MATHEMATICAL MODELLING- AN ASSESSMENT TOOL OF CHEMICAL RISK

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1.Introduction

The concentration of occupational toxic substances must be known in order to ensure an accurate assessment of the risk and of the exposure to chemical dangerous substances’ impact upon human health.
Knowing chemical substances’ levels in the occupational environment means knowing the concentrations of chemical agents in areas close to the source, in areas were workers are placed permanently or periodically, in frequently used areas or passing places, in remote areas from the sources.
This sum of areas represents in fact information upon agents’ diffusion and circulation in the working space. According to present technologies, by monitoring the working environment, this information cannot be obtained in real time, they are not exhaustive and require a great human and financial effort.
Mathematical modelling represents the less expensive way of measuring the level of chemical agents in the working atmosphere.
The application on a large scale of mathematical modelling increased with the development of computers. Today, when discussing mathematical modelling, usually the use of computers is understood and no longer specified.
The ventilation system, the space geometry and the characteristics of the generating source influence the agents’ dispersion in the working space. In fact, the movement in any fluid can be described in a unitary manner by establishing one of the most important equations, for describing the matter, the diffusion equation. The equation expresses the plausible, intuitive result, according to which the inequalities in diffusion tend to smoothen and the distribution becomes uniform.
Starting from these certainties I developed a mathematical model of chemical agents’ dispersion in “small spaces”, called RRs model. This model can be used to predict the concentration field of chemical agents in a defined space.

2. General equations of the model

Real situations that involve fluids’ flowing and mass transfer (the diffusion of agents in small spaces) are controlled by the principles of conservation of the mass, movement, energy, chemical species and others. These principles are expressed in the form of partial differential equations and represent the basic equations of the developed model.

1) The continuity equation, that expresses the conservation of fluid mass.
2) Navier-Stokes equations, expressing the balance of the movement quantity.
3) Diffusion-convection equations

The flowing and diffusion equations can be solved analytical, analogical or numerical for many simple cases. Results can be applied, with some corrections, to a much larger class of phenomena.

3. The calculus program

Taking into account the complexity of the problems set in the model and the available computers, I chose TURBO PASCAL language to write the program.
The entry data of the program are displayed in 3 windows:

1. general data – the dimensions of the "small place", the number of increments in length, width, air holes, the atmosphere status, diffusion coefficient and the maximum number of iterations.
2. extreme conditions – the number of increments that border the air holes and the airflows that pass through them.
3. pollutant sources – the pollutants flows are introduced in the points determined by the values of increments.

In the 2D representation, the program plots:

- the border of the "small space"; the positions of entry and exit holes;
- the position of the agents' generating sources;
- the areas of pollutant's izoconcentration;
- air (gas) flow lines;
- the grid that sets the partition in increments
- the lines of pollutant's izoconcentration;
- the grid and number of increments;
- the values of flow potential through the grid holes;
- the debits of pollutant sources;
- the concentration in the point where the mouse cursor points.

In the 3D representation, the program displays a perspective picture of the field of concentrations and is able to modify the dimensions of the concentration's alleviation.

4. The validation of the mathematical model

he concentrations obtained with the mathematical model, having as entry the physical-chemical characteristics of the sources and the characteristics of the defined space, allow to estimate the risk of occupational exposure by comparing those concentrations with the threshold limit values measured at the work place.
In these conditions we must validate the mathematical model of agents' diffusion in small places, with actual measures of the concentrations of agents in an industrial working place "HALL", were activities of car adjusting and repair take place.
Taking into account the type of industrial activity in the HALL, we established the moments and the point for simultaneous and continuous measurements of the main resulted agents' concentrations: carbon monoxide and azotic oxides. The agents' concentrations were measured with NDIR – an infrared analyzer with crossed flow modulation, HORIBA-ENDA Transportable -1000 Series Type.
The concordance between the measured and modeled values is satisfactory.

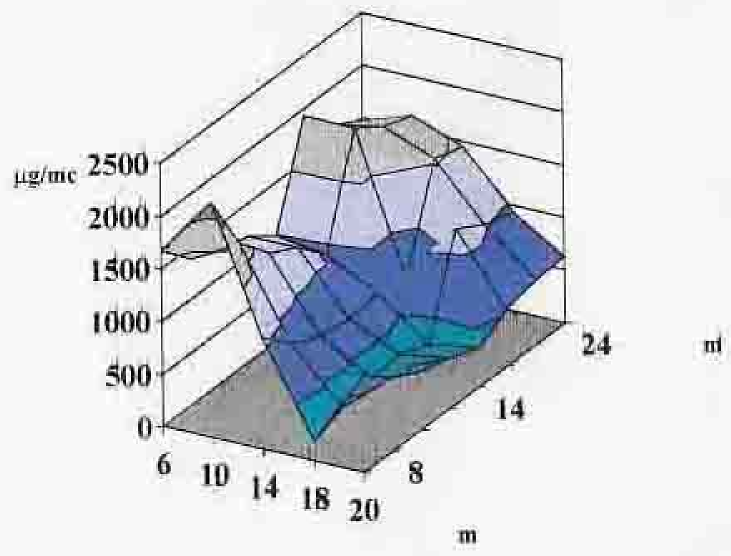

fig.1 Area's modelated circulations

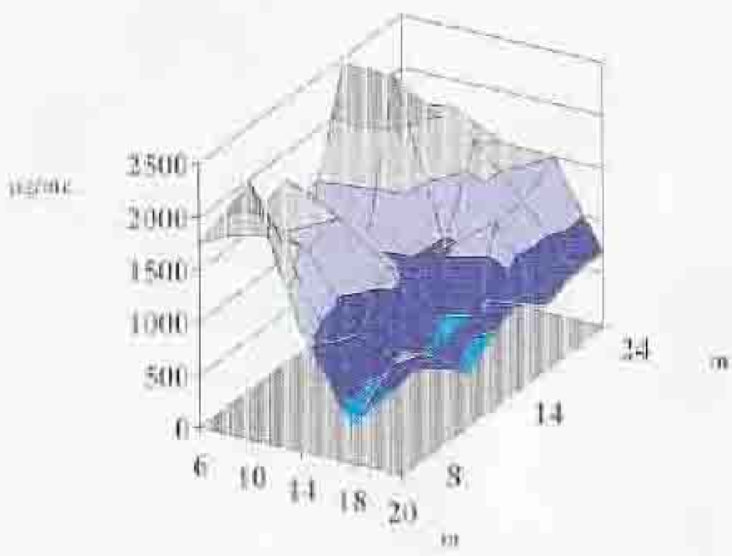

fig.2 Area's measured concentrations

From Fig. 1-2 we observe the following:

- modeled and measured fields are uniform
- there is an underestimation of modeled concentrations both in the neighborhood of agents' generating sources and in the dilution areas.

fig.4 Carbon monoxide concentartions field-hall no.1-3D representation

fig.3 carbon monoxide concentrations field-hall no.1-2D representation

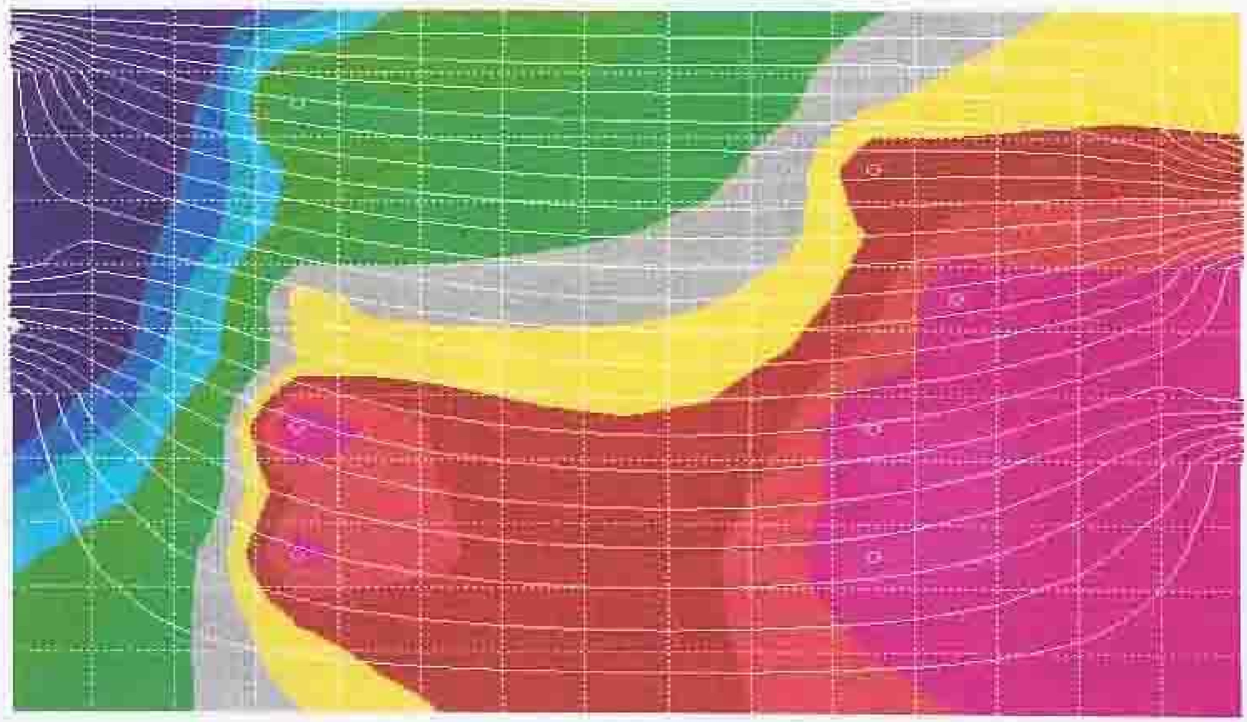

Fig. 3-4 presents the simulated concentrations' field showing that the use of this program is friendly and suggestive.

5. Conclusions

The RRs mathematical model is an interesting instrument that assesses the concentrations of physical-chemical agents in the working environment.

It is the first model of this type developed in our country, with applications in the industrial toxicology activity. The model quickly offers information and information is “power”. In other words, it provides savings (of time, staff and financial) and information. With its help it can be achieved:

- the revision of work place’s monitoring methodology, by accurate establishment of the points of agents’ measurement;
- appraisal of chemical risk in the designing phase of an industrial unit with the direct involvement in the health and safety at work policy;
- obtaining information related to ventilation system of the defined space, that are necessary both in the designing phase, as well as a control instrument for all decision makers in occupational safety;
- the possibility of sorting at sectorial level of air’s quality status in the working areas
- the main purpose of this paper is the development of a “new way” of assessing the surrounding environment’s health status, starting from the concept that “surrounding environment’s therapy” must be the foundation of population’s health status.