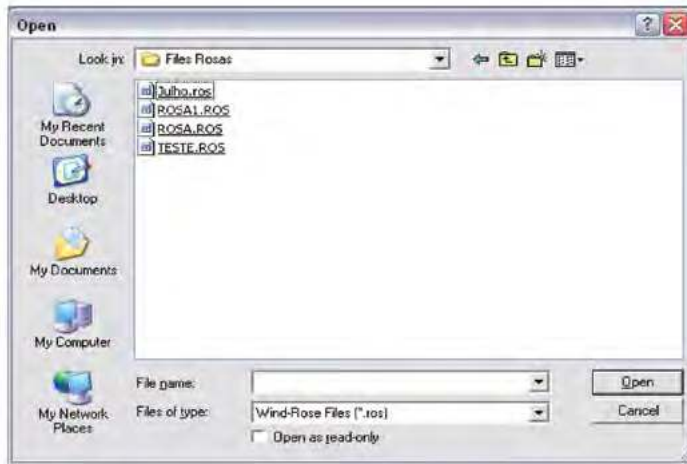
Image 7: Dialog for the selection of data file.
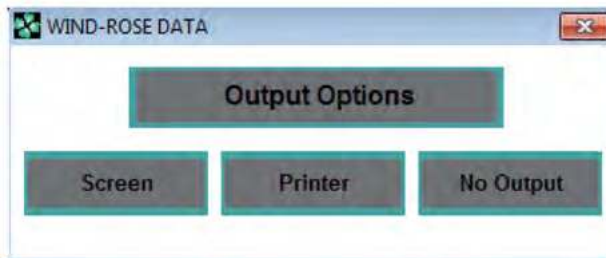
Image 8: Dialog with the data output options.

visible dialog boxes will be closed, and a new one will be opened providing the option to view, print or do nothing with the read information.

If the user wants to create a simulation with new data, choosing the New Data option will lead to dialog windows in which all the necessary information can be inserted. A description of the information in each type of data files will be made below.

1.2.1 Meteorological Data

Meteorological conditions are characterized by wind roses, up to 6 per file, as there are 6 stability classes. Each rose can be defined by up to 16 directions of wind (sectors), each with up to 6 wind classes.

The sum of the % of the persistence of each wind class along the various directions of a particular wind rose represents its % of global occurrence.

$$
\begin{bmatrix}
dTdZ_E \, , dTdZ_F \, , Hi \, , Fl \, , FD \\
"Estab_R \, , Freq_R \, , NSect_R \, , NCV_R \, , [Dir_R] \, VV_{1R} \, ,..., \, VV_{NCV_R,R} \\
Pers_{1,1,R} \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots Pers_{NCV_R,1,R} \\
\vdots \qquad\qquad\qquad\qquad\qquad\qquad \vdots \\
\vdots \qquad\qquad\qquad\qquad\qquad\qquad \vdots \\
\vdots \qquad\qquad\qquad\qquad\qquad\qquad \vdots \\
Pers_{1,NsectR,R} \cdots\cdots\cdots\cdots\cdots\cdots Pers_{NCV_R,NsectR,R}
\end{bmatrix}
$$
$$R = 1, NR$$

The previous scheme represents the file structure of meteorological data, (**ros** files), where the meaning of the parameters are as follows:

- dT/dZ_E and dT/dZ_F represent the potential temperature gradients for stabilities E and F, with default values of 0.02 and 0.034 K.m^{-1};
- *Hi* is inversion height (if the inversion height is not to be used, then set it to a large positive number);
- *Fl* and *FD* are flags respectively for inversion (0 to disregard, –1 to enforce) and correction for sampling time (0 if ≤24h, –1 otherwise);
- *Estab$_R$* is the Pasquill-Gifford stability class, being one of the following (A, B, C, D, E, F);
- *Freq$_R$* is its fraction frequency of occurrence of each stability (a real number between [0 1]), *NSect$_R$* is the number of wind sectors (an integer between [1 16]), *NCV$_R$* is the number of wind classes (an integer between [1 6]);
- *DIR$_R$* is the wind direction relative to Geographic North (a number between [0 360[). This variable only exists for a single wind direction;
- *VV$_{1,R}$* to *VV$_{NCVR,R}$* is the average wind speed for each wind class (m/s);
- *Pers$_{1,1,R}$* to *Pers$_{NCV,NsectR,R}$* are the corresponding frequencies of occurrence (persistences) of wind class *i* in wind sector *j*. The sum of all wind frequencies of all sectors and for all stabilities must be a number ≤1. The reason why this number may be lower than 1 is because of the possible occurrence of very low wind speeds (< 1m/s) that are not accounted for in the dispersion simulation (please refer to Model Highlights, Meteorological Data).

Image 9 presents an example of a **ros** file, containing 1 wind rose of B stability with an overall frequency of occurrence of 9.76%, with 16 sectors and 6 wind classes per sector.
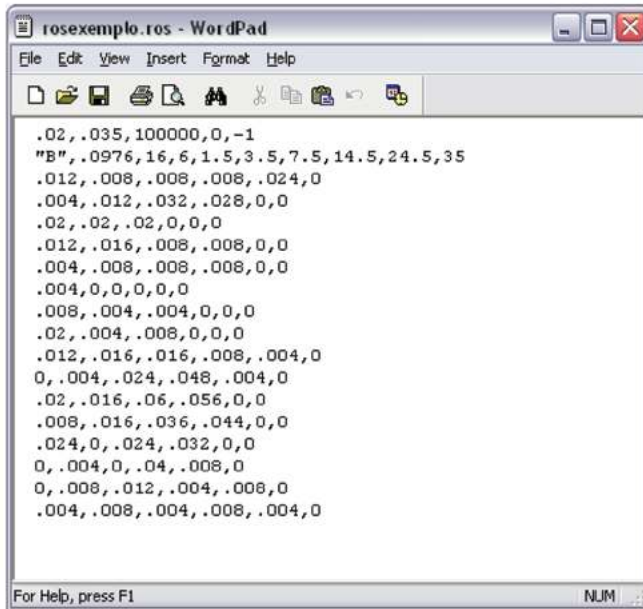
Image 9: Contents of a **ros** file.

1.2.2 Dispersion Data

The files with the dispersion data (**disper** files) present the following data:
- Equations used for the calculation of the dispersion coefficients in the horizontal transverse direction relative to the wind (σ_y) and vertical direction (σ_z);
- Parameters for each one of those equations according to the stability;
- Sampling time related to the parameters and equations.

The following scheme presents the file structure concerning the dispersion data, where *Tamst* represents the averaging time corresponding to the standard deviations of the plume concentration distributions. If different stacks are simultaneously evaluated, there may be some reason to use stack-discriminating dispersion equations, obtained with different sampling times. In that case, the largest sampling time should be used for all, usually 60min for short term estimates.

$$
\begin{bmatrix}
\text{Eqy} \\
ay_A \;,\; by_A \;,\; cy_A \\
\vdots \;,\; \vdots \;,\; \vdots \\
\vdots \;,\; \vdots \;,\; \vdots \\
\vdots \;,\; \vdots \;,\; \vdots \\
\vdots \;,\; \vdots \;,\; \vdots \\
ay_F \;,\; by_F \;,\; cy_F \\
\text{Eqz} \\
az_A \;,\; bz_A \;,\; cz_A \\
\vdots \;,\; \vdots \;,\; \vdots \\
\vdots \;,\; \vdots \;,\; \vdots \\
\vdots \;,\; \vdots \;,\; \vdots \\
\vdots \;,\; \vdots \;,\; \vdots \\
az_F \;,\; bz_F \;,\; cz_F \\
\text{Tamst}
\end{bmatrix}
$$

The following image presents an example of a **disper** file:

Image 10: Contents of a **disper** file.

1.2.3 Source Data

The files regarding the source characteristics and emission data are **fon** files. These contain information on the characteristics directly related to the sources:
1. Spatial position (arbitrarily fixed at [0,0] for one of the sources)
    1.1 Abscissa (m)
    1.2 Ordinate (m)
    1.3 Height (m)
    1.4 Altitude (m)

2. Mass Flow of pollutant (g/s)

3. Plume rise equation
    3.1 Holland
    3.2 Moses-Carson
    3.3 Davidson-Bryant
    3.4 Briggs
    3.5 Briggs with thermal energy of the plume
    3.6 Actual known plume rise

4. Depending on the choice made in 3, it is also necessary to know:
    4.1 Holland, Davidson-Bryant, Briggs
        4.1.1 Temperature of the exhaust gases (K)
        4.1.2 Stack exit velocity of the gases (m/s)
        4.1.3 Stack inner diameter at release height (m)
    4.2 Moses-Carson
        4.2.1 Thermal power of the gas (MW)
        4.2.2 Escape velocity of the gases
        4.2.3 Stack inner diameter at release height (m)
    4.3 Briggs (knowing the value of thermal energy)
        4.3.1 Thermal energy of the gas (MW)
    4.4 Known plume rise
        4.4.1 Plume rise (m)

5. Choosing Holland or Moses-Carson, the user can either provide them or else use a default multiplicative correction factor for these equations:

Table A1. Correction factors by default for Holland and Moses-Carson equations

	Stabilities	A	B	C	D	E	F
Correction Factor	**Holland**	1.20	1.10	1.05	1.00	0.90	0.80
	Moses-Carson	2.65	2.65	1.08	1.08	0.68	0.68

Table A2. Power Law default correction factors

Stabilities	A	B	C	D	E	F
Power Law Coefficient	0.10	0.15	0.20	0.25	0.25	0.30

Besides information about each source, these files also contain the temperature and atmospheric pressure and the values of Power Law coefficients for each stability. Default values may be presented. Alternatively, the user may also provide them.

The diagram below represents the **fon** file structure, where the number of sources (NF) is limited to 50:

$$\begin{bmatrix} Pot_A , Pot_B , Pot_C , Pot_D , Pot_E , Pot_F \\ NF , PAtm , TAtm \\ cx_f , cy_f , alt_f , cota_f , caud_f , eqse_f , [x]_f \\ [fc_A , fc_B , fc_C , fc_C , fc_E , fc_F]_f \\ \qquad\qquad\qquad f = 1, NF \end{bmatrix}$$

- Pot_x represent the power-law correction factors for the wind speed variation with height (see Eq. [1]) as a function of stability, in this case those from Table A2;
- NF is the number of sources, $PAtm$ and $TAtm$ are respectively the barometric pressure (Pa) and the ambient temperature (K), both obtained at 10m height;
- cx_f and cy_f represent the terrain coordinates for source f;
- alt_f and $cota_f$ are respectively the stack physical height (m) and altitude (m);
- $caud_f$ is the pollutant emission rate (g.s^{-1});
- $eqse_f$ is the equation # for plume rise estimates. If the plume rise is known, then $[x]_f$ is its value.

The following image presents an example of a **fon** file with 5 sources, in which the Power Law coefficients provided by default are used, and the Davidson-Bryant equation is used to calculate the actual height of the plume:
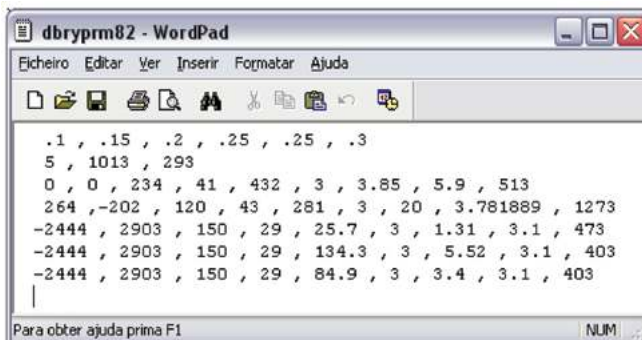
Image 11: Contents of a **fon** file.

1.3 Data Validation

1.3.1 File Validation Menu

This option in the main menu allows the user to "manually" create/modify data files, independently of the program. The construction of a new file implies the use of an application which creates files with the **txt** extension. Existing text files can be modified in any word processor.

Files are validated by activating the File Validation button in the main menu. **Image 12** shows the dialog presented to the user. This dialog should select the type of file to validate. The next step is locating the file in the computer. In case the selected file is not a **txt** file or one of the types of data files allowed, or if there is no agreement between the type of the chosen file and the type to validate, an error message is presented, and the dialog is closed. If the validation is successful, further files can be validated or the menu can be closed by selecting the Exit button.

For example, file validation can be used to create all atmospheric stabilities that are coherent with wind-speed data (Table 1), using the *Wind-Roses* button (Image 12), without having to manually enter all stabilities. It can also be used if the user wants to input new dispersion or plume-rise equations, respectively activating the *Dispersion* and *Sources* buttons.
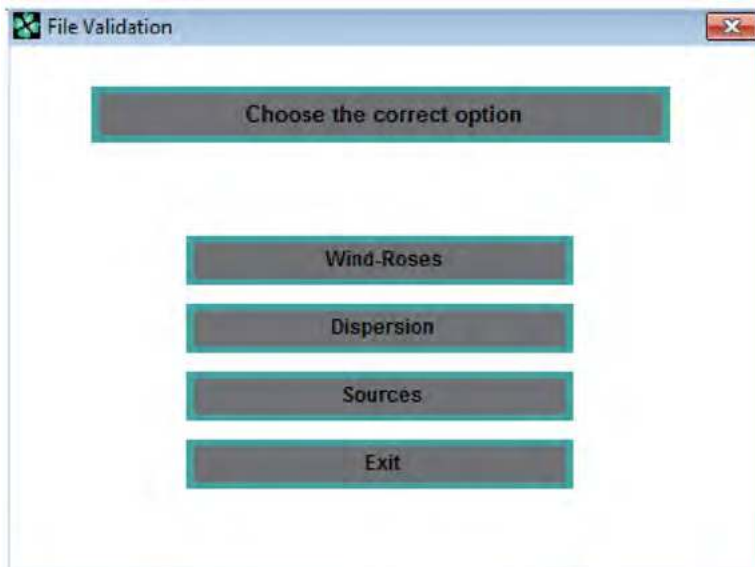
Image 12: Dialog for file validation.

1.4 Simulation

After choosing all data needed, viz. **rose**, **disper** and **fon** data, it is possible to simulate pollutant dispersion. The program offers the user several possibilities:
* Calculation of concentrations in points specified by the user;
* Calculation of isopleth maps;
* Determination of the value of the maximum concentration and respective location using optimization algorithms [2, 3, 19].

Next, a brief description of each one of these menus is presented.

1.4.1 Concentration Estimates Menu

When choosing this menu, a dialog window similar to the one in **Image 13** is presented.

The first decision to be made regards the mapping for which the calculation of the pollutants' concentration is specified. The calculation target points can be provided in three different ways: by specifying coordinates for each point, by graphically choosing points on the map and by choosing some grid.

Image 13: Estimation of concentrations at user-defined points.
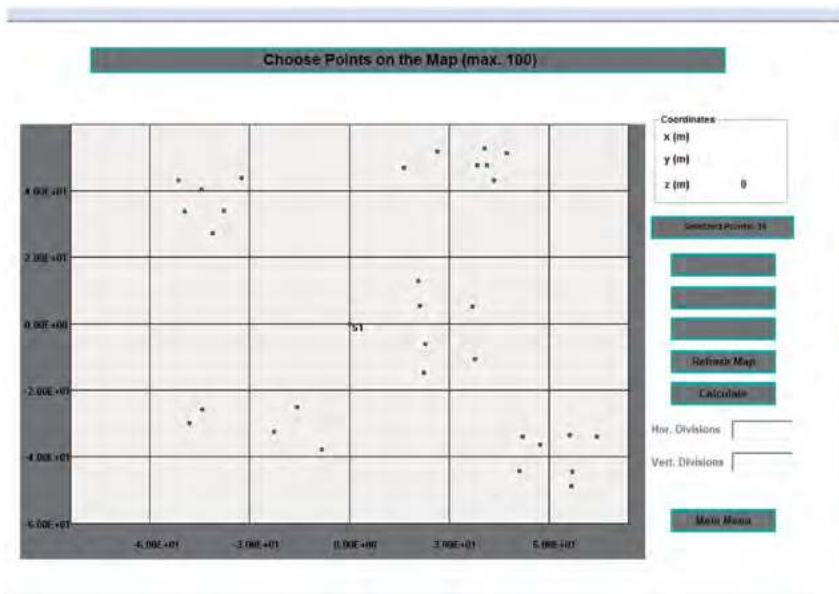
Image 14: Selection of points on the map.

Regardless of the choice, a maximum number of 100 points can be set. In addition to defining different points, it is also necessary to: define corrections for the sampling time and for plume-rise equations, otherwise the default values built into IMDIS will be used; a method for estimating the transport wind speed should be selected, either at the effective stack height or as a plume vertical integration average (depending on atmospheric stability and downwind distance from the source); for multiple sources, the contribution from each source to pollution can also be calculated at the different points.

Once the necessary definitions have been made, the above dialog is automatically closed. If the different points have been introduced through the specification of coordinates, the dialog with the different output options will be presented (see **Image 8**); if any other option has been chosen, a window of larger dimensions will be presented. This window will contain the map with the different sources, and you can select the points at the desired location or define a grid on which the calculations will be made, by simply using the computer mouse. The *x* and *y* point coordinates are continuously updated under the mouse pointer, and are displayed on the top right corner of the window.

Image 14 shows that there are commands which allow the boundaries of the *x* and *y* coordinates on the map to be changed: *Zoom In*, to reduce the area represented by the map; *Zoom Out* to expand the area (birds' eye view) or *Move Center* to modify the central point in the map. These options are only available before the final selection (points or grid) on the map has been carried out. To make new definitions or reset the original map, the *Refresh Map* button should be used. After defining points,

pressing the *Calculate* button will cause the program to calculate concentrations and present the results. If a grid has been set, its number of vertical and horizontal divisions must be given before any calculations are made.

1.4.2 Concentration Isopleths Menu

Choosing this option allows the drawing of maps with the same concentration. One interesting versatility of *IMDIS* is the possibility of obtaining concentration isopleths regarding a given situation or average values of several situations, for example, using average daily measurements to compute weekly estimates.

Image 15 shows the menu made available to the user when the *Concentration Isopleths* button in the main menu is selected. The results of the computed concentrations are stored in text files that can be later retrieved. To see these results in a graphic form, the *Draw* option must be selected. If the file with the results regarding the situation of interest is not yet available, the *Estimate* option must be chosen instead.
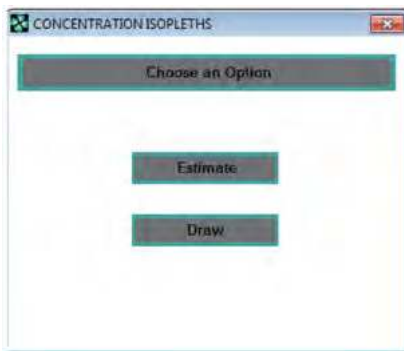
Image 15: Isopleths main menu.

When choosing to calculate the (new) isopleths, a new menu appears, containing several options:
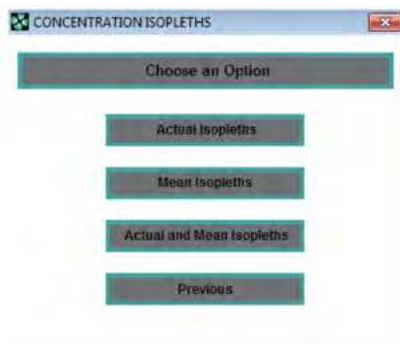
Image 16: Menu related to the calculation of isopleths.

Actual Isopleths, to carry out the calculation of a given situation. After choosing this option, the name of the file which will store the results has to be given;

Mean Isopleths, to determine average values of concentrations between two situations with different conditions, for example, on two consecutive days. In this option, the name of the existing file must be provided (this is a read-only file and will not undergo any changes). The data in this file will be averaged with the data for the current situation. It will also be necessary to define the name of the new file which will contain the average values that the new situation has contributed to;
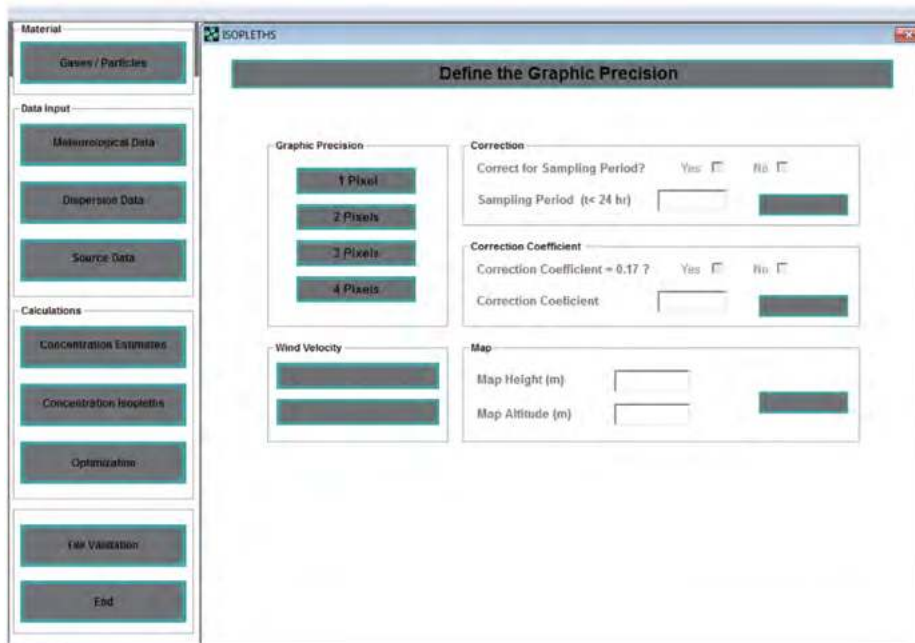
Image 17: Dialog in which the accuracy of the calculation of concentration isopleths is set.

- Actual and Mean Isopleths, this option must be chosen when you wish to know the results of the new chosen situation, in addition to calculating the average concentrations. In addition to the information supplied in the previous situation, it is also necessary to define the name of the file which will store the data for the current situation.

After choosing one of the calculation options, a new window is presented, where the precision for the calculation is set. The most precise situation corresponds to every pixel being calculated. This situation corresponds to assigning a pair of coordinates (*x, y*) to each one of the pixels that represents the space of the map on the screen. Smaller resolutions can be chosen, with the benefit of a faster execution time. For

example, a 2 Pixels choice will run 4 times faster than a 1 Pixel one, and a 4 Pixels will be 16x faster, although the image will be more blurred.
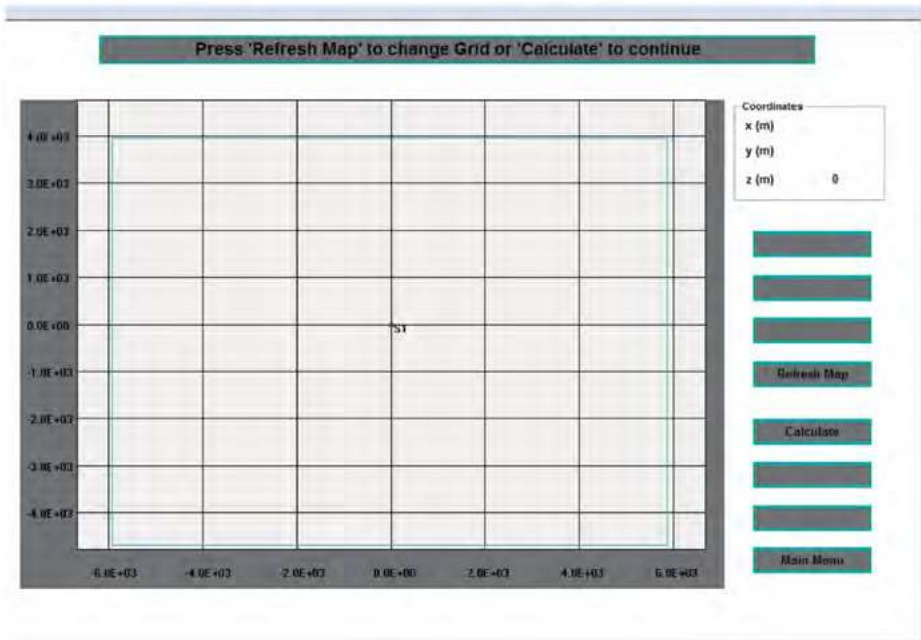
Image 18: Definition of the space in the map for concentration isopleths calculation.

The next step is the definition of a grid that outlines the space in which the calculations will be carried out. The dialog box shown in **Image 18** is similar to that presented in **Image 14**.

To define the grid, the left mouse button in the initial point of the grid must be pressed. Then, the mouse pointer must be moved in the desired direction, which will cause a box outlined by a green line to be created. When the grid has the desired size, the same mouse button should be activated again, and the grid is set. To start the calculations, the *Calculate* button must be pressed.

Image 19 shows the general aspect of the program during the calculations. This task can be time-consuming, from short to longer periods of time, according to the complexity of the data and to the calculation resolution. For a better idea of the time needed to complete the calculations, a progress bar is placed along the bottom of the window. When the calculations have been completed, this window is automatically closed, and the isopleths main menu appears (**Image 15**). By selecting the Draw option, the previously calculated file is uploaded and the map can be drawn.
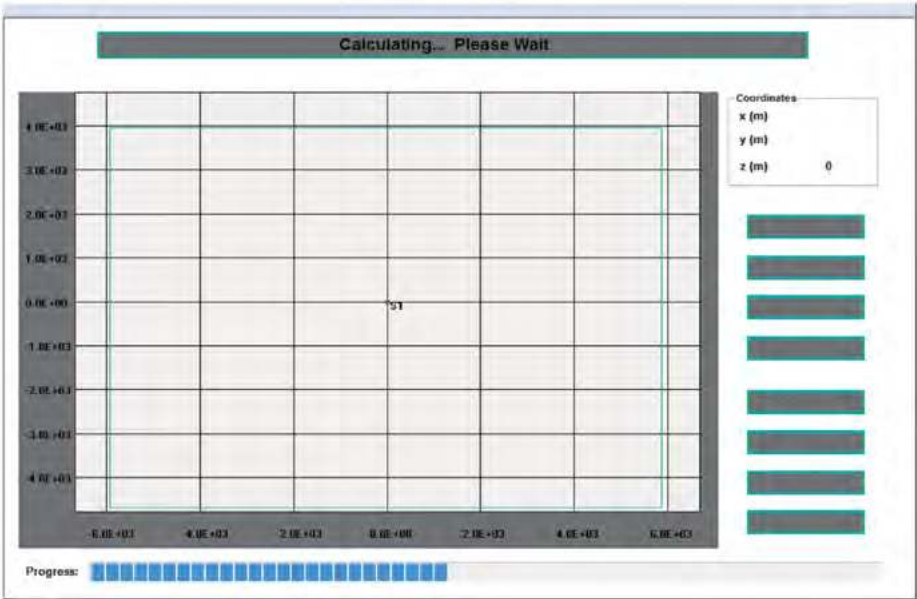
Image 19: Evolution of the calculation.

From the moment the drawing is completed, there are two available options: *Copy Map* or *Isopleths Listing*.
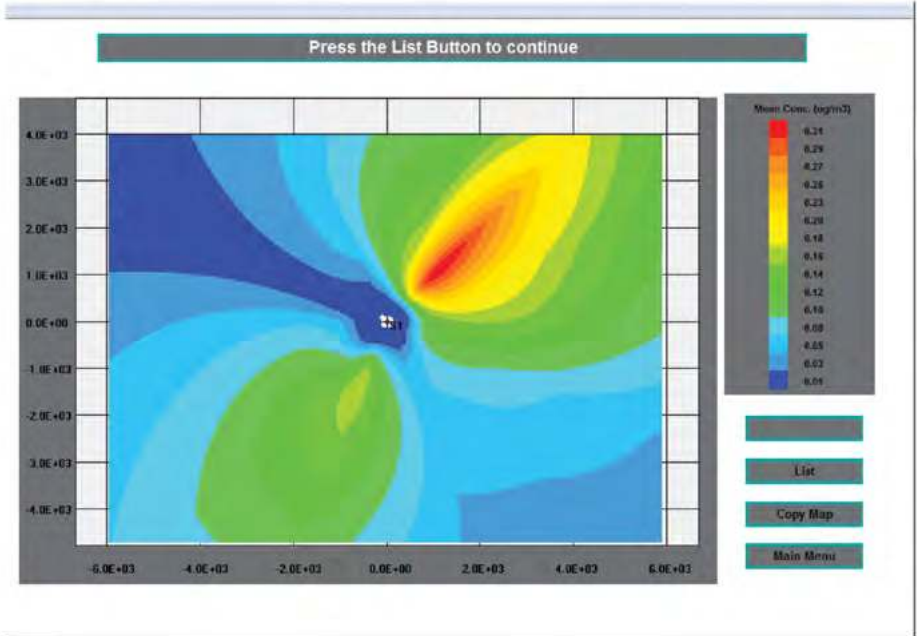
Image 20: Map copied to the Windows Clipboard.
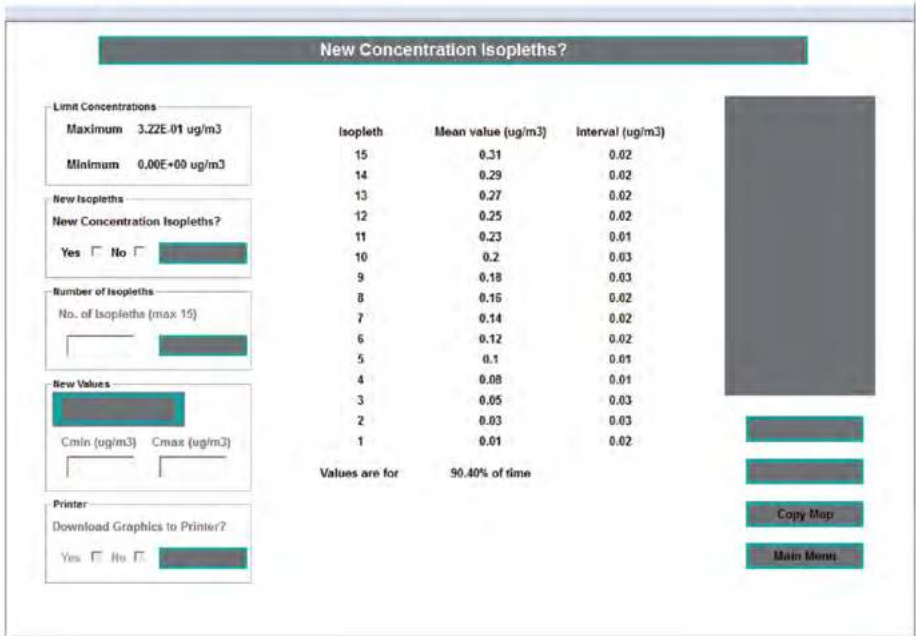
Image 21: Isopleths listing.

1.4.3 Optimization Menu

Choosing this option offers different possibilities of calculating the maximum concentration. According to the data, the downwind x coordinate, the x coordinate plus the critical wind speed, the (x, y) coordinates, or the (x, y) coordinates plus the critical wind speed.

The optimization menu is similar to the one presented in the following image:
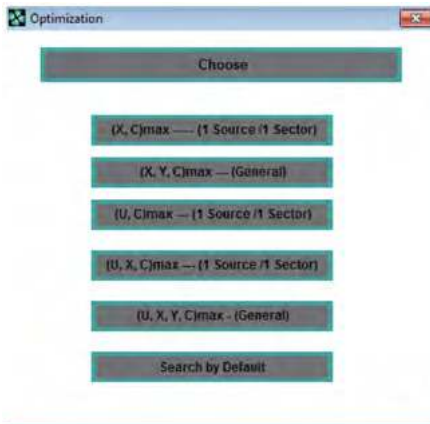
Image 22: Main menu for optimization.

There are specific options for cases in which there is only one source, and the roses only have one sector. There are options that seek the point of maximum concentration in regions chosen by the user. The *Search by Default* option includes two search options for the global maximum.

The following image presents the result of the maximum concentration search using the (*X, Y, C) max (General)* option in the sub-menu of the Search by Default option.

Image 23: Results of maximum concentration for a specific simulation.

With the purpose of better illustrating how to use *IMDIS*, a specific example containing every step necessary to use the options of the program is considered below.

2 *IMDIS*: User Manual Example

2.1 Material Selection

- Choose the *Gases/Particles* options in the main menu.
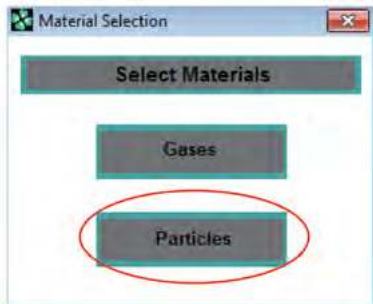
By selecting the *Particles* option, we need to set the average particle size. Regardless of the option chosen in this menu, the last property to set is the background concentration of the pollutant.
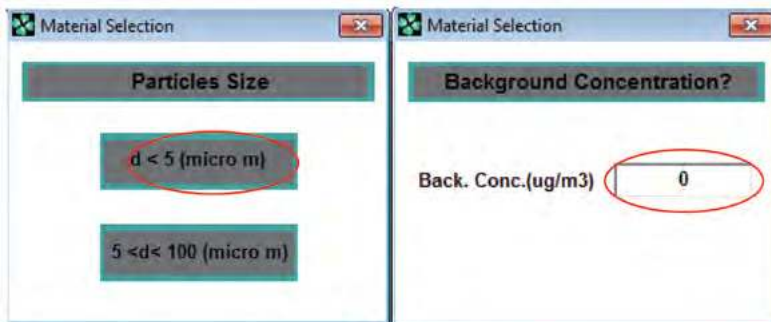
2.2 Data Entry

2.2.1 Meteorological Data

- Choose the *Meteorological Data* option in the main menu and select the *New Data* option in the *Get Wind-Rose Data* sub-menu. If the data files already exist, select the *Data in Disk* option.
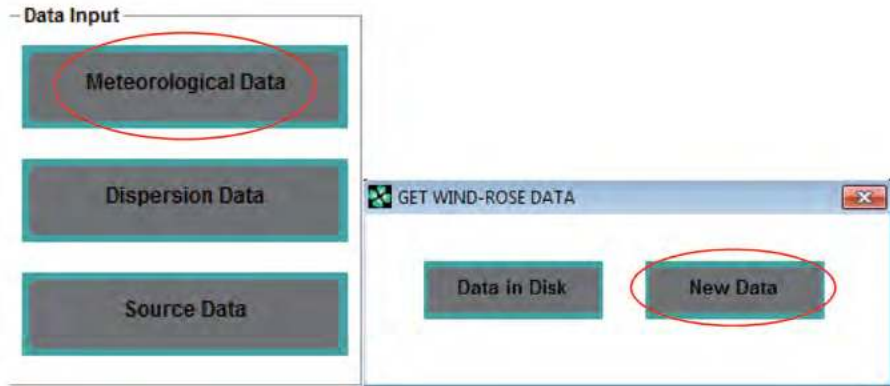
- The new dialog allows the input of all data related to the wind rose to be created. Whenever there's a visible dialog window, the buttons of the main menu remain inactive (dimmed).

- Fields are to be sequentially filled in. Initially, only the field that allows the definition of the average time is available. Once set, the next field becomes available. The possible maximum number of wind roses to be set is 6 per file, corresponding to the six atmospheric stability classes of Pasquill-Gifford scheme.

- After the number of wind roses has been set, the fields related to their properties are made available. If only one wind rose is set, the field corresponding to the frequency is dimmed, because its value must equal 1. By defining a number of roses larger than 1, all properties for each rose will be separately set.

- Along the top of the window, there is a space containing messages with instructions for the user. If data outside the allowed limits are introduced, an error message will appear. The program will only proceed when data are properly introduced. The transition to the next field can be made in three separate ways: using the Enter key or the Tab key on the keyboard or through a mouse click. This will quickly become very intuitive.
- Once all properties of the wind rose have been set, the corresponding fields become inactive, and you can proceed to fill in the wind speeds (maximum and minimum) for the number of classes defined for the wind rose under construction.

- The next step is defining the persistence of each wind class in each of the defined wind sectors. By filling in the last field of the current sector, the fields will be cleared, and the persistence of the following sector must be filled in. For user guidance, there's an indicator of the sector being defined.

Frequency

Sector Nr 1		
Class 1	**Class 2**	**Class 3**
.00046	.00023	0
Class 4	**Class 5**	**Class 6**
0	0	

(...)

- If the rose's stability is E or F, the determination of the potential temperature gradient in the atmosphere is needed. The default value can be used, or a new value can be set. The Ok button only becomes available when all information is set.

Temperature Gradient

dTpot/dz by default?   Yes ☑   No ☐

dTpot/dz (K/m)   0.02   Ok

Temperature Gradient

dTpot/dz by default?   Yes ☐   No ☑

dTpot/dz (K/m)

- When concluding the definition of the wind rose properties, the user will receive instructions to press the button which enables the definition of the next wind rose. All the previously completed fields will be erased, and the definition of a new wind rose will be started in a similar way to that previously filled in. There is also a *Repeat Data* button which enables the user at any point to return to the *Get Wind-Rose Data* sub-menu and restart the process.
- When all wind roses have been defined, the user must press the *Finish* button. It is also necessary to determine if a temperature inversion takes place. If it does, you have to define the height at which it occurs.

Temperature Inversion

Temperature Inversion?   Yes ☐   No ☐

Inversion Height (m)

- The next step is storing the data in a file. To do so, simply activate the *Save Data* button. A window in which you can choose the location on your computer where you want to save the file will appear.
- If a valid file name was not introduced, the user will be informed and will have the option to re-select the name and location of the file.

- After the meteorological data has been created, the window is closed, and a new sub-menu with view information or send to printer options will appear:

- Choosing the data output option for the screen:

2.2.2 Dispersion Data

- Choose the *Dispersion Data* option in the main menu and select the *New Data* option in the *Get Dispersion Data* sub-menu. If the data files already exist, select the *Data in Disk* option.

- The new dialog allows the introduction of the correct dispersion data.

- First, you must choose the equation for the calculation of σ_y. By moving the mouse cursor over the buttons corresponding to each of the equations, the respective equation and its dependence on each parameter will appear to the right.
- By selecting, for instance, Green's equation, the fields for the parameters on which the equation is dependent become active. By introducing all the values of the parameters for the stability class A, the *Stability>>* button becomes active and must be pressed in order to proceed with the introduction of data for the other stability classes, otherwise the default values built into *IMDIS* will be enforced.

- After defining all the required data, pressing the *Finish* button activates the equation for the calculation of the vertical dispersion coefficient, σ_z. This is performed in a way similar to σ_y, as described before.
- The last piece of data to be introduced is the sampling time for which the introduced data is valid.
- The next step is storing the data in a file. To do so, activate the *Save Data* button and choose the location where you want to save the file.
- If a valid file name was not introduced, the user will be informed and will have the option to reselect the name and location of the file.
- After the process of creating meteorological data is finished, the window is closed, and the sub-menu with information view or send to the printer options will appear.
- By choosing the data output option for the screen, we obtain the following image:

2.2.3 Pollutant Emission Data

- Choose the *Source Data* option in the main menu and select the *New Data* option in the *Get Source Data* sub-menu. If the data files already exist, select the *Data in Disk* option.

- The new dialog allows the introduction of all data related to the sources.

- The Power Law coefficients are provided by the program. However, new values can be defined by the user by activating the *No* selection box.

- After the definition of the Power Law coefficients (default or otherwise), pressing the Ok button activates the fields for specifying atmospheric pressure and temperature, supposed to be taken at 10m height.

The next step is the definition of the number of stacks, which must be an integer between 1 and 50.

- Choosing the calculation model for the plume rise can be made in two different ways: stack by stack, by selecting the *Yes* box in the image below, or assigning the same model to all stacks (*No* box).

- If the chosen model is Holland or Moses-Carson, values for the equations' correction factors will be necessary. Such values may be provided by the program or provided by the user.

- The next piece of data is related to the existence or non-existence of a *Flare*. In case the emission point is a flare, it is necessary to define the thermal energy and molecular weight of the gases.

Flare

Flare? Yes ☑   No ☐   Ok

Thermal Energy (MW)   Mean Molecular Weight

- All that is left to be defined are the properties that are specific to each source, such as the *x* and *y* coordinates, stack physical height, stack altitude and mass flow released, and also gas temperature at stack tip, gas velocity at stack tip and inside stack diameter.

Source Properties

Coordinates (m) x [　] y [　]

Source Height (m) [　]

Source Altitude (m) [　]

Mass Flow (g/s) [　]

Other Properties

Tgases (K) [　]

Vel (m/s) [　]

Diam (m) [　]

- For example, using the following data, with Holland´s plume rise estimates for both of 2 different sources:

- If the plume rise is known, its value should be used instead of estimating it through one of the above formulas.
- If the source has been identified as a flare, there is no need to define any more data. The next stage is defining the next source by pressing the *Next Source* button:

- The final step is storing the data in a file. To do so, simply activate the *Save Data* button, where the location on the computer can be selected.
- After the process of creation of source data has finished, the window is closed, and the sub-menu with the output options will appear. In this case, with output to the screen, the following appears:

2.3 Simulation

All *IMDIS* calculation options are accessible from this sub-set of the main menu. Calculations can only be made after loading all necessary files. Otherwise, a warning message will appear:
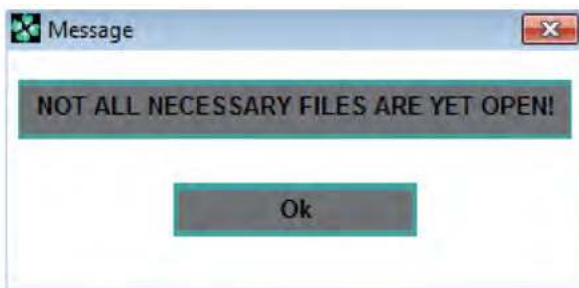
2.3.1 Estimation of Concentrations
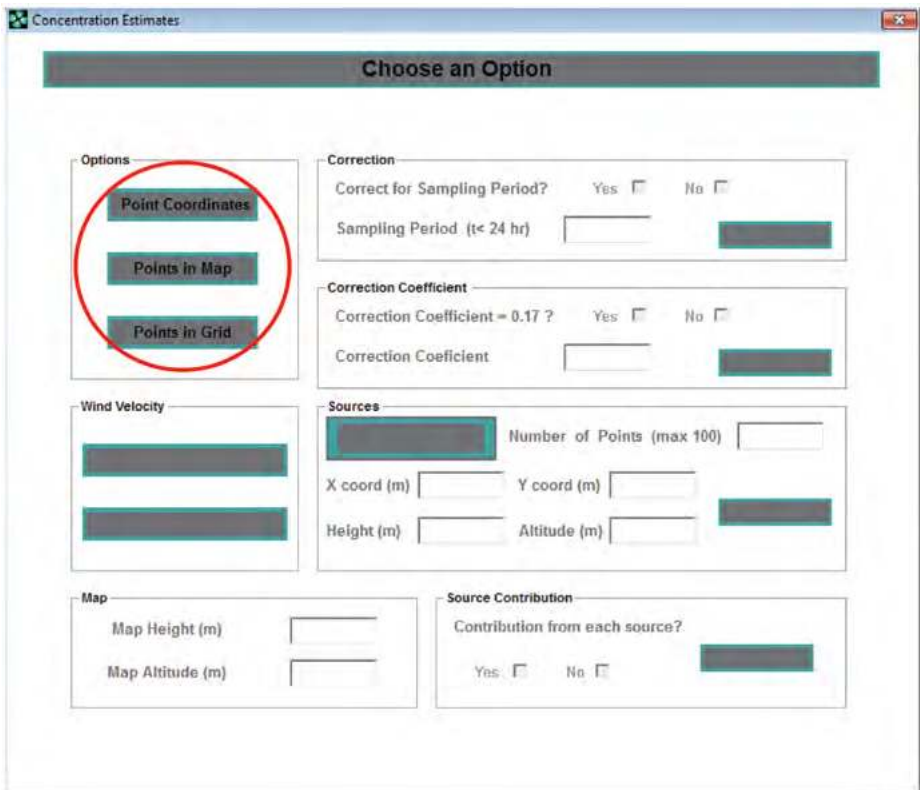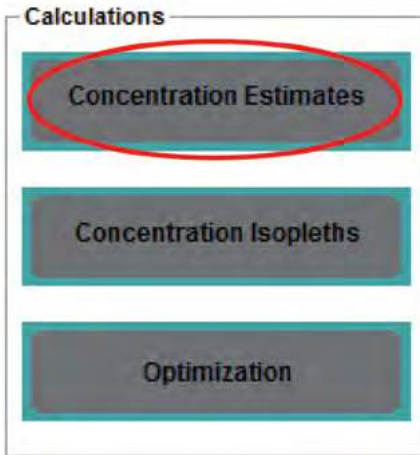
- The calculation of concentrations can be carried out in three different ways. The user will have to choose between specifying coordinates for the points, points on the map or defining a grid on the map. Regardless of the choice made, the user needs to determine if he intends to correct the sampling time. If that is the case, a value for the correction coefficient that may or may not be provided by the program must be defined.
- The next step is to choose a model for wind speed calculation, either at effective stack height or integrated as a function of distance from the source (thought to be more accurate):

- If Point Coordinates option has been chosen, a number of points (up to 100) is defined. The procedure is similar to that described in similar situations: there is an indicator of the point for which information is being entered; once all the necessary fields have been completed, an increment button becomes active and allows to sequentially determine all points.

- If the grid option has been defined, a maximum of 10x10 points equally spaced on the chosen map can be estimated, after specifying both map altitude and height (meters above stack altitude):
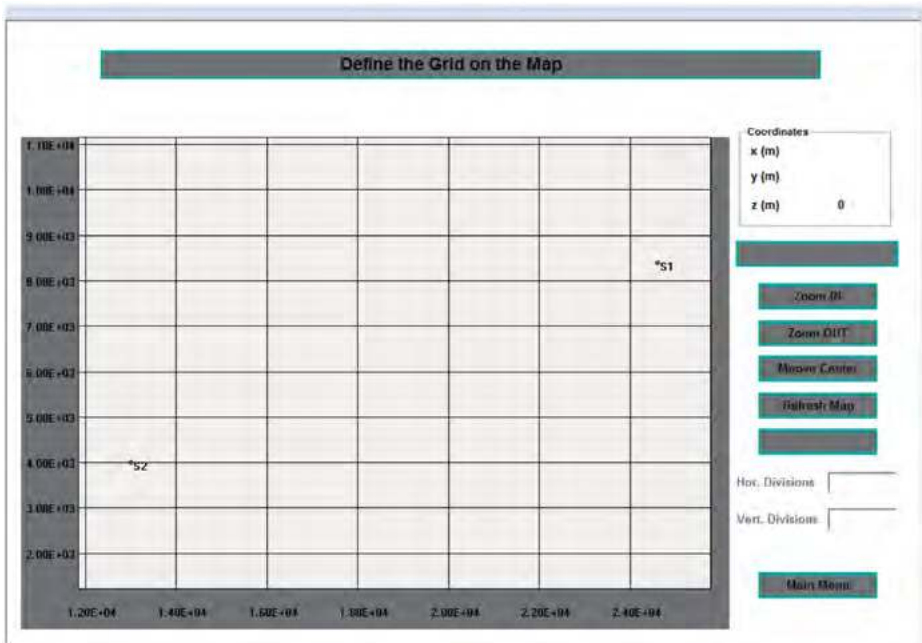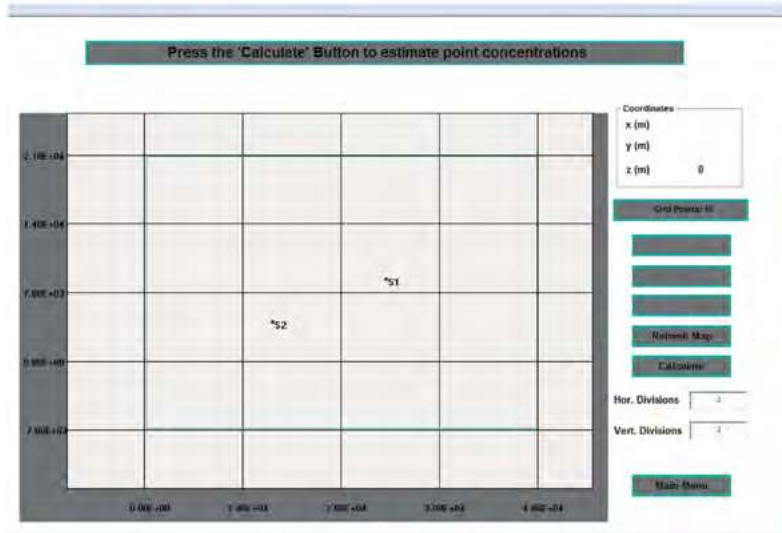

- If the file with the source data has information about more than one source, there is the possibility of calculating the contribution from each source to pollution at a given point.

For any choices that imply the selection of points on a map (directly or through a grid), a new window is presented. The map allows for various actions:
  – Visualizing the *x* and *y* coordinates by hovering the mouse over the map (1)
  – *Zoom In* (2), which allows reducing the area represented by the map
  – *Zoom Out* (3), which allows expanding the area represented by the map
  – *Move Center* (4), which allows selecting (by clicking) a point to be the center of the map
  – *Refresh Map* (5), to restore the initial map or eliminate possible selections that are eventually made.

- If the selection of points was the chosen option, the mouse cursor must hover over the map, and the left mouse button must be pressed in the desired places. The selected point will be marked in that place. At the end of the selection, the *Calculate* button must be pressed for the calculation to be carried out.

- If the definition of a grid was the chosen option, a click must be made to define the first vertex of the grid. Then, moving the cursor will define a green lined-box. When the grid has the desired size, a second click must be made to fix the grid. After the grid has been defined, the *Next* button must be pressed to define its number of divisions. The definition of a grid implies inserting a number of vertical and horizontal divisions to define crossing coordinates. The product of the two divisions must not exceed the maximum value (100 points).

Concentration Results

Rose Nr 1   Stability B

Point	x coor (m)	y coor (m)	Height (m)	Conc (ug/m3)
1	160.1	-6787	0	0
2	13400	-6787	0	0
3	26640	-6787	0	0
4	39880	-6787	0	0
5	160.1	2457	0	0
6	13400	2457	0	0
7	26640	2457	0	0.516
8	39880	2457	0	0.19
9	160.1	11700	0	0
10	13400	11700	0	0
11	26640	11700	0	0
12	39880	11700	0	1.14
13	160.1	20940	0	0
14	13400	20940	0	0
15	26640	20940	0	0
16	39880	20940	0	0

Values are for   100.00% of time

% Contribution of each source

Stability B

Point	Source 1	Source 2
1	0.00	0.00
2	0.00	0.00
3	0.00	100.00
4	0.00	100.00
5	0.00	0.00
6	0.00	0.00
7	0.00	100.00
8	7.98	92.02
9	0.00	0.00
10	0.00	0.00
11	0.00	100.00
12	99.68	0.32
13	0.00	0.00
14	0.00	0.00
15	0.00	0.00
16	1.05	98.95

- By carrying out a selection operation on the map, operations 2, 3 and 4 of for map manipulation become unavailable. If the original map is replaced (operation 5 to refresh map), they will become available again.
- After the calculation finishes, the window is closed and the sub-menu with information on output options will appear.

2.3.2 Concentration Isopleths

In this menu, the concentration isopleth maps can be obtained.
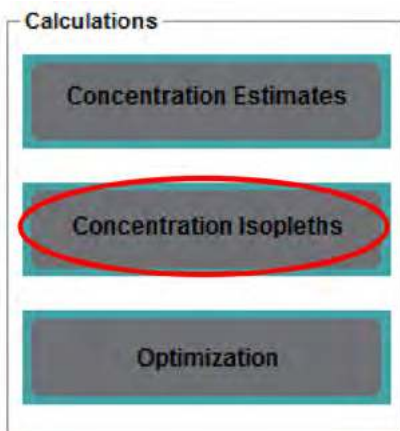
- To build a new results file, choose the *Estimate* option:
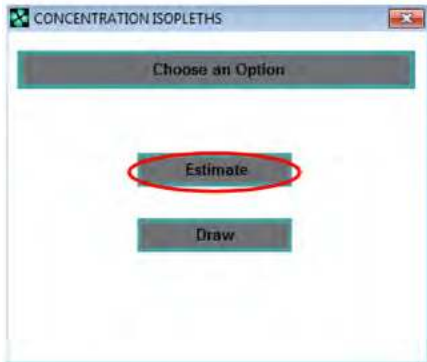
In the sub-menu depicted in the following image, the choice must be made according to the intended purpose of the simulation:
- If the user intends to simulate a new situation, the *Actual Isopleths* option must be chosen;
- If the user wants to determine the average values between an existing situation and a new situation, e.g., two days in a row, the correct choice is *Mean Isopleths;*
- The *Actual* and *Mean* Isopleths option must be chosen if the conditions are the same as the previous case and if both the actual and combined data is of interest.
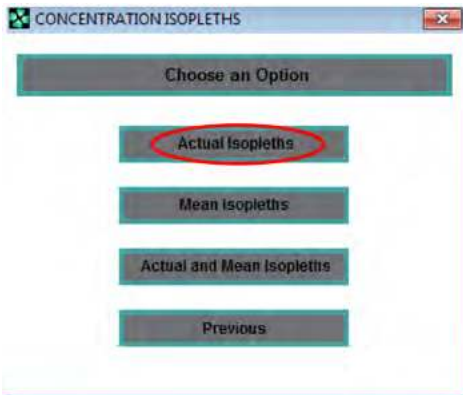
- By choosing the first option, the user only has to define the name and computer location of the file to store the results. In the second and third options, the location of the file with the existing results and the name and location of the file to store the averaged results must be both provided. In the third option, the name and location of the files to store the results of the new situation has also to be provided.
- For instance, when choosing the situation above, the user is asked to name the results file.

- After the definition of the file, a new dialog window appears. The first decision is related to the choice of resolution with which the calculations will be carried out and which varies between 1 and 4 pixels. The more accurate situation is option 1 pixel. This corresponds to assigning a pair of coordinates (x, y) to each one of the pixels that represents the space of the map on the screen, for which the concentration will be calculated. Smaller resolutions can be chosen to speed up execution, but more blurred concentration maps will result.
- Selecting the option 4 pixels:
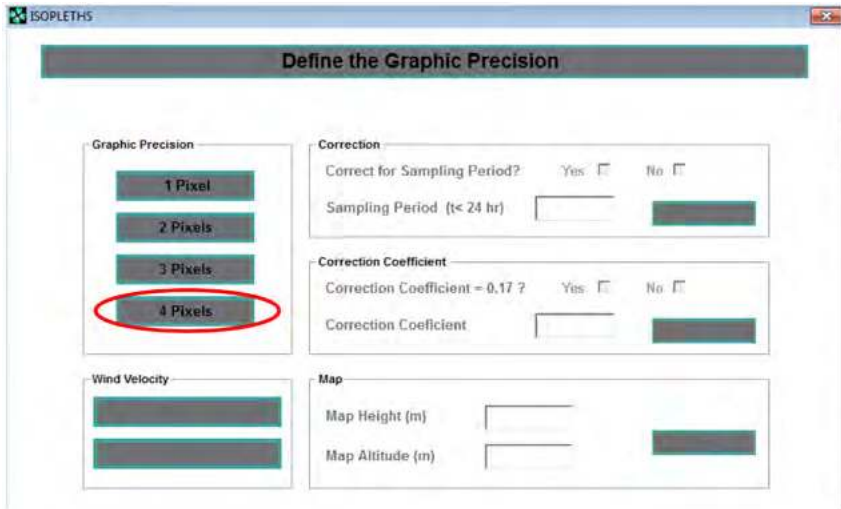
- Next, the user needs to determine if there is intention to correct for sampling time. This may be necessary due to mismatching between averaging times used in the formulas for σ_y and σ_z, usually 10–60 min, and the averaging time corresponding to the calculated concentrations, viz. [1 24]h. If that's the case, the user will have to define a value for the correction coefficient that may or may not be provided by the program.
- The next step is to choose a model for wind speed calculation.
- Finally, receptor map elevation and level must be defined.
- By activating the Next button, a new window with the map appears. The map allows for various actions:
  - Visualize the (x, y) coordinates by hovering the mouse over the map (1)
  - *Zoom In* (2), which allows reducing the area represented by the map
  - *Zoom Out* (3), which allows expanding the area represented by the map
  - *Move Center* (4), which allows selecting (by clicking) a point to be the center of the map
  - *Refresh Map* (5), to restore the initial map or eliminate possible selections that are eventually made.
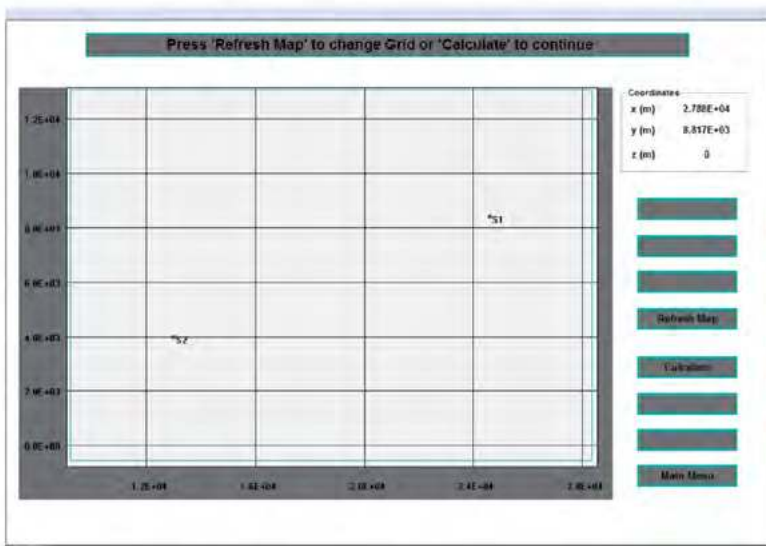
- A grid is defined starting with a click to define the first vertex of the grid. Then, moving the cursor will define a green lined-box. Move the cursor until the grid reaches the desired size and click again to define the last vertex.
- Press the *Calculate* button to start the calculation.
- At the end of the calculation, the window represented in the previous image is closed, and the isopleths sub-menu appears again.
- Activating the Draw button in this window and the following window, the program draws the concentration isopleths map:
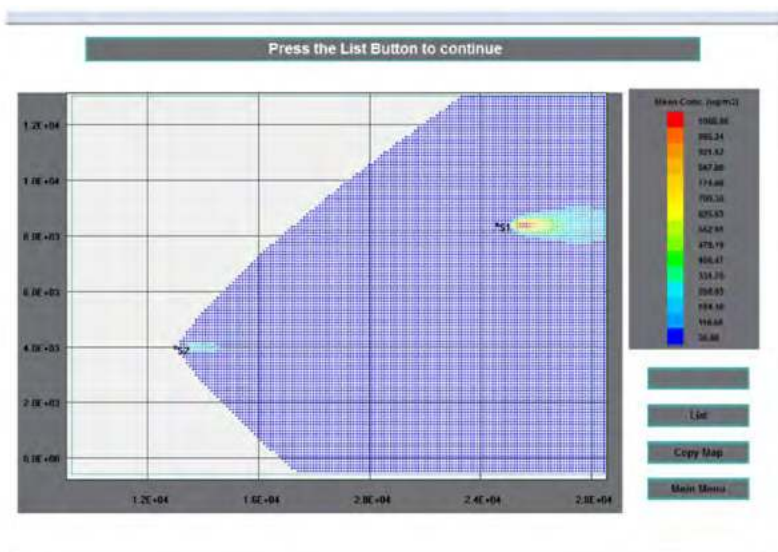
- On the bottom right corner of the window, there are two buttons which enable further functionality:
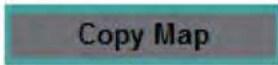
- The List button lists the isopleths' values.
- The Copy Map button allows the map to be copied to the Windows Clipboard, enabling it to be included in other applications.

By pressing the List button, the map disappears, and a table summary appears containing the average values of the various concentration isopleths.

New Concentration Isopleths?

Limit Concentrations

Maximum 1105.82 ug/m3

Minimum 0.00E+00 ug/m3

New Isopleths

New Concentration Isopleths?

Yes ☐ No ☐

Number of Isopleths

No. of Isopleths (max 15)

New Values

Cmin (ug/m3) Cmax (ug/m3)

Printer

Download Graphics to Printer?

Yes ☐ No ☐

Isopleth	Mean value (ug/m3)	Interval (ug/m3)
15	1068.96	73.72
14	995.24	73.72
13	921.52	73.72
12	847.8	73.71
11	774.08	73.71
10	700.35	73.73
9	626.63	73.73
8	552.91	73.72
7	479.19	73.72
6	405.47	73.72
5	331.75	73.71
4	258.03	73.71
3	184.3	73.73
2	110.58	73.73
1	36.86	73.72

Values are for 100.00% of time

Copy Map

Main Menu

- New values for isopleths can easily be provided, defining further ranges and locations of interest.
- By choosing a new region to plot the isopleths, using the maximum definition (1 pixel), we get the following pictures:
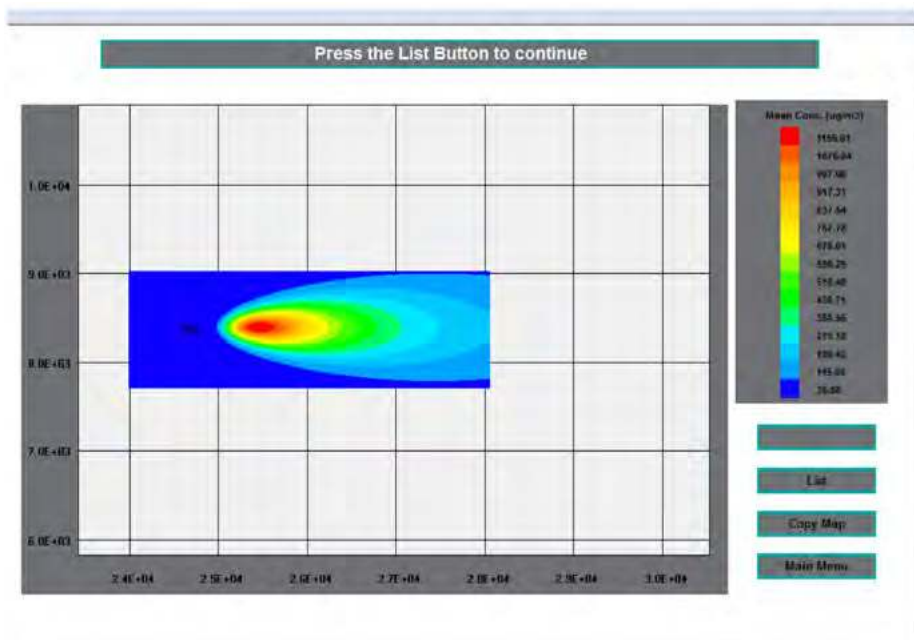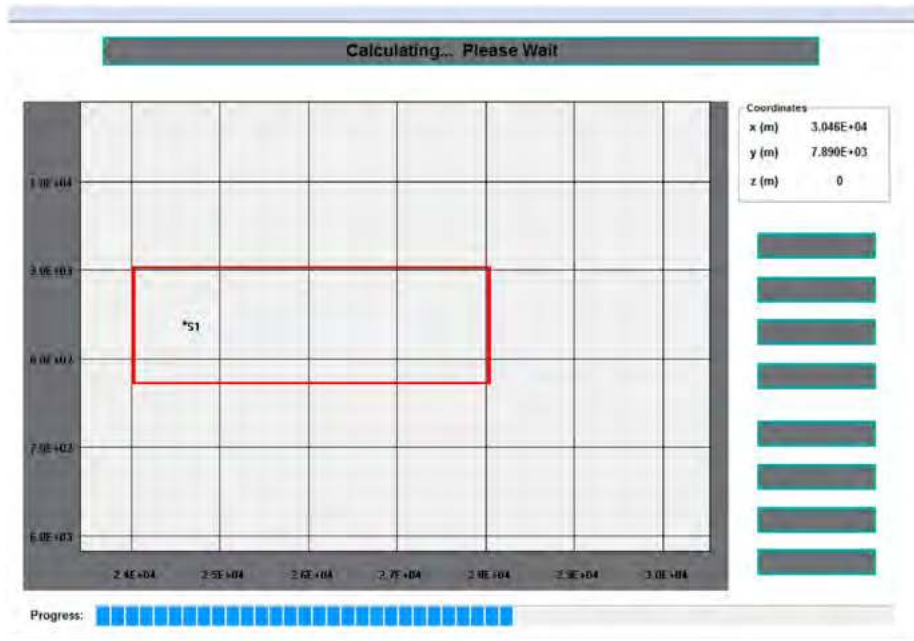
- A subgroup of isopleths can now be chosen at will. For example:
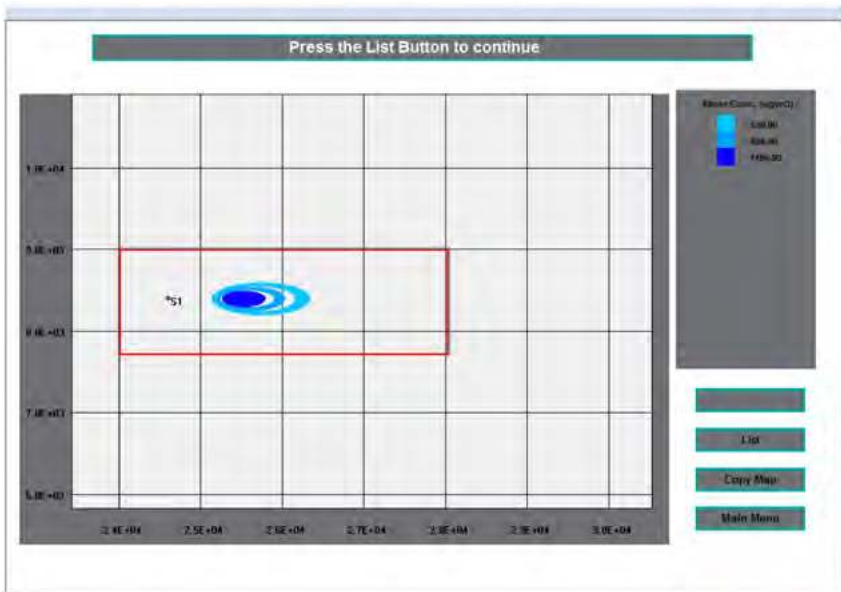
2.3.3 Optimization

A better and faster way to produce useful isopleths is to first find out where the maximum concentration occurs. Choosing this option offers different possibilities of calculating the maximum concentration value of pollutants.

- When pressing the Optimization button in the main menu, the following dialog appears:
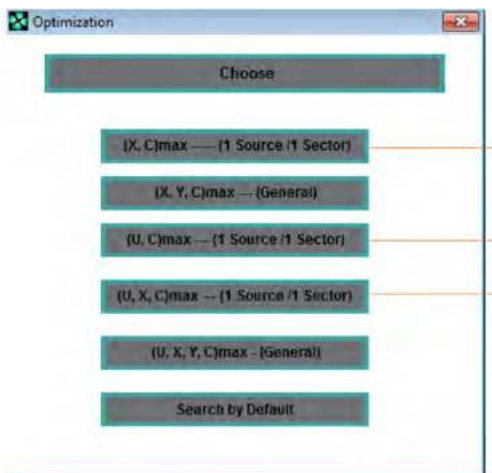
- The three options marked in the image above are only valid for situations in which there is only one source, and the wind roses have only one sector. In case the data doesn't respect these specifications, and one of these choices is made, an error message appears, and after some time the window is closed.
- By choosing a valid option, regardless of what that is, the user needs to determine if there is the need to correct for sampling time. If that's the case, a value for the correction coefficient that may or may not be provided by the program has to be defined. The next step is to choose a model for wind speed calculation, and finally, map elevation and level must be defined:


- If the second or fourth option in the Optimization sub-menu '(X, Y, C)max---General' and '(U, X, Y, C)max---General' respectively have been chosen, by activating the Next button in the image above a window with the map appears. The map allows for various actions, as already described before.
- A grid is defined starting with a click to define the first vertex of the grid. Then, moving the cursor will define a green lined-box. Move the cursor until the grid reaches the desired size and click again to define the last vertex.
- Press the Calculate button to initiate the calculation.
- After defining the grid, in case the selected option was *(X, Y, C)max---General* or *(U, X, Y, C)max---General* in the Optimization sub-menu or after clicking the Next button in the case of the other options, a new window appears:
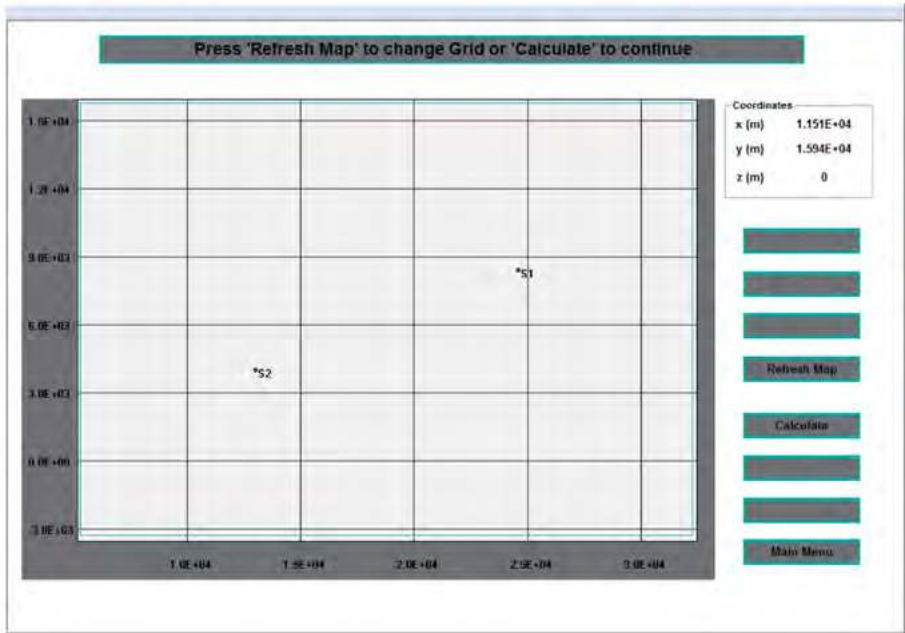
- After pressing the Calculate button:
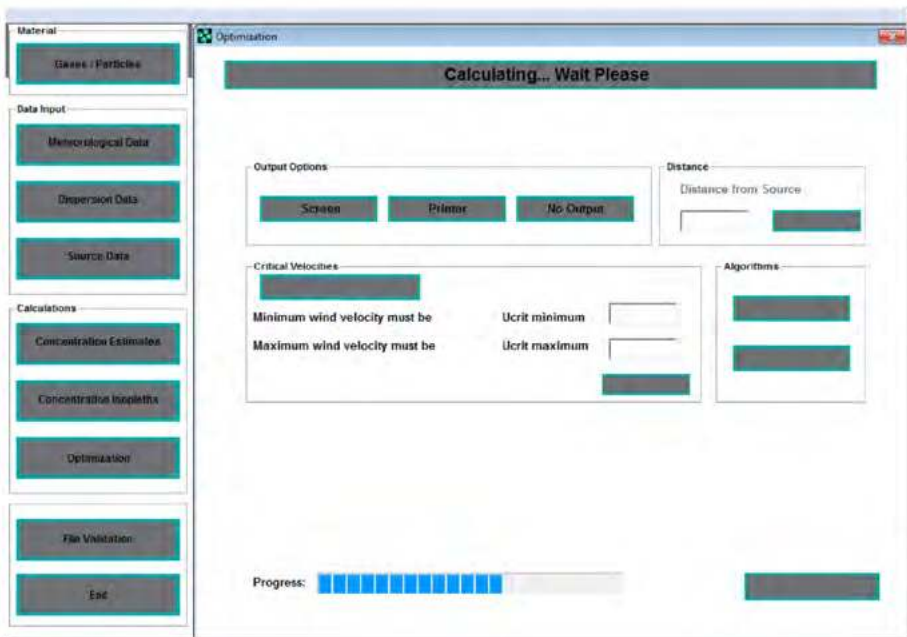
- The operation of the program will vary according to the optimization option. For example, choosing *(X, Y, C)max---General*: After setting the result output mode, the results are shown on the screen.
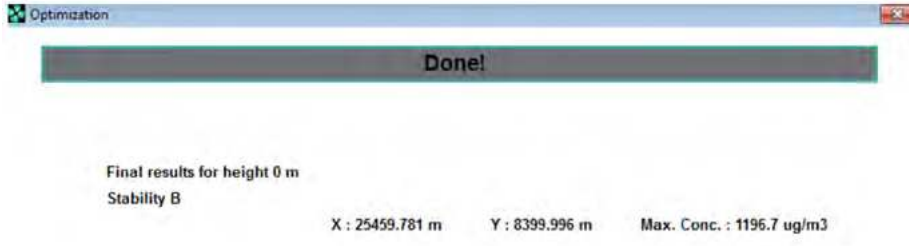

It should be noted that this result is very similar to the one obtained above for the maximum valued isopleth.

All the other options available in IMDIS have a similar operating scheme, and it should by now be fairly easy for the operator to run these options. It should be stated that all options where *U* occurs refer to the critical conditions, however unlikely they may be to occur:
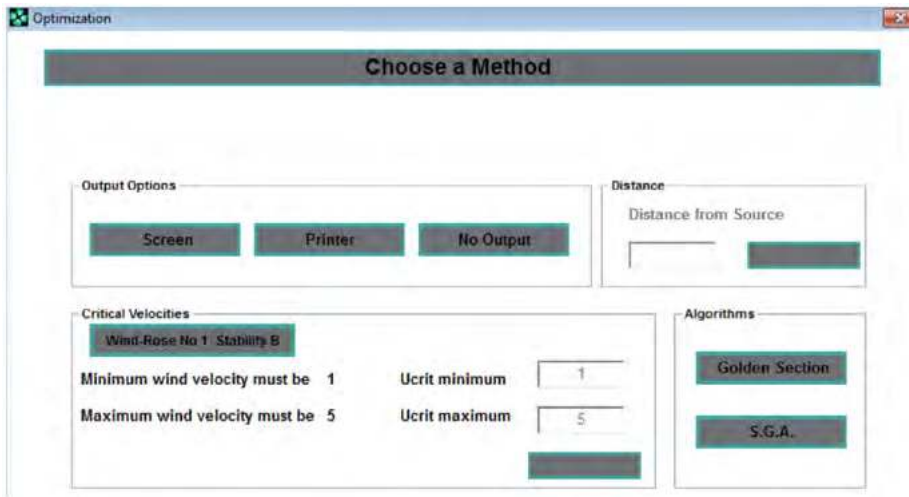
By choosing the Golden Section algorithm, one obtains the following critical conditions:
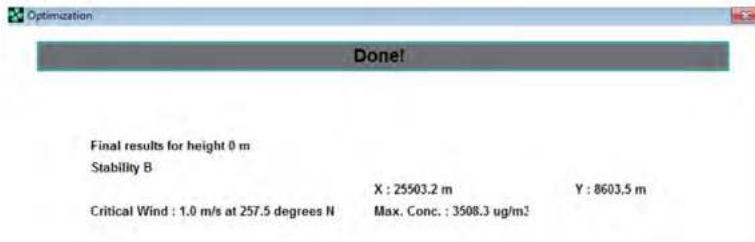

while by choosing the SGA algorithm:

Although the critical wind speed is the same from both algorithms, the wind angle is not, and this affects the location and maximum concentration. For confirmation, the next figure shows the isopleths obtained by using the meteorological data from the SGA optimizer.
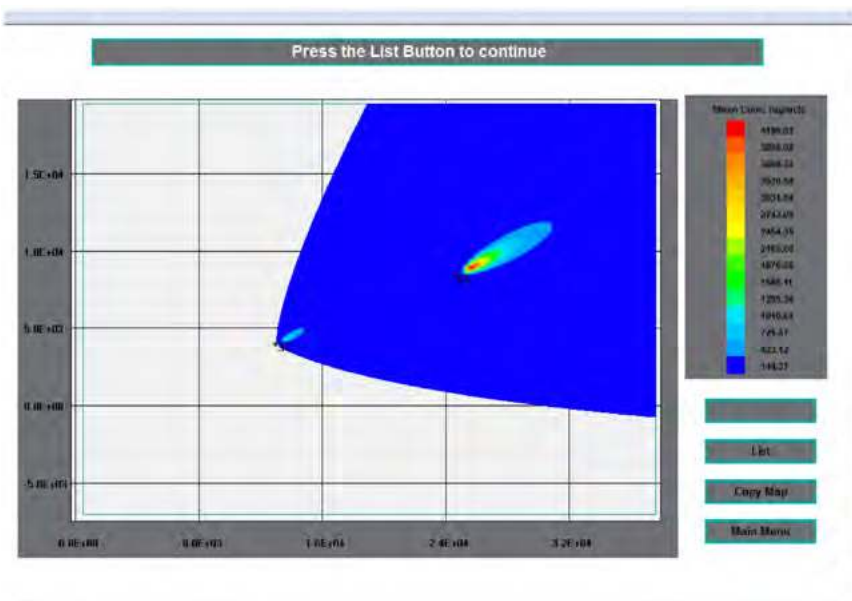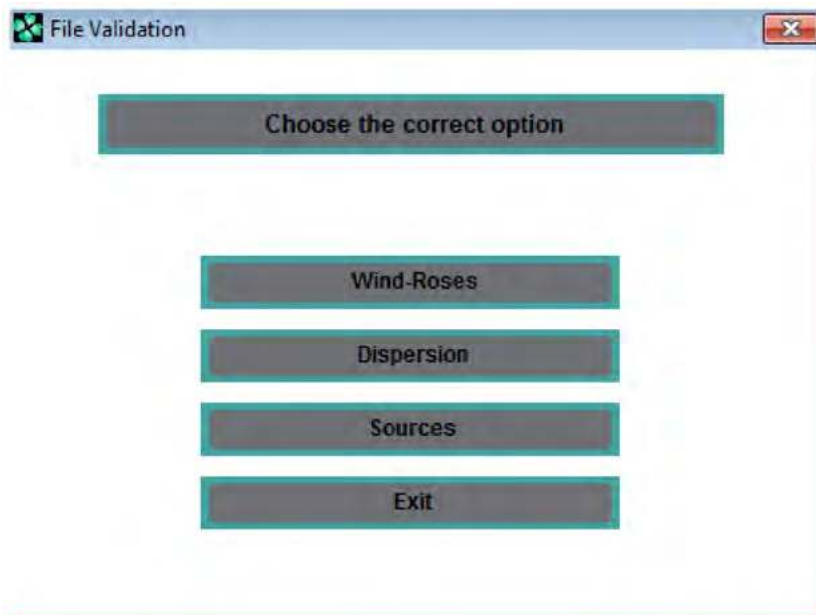
2.4 File Validation

This option in the main menu allows the user to manually create/modify data files, while respecting the file formats for the program to work. Files that can be validated are of types ***.txt**, ***.ros**, ***.fon** and ***.disper**.
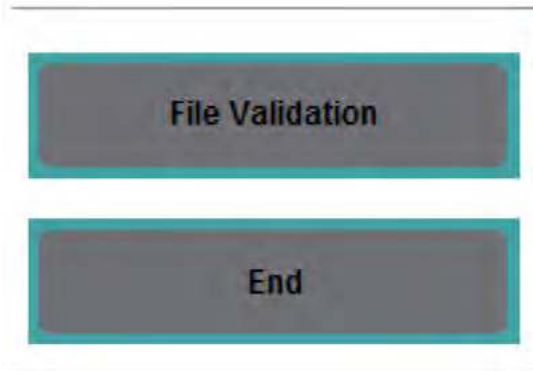
- The first step is to choose the type of file you intend to validate:

- Next, locate the file to be validated. In case the validation has been successfully carried out, the user will be asked of other files needed to be validated.
- In case the selected file is not valid, an error message appears, and the window is closed moments later.

2.5 End of the Session

To close the program, press the End button in the main menu.

2.6 Operating Requirements

For the good operation of the application, there are two requirements that must be taken into consideration, which are related to definitions external to the program:

• The screen's resolution should be 1024 x 768 so that the dimension of the main window of the program takes up all the space on the screen.
• The regional option for the numbers (control panel) must be set to English (United Kingdom).