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Paper from: *Development and Application of Computer Techniques to Environmental Studies*, CA Brebbia and P Zannetti (Editors).
ISBN 1-85312-909-7

An integrated applied research utilising fluid-dynamic software as support to medical enquiry into health problems by air pollution

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Abstract

In environmental matter a good tested fluid dynamic software is the right tool not only to detect the fallout trend of pollutant gases emitted by industrial plants but to give also reliable information to the medical-team both about probable sensible targets of pollution and maximal dose of possible inhalation for each people living in a considerable neighborhood of emission sources.

Paper wants to show the results of an inquiry commissioned by CE.RI.CA (Research Center for Environment Conservation) to the aim to discover the relationship between the fallout of gaseous pollutant emitted by petrochemical plants into the urban area, and the checkable pathologies of resident population in Melilli town (Italy).The enquire has been developed in three steps:

- The localization of high risk areas has been achieved making use of fluid dynamic ADREA-3D computer code.
- The validation of data of pollution coming from numerical simulations of computer code has been done through comparison with data recorded by networks of environmental steady stations, that is: CIPA (Industrial Consortium for Environmental Protection), District of Siracusa City and Enel networks.
- The correlation between pollutant concentrations and respiratory pathologies and diseases has been carried out through " questionnaire method" by medical team.

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1 Risk areas

To discover risk areas, as regard pollutant fallout into investigated territory, has been used the ADREA-HF [1] computer code, already tested by Energetic and Environmental Division of D.I.I.M. [2] [3] in order to study fluid-dynamic, diffusion and fallout of heavy gas.
Gaseous pollution hitting Melilli town comes from emissions of many petrochemical plants located in the industrial area of Priolo Gargallo.
Figure 1 shows area interested by petrochemicals plants, Melilli town and location of environmental steady stations.

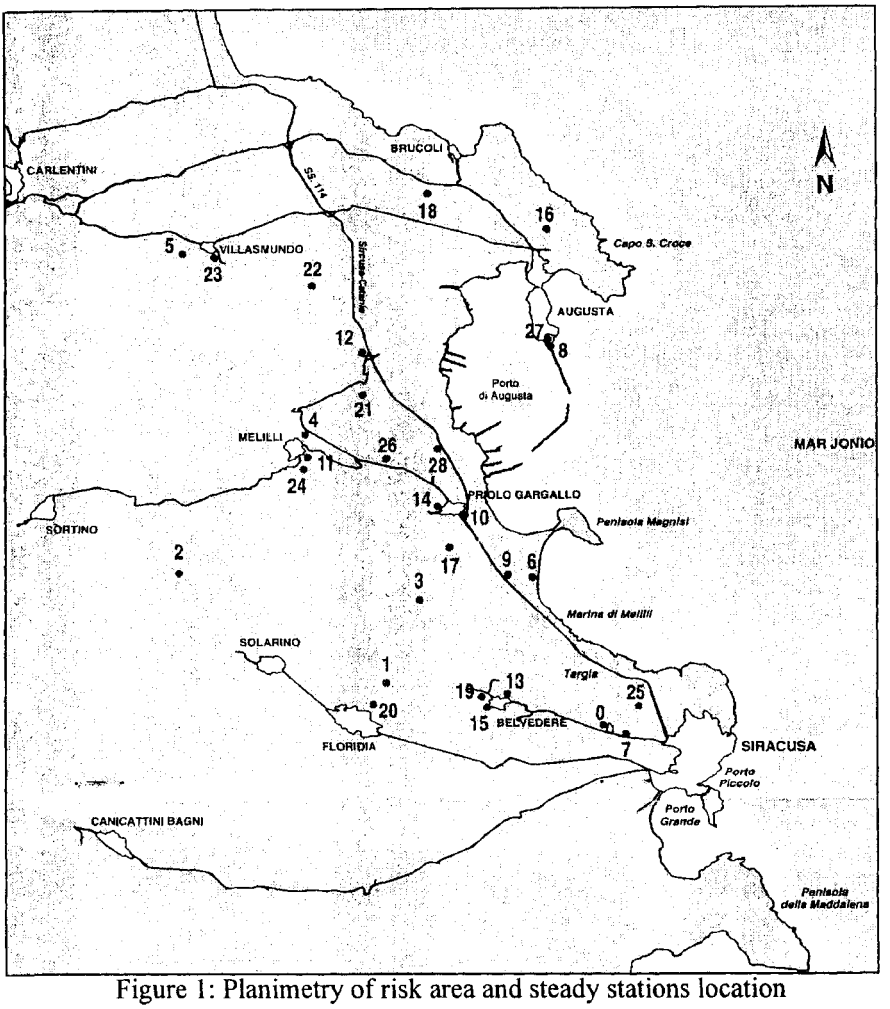

Figure 1: Planimetry of risk area and steady stations location

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Computational domain of computer code, that is a three dimensional domain, has been built taking in account all the territory of Melilli town and the rising above atmosphere, as follows:

- for the X direction: 1.800 meters;
- for the Y direction: 1000 meters;
- for the Z direction : 563 meters

In order to have right information about the fluid-dynamic of pollutants people took in account the presence of natural and anthropic obstacles, that is the ground orography, the localized buildings and the built-up area. Orography, that causes variations in the ground of computational domain, has been considered by surveying the hisoypses on cartography and by subsequent data verification through a reasonable number of altimetric readings in identified points of investigated area. In order to define anthropic obstacles, that is existing buildings, people subdivided the checked area in five sub-areas in function of height of buildings as follows:

- from ground 0.00 to 4.00 m; up to 6.00 m, up to 10.00 m, up to 12.00 m and up to 15.00 m.

This subdivision covers entirely all building typologies of Melilli built-up area.

Three dimensional modelling of orography has been obtained through triangulations, each of them defining an oriented plane inside the domain that constitutes the ground configuration of computational domain.

Modelling of built-up area has been obtained through closed quadrangulars surface, each of them defining an horizontal plane inside the domain that constitutes the roof-tops of buildings.

Particular attention has been reserved to modelling the streets too as they represent preferential ways for the diffusion of pollutant.

In this way have been defined a total of n. 251 obstacle, as follows:

- n.124 obstacles define the ground of computational domain identifying not building areas;
- n. 103 obstacles identifying built-up area;
- n. 124 obstacles identifying the scattered buildings.

Fluid-dynamic computation needs previously partition because people must define the different roughness of surfaces and to define also the several boundary conditions for temperatures, thermal fluxes, velocities and so on. In this way all the defined surfaces have been classified in four different regions of roughness, in function of its own superficial irregularities as shown in Table 1.

Table 1: Region's roughness

Region number	Roughness	Surfaces
1	0.75	Ground
2	0.40	Built-up area
3	0.05	Scattered buildings
4	0.00	Bounding surfaces of domain

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The representation of so modelled calculus domain is shown in figure 2.

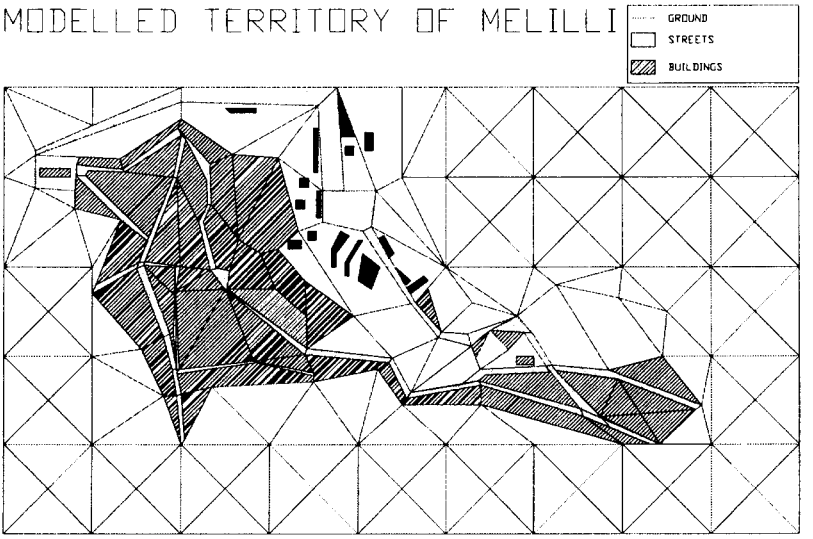

Figure 2: Planimetry of domain calculation and schematizing obstacles

Calculus grid has been obtained in function of the dimensions of domain, considering as adder of many sub-volumes called "cells", in function of maximum and minimum dimension of cells too and utilizing one constant ratio to define dimensional variations of the same cells.
In this way the calculus grid presents:

- n°59 cells in X-direction
- n°41 cells in Y-direction
- n°24 cells in Z-direction

The whole volume of domain, therefore, has been subdivided in n. 58056 cells, and among these:

- n°15547 cells are "inactive cells" as not interested by air-flow because they are full contained inside obstacles and they not influence fluid-dynamic of gaseous pollutants;
- n°19545 cells are "partially active cells" as partially interested by presence of obstacles, and so not fully interested by air-flows;
- n°22964 cells are "fully active" cells as fully interested by air-flows.

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By this subdivision of the volume domain total amount of cells interested by air-flow, and for this reason subjected to the governing equations, have been n°42509.

All geometrical data of domain have been processed by Delta-B sub code [4]. This sub-code permits both to define and to input in main computer code some calculus data as like as number of boundary surfaces, its dimensions, its orientation, its geometrical characteristics and its typologies.

After Delta-B sub-code processing, n°581 boundary surfaces have been generated as follows:

- the surfaces from n.1 to n°576 are surfaces bounding each obstacles (solid surfaces: ground and buildings);
- the surface n° 578 is the vertical surface through which pollutant gaseous come into the volume domain;
- the surfaces n° 577, n°579 and n° 580, are the lateral surfaces of domain (air surfaces)
- the surface n° 581 is the ceiling-plant of domain (air surface).

2 Basic simulation hypothesis

In aim to discover the critical conditions about air-pollution in Melilli town, people took in account several hypotheses as follows:

- the main direction of inlet of polluted air takes place through a vertical surface (surface, n° 518) with dimension 1000 meters in length and 563 meters in elevation. Geographic orientation of this surface has been chosen so that its normal vector results parallel to the direction of the "critical wind".
- The direction and the intensity of the "critical wind" is that one causing the most significant effects of pollution into Melilli town with reference to the positions of polluting source too.
- The intensity of the "critical wind" has been chosen in such way to satisfy at the same time to three conditions:

- to belong to data registered by meteorological steady stations located near Melilli;
- to be so strong to cause the transportation of pollutant from the emission sources (Priolo Gargallo) to built-up area (Melilli town);
- to be more or less constant in direction and intensity for some periods of time during the day, otherwise the transport of pollutant could happened further or before the built-up area.

The results of analysis on the data carried out by CIPA environmental network in the period from 1995 to 1997 showed the "critical wind" is that one blowing from the East direction with an intensity of 3.00 m/s.

- The SO_2 gas has been chosen as "tracer gas" to estimate air pollution into investigated domain.

In order to define the concentration of SO_2 coming through inlet surface, as previously referred, people extrapolated the value of 800 $\mu g/m^3$ from data

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registered by environmental steady stations (CIPA, ENEL, and District of Siracusa, networks).

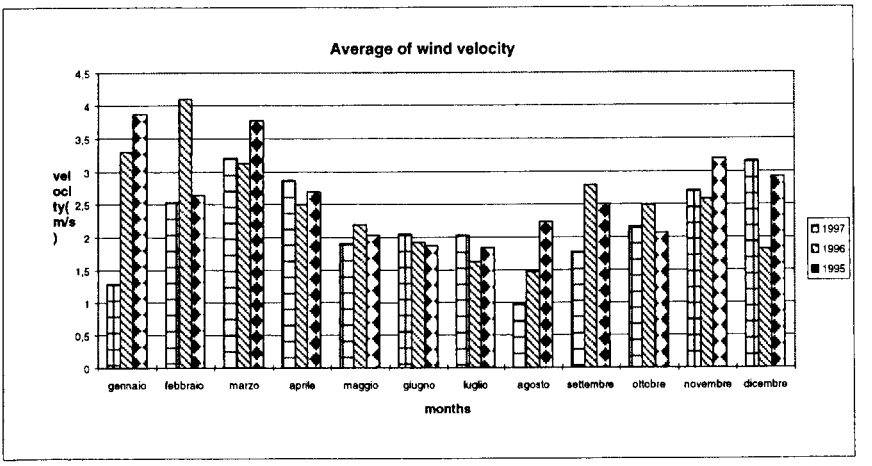

Figure 3 - Wind data registered by steady stations

Figure 4 shows the SO_2 concentration data registered by steady stations during the years from 1995to 1997.

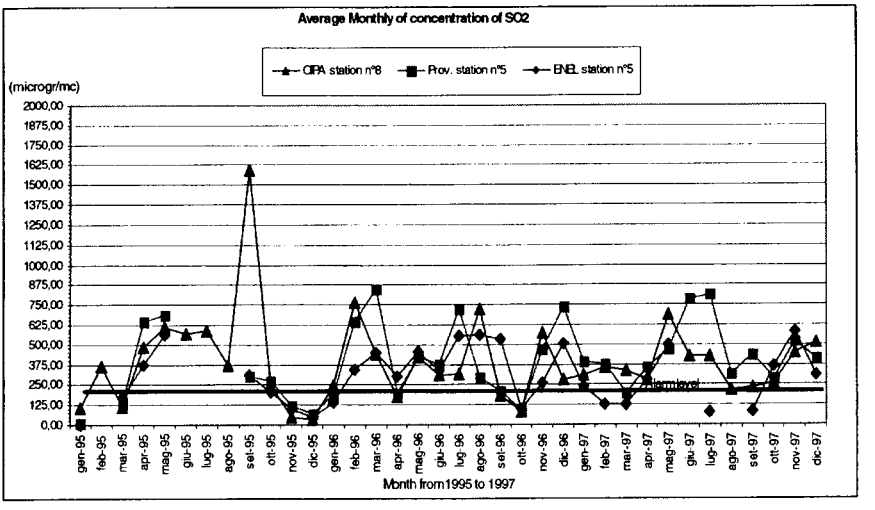

Figure 4 - SO_2 concentration data registered by steady stations

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- The adopted inlet velocity of SO_2 coming into domain through inlet surface has been the same of that one of the "critical wind", that is 3.00 m/s.

3 Simulation model and calculation strategy

ADREA-HF code is based on the finite volume concept in Cartesian Co-ordinate system. Conservation laws and related equations are applied to a defined three-dimensional atmospheric domain. The set of governing equations for the mean flow field parameters are expressed in tensor notation and reported as follow:

- Mixture mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \qquad (1)$$

- Mixture momentum :

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\rho K_{mj} \frac{\partial u_i}{\partial x_j}\right) + \rho g_i \qquad (2)$$

- Mixture energy :

This equation is expressed in terms of internal energy and temperature:

$$\frac{\partial \rho e}{\partial t} + \frac{\partial \rho u_j e}{\partial x_j} + P \frac{\partial u_j}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho c_p \frac{K_{mj}}{\sigma_h} \frac{\partial T}{\partial x_j}\right) \qquad (3)$$

- Heavy fluid mass transport :

This equation is expressed in terms of the mass fraction transport:

$$\frac{\partial \rho q_w}{\partial t} + \frac{\partial \rho u_i q_w}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho \frac{K_{mj}}{\sigma_h} \frac{\partial q_w}{\partial x_j}\right) \qquad (4)$$

where:

ρ = fluid density, e = fluid mixture internal energy, C_p = fluid mixture specific heats, P = fluid mixture total pressure, g_i = gravity acceleration component in the i-direction, u_i = general expression for the velocity components (u,v,w), x_i = general expression for the distance (x,y,z), Km_i = momentum eddy viscosity in the i-direction, q_w = heavy fluid mass fraction, σ_h = effective Prandtl number,

Turbulence closure modelling is based on the gradient transport hypotheses and involves application of the eddy viscosity/diffusivity concepts.

The one-equation model has been adopted for the solution of the transport equations, this model utilizing turbulence relates quantities such as turbulent kinetic energy (K) and turbulent energy dissipation (ε).

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Turbulent kinetic energy has been obtained through the solution of transport equations, while turbulent energy dissipation (ε) have been calculated by semi-empirical relations [1].

The temperature variations follows a linear decrease with height corresponding to neutral stability conditions.

4 Computational steps

Owing there are too many complex equations to solve, it need to subdivide computational procedure in three different steeps, that is:

a) 1-D velocity profile calculation;
b) 3-D steady state wind field calculation;
c) 3-D dispersion calculation.

In the first step of calculus people solves a mono-dimensional problem in order to define a field of velocity along Z-axis.

In the second step people utilised the previous field of velocity as starting condition to solve the three-dimensional flow equations except for heavy fluid mass transport equation.

In the third step people utilizes data of velocity field coming from the solution of second problem and solves in this step also the equation of heavy fluid mass transport equation.

By this procedure people obtains the values of concentrations of polluting gas in the whole domain of calculus and for not steady state conditions.

5 Location of zones where to focalise the medical screening

Negative effects of air pollution on health are function both of exposure times and of concentration of polluting substance to which human target is submitted.

If, in first hypothesis, people assumes as constant value the time of exposure to air pollution for all inhabitants of Melilli, than there is a direct correlation between amount of pollutant concentration and probability of the onset pathologies.

Since the fallout heavy gas forecasted by computer model shows different values of concentration into the various zones of Melilli territory, it mean that there are different probabilities of the onset of health problems among inhabitants of investigated territory.

Therefore, it has been necessary to forecast in which zones of built-up area it could be more opportune to carry out the medical screening by "questionnaire method". In this way it has been necessary to set-up one "hierarchization of probabilities" of the onset pathologies in function of the zone of residence of inhabitants, so that the medical team has been able to carry out the screening among the inhabitants of that zones showing more probability to be hit by air pollution.

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The procedure to building the "hierarchization" has been as follows:

- People choose as zones with maximum probability (Pmax =100%) that ones were computer model forecast fallout of pollutant gas over 250μg/m^3, that is the alarm concentration for SO_2 in Italian normative.
- People fixed ten intervals of values of gas concentrations, each of them wide 25 μg/m^3 , between zero value and 250 μg/m^3.
- On the ground of fallout data forecast by computer model in all Melilli territory people bounded the sub-zones of territory where the values of the gas concentrations have been included in previous ten interval of concentrations.
- For each one of that sub-zones has been computed pertaining weighted average of gas concentrations as follows:

$$\overline{Cj} = \frac{\sum Cij * Aij}{\sum Aij} \qquad (5)$$

where:

$\overline{Cj}$ = weighted average of gas concentration computed for j-zone;

Aij = value of i-plane surface included in j-zone;

Cij = concentration of gas pollutant forecasted by computer model into i-surface;

ΣAij = summation of values of the i-plane surfaces included in j-zone.

i = varying in function of forecasted punctual concentrations;

j = varying from 1 to 10.

- People computed probability of the onset of pathologies for each j-zones through linear interpolation as follow:

$$Pj = \frac{\overline{Cj}}{C\,\mathrm{max}} P\,\mathrm{max} \qquad (6)$$

where: Pmax = 100% and Cmax = 250 μg/m^3

The values of probability for each of ten intervals of gas concentration coming from formula (6) are shown in table 2.

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Table 2 – Probability of the onset of pathologies

Range of concentrations	Wide of interval ΔC	Probability of the onset
> 250	25	100.0
225 ≤ C ≤ 249	25	99.6-90.0
200 ≤ C ≤ 224	25	89.6-80.0
175≤ C ≤ 199	25	79.6-70.0
150≤ C ≤ 174	25	69.6-60.0
125 ≤ C ≤ 149	25	59.6-50.0
100 ≤ C ≤ 124	25	49.6-40.0
75 ≤ C ≤ 99	25	39.6-30.0
50 ≤ C ≤ 74	25	29.6-20.0
25 ≤ C ≤ 49	25	19.6-10.0
0 ≤ C ≤ 24	25	9.6-0.0

Two examples of "hierarchization" of the zones with different fallout into territory of Melilli town are shown in figures 5 and 6. for two different plane along Z-axis

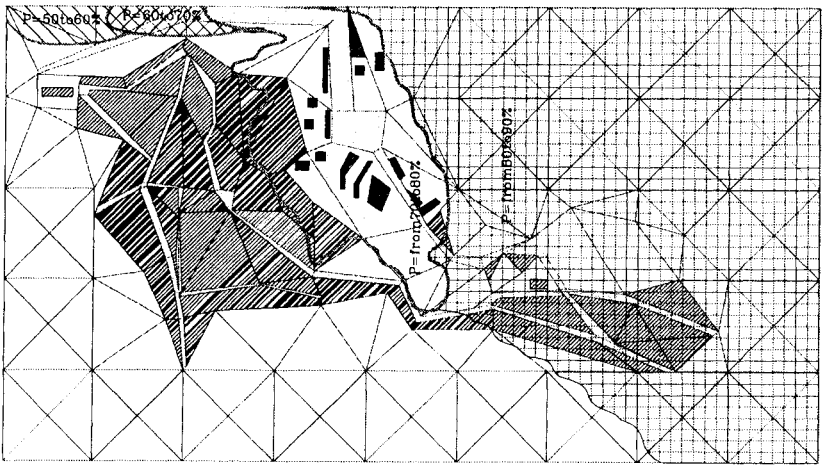

Figure 5 - Hierarchization of the zones for Z = 255.00meters

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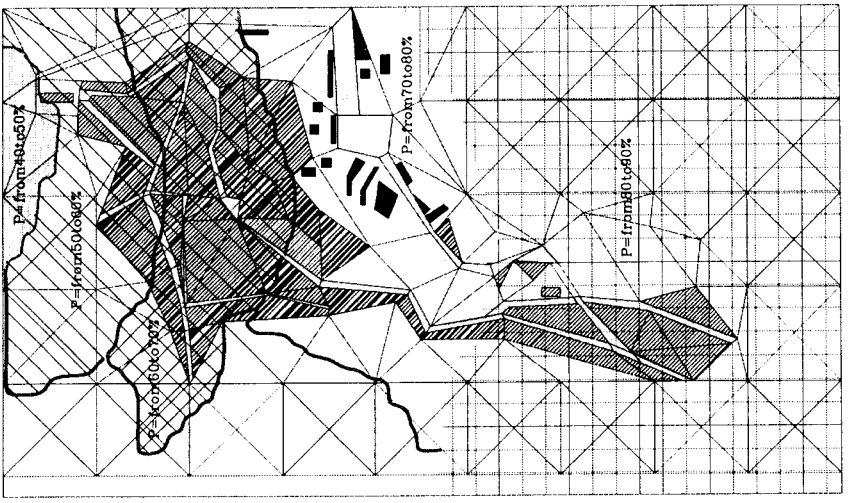

Figure 6 - Hierarchization of the zones for Z = 330.90 meters

6 Comments

- The choice of origin of scale of probability, that is 100%=250 μg/m^3, do not alter the effectiveness of data carried out as the "hierarchization" will serve only to create the comparison in terms of probability between zones of built- up territory subjected to different degree of pollution and people do will not to give real amount of pollutant shoot-down in each zone.
- People considers SO_2 as not a reactive gas, both chemically and in physic way, during the phase of convective diffusion. This hypothesis is not quite true because the variation of some parameters (relative humidity, air temperature, presence of other substances in the air and so on) could be cause modification of SO_2 concentrations. To neglect the probably reactions of SO_2 really it is not important to the aim of computing, in fact people must consider the forecast coming from modelling as upper limit of fallout of SO_2 concentrations and this consideration can not change the hierarchy of zones in terms of the onset of pathologies.
- There is different sensibility for each human-target in function of his age, his state of health and so on, but all these kinds of parameters have been took in account in medical screening of research.
- The hypothesis that all the people have been exposed for the same period of time to polluting gas it is not quite true, but this do not alter the significance of "hierarchization" on the ground that the aim of computing has been only to give to medical team indications about the places of Melilli town where to direct their own efforts for the questionnaire screening.

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7 Results

The used technique of investigation offers considerable advantages in the case of medical screening particularly when very much samples must be investigated and, in addition, they are scattered along a wide area.

The use of predictive fluid dynamic environmental computer code gave the possibility to have an aimed enquire directing medical team's effort only towards the zones of territory where there is the greatest probability to have polluting fallout and, in this way, to find the human-targets really impacted by pollution.

In shorts terms, it mean financial savings and, above the all, time savings especially when people's health is at stake. Medical team addressed "questionnaire method" to that ones sub-areas showed by "hierarchization" and obtained very remarkable information about correlations between polluting coming from petrochemical plants of Priolo Gargallo and both bronchial and allergic pathologies of people living in Melilli town.

Unfortunately in this paper there is no room to show the model of adopted questionnaire, the correlations between the pathologies carried out by medical team among people dwelling in each zone and the probability of polluting fallout calculated by fluid-dynamic code and so on.

However all these matters surly will be shown in the second part of paper in the next Envirosoft Conference.

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