A NUMERICAL TOOL FOR THE PREDICTION OF A TOXIC CHEMICAL SUBSTANCE DISPERION AT THE WORKPLACE

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INTRODUCTION

PVC is prepared by suspension, emulsion or bulk polymerisation of Vinyl Chloride Monomer (VCM). This latter chemical has been linked with a series of hazards concerning Safety and Hygiene. More specifically, in high concentrations VCM acts as an anaesthetic and causes skin burns by rapid evaporation and consequent freezing. When exposed to heat or flame it is dangerous and its vapours can explode. Furthermore, it emits highly toxic fumes of phosgene upon thermal decomposition and reacts violently with oxidizing materials. Besides these hazards that are connected with high concentrations, VCM is also dangerous in minute concentrations as it is a recognized carcinogen which attacks, particular the liver. Safety and hygiene rules apply not only to VCM polymerization plants but also to PVC processing factories, since the traces of monomer trapped in the PVC resin during polymerization can be evolved from the molten resin at the processing stage. Many directives have also been issued to protect human health against the possibilities of VCM migration from the packaging of foodstuff. Thus, the EEC directives consider the concentration of 0.01 mg VCM per kilogram of resin as an upper safety limit for the final product. The evolution, during the last decade, of a large number of multidimensional, multiphase models and solution techniques for simulating fluid flow and transport processes, coupled with the development of modern high speed / low cost computers and workstations has made it possible to use new CFD methods to assess the effectiveness of ventilation provisions in industrial and other buildings.

In this work, the VCM concentrations around the blending installations in a PVC-pipe production plant were measured. In particular, the concentrations above two high speed mixers and three ribbon blenders have been determined. These measurements allowed the development and validation of a model describing the distribution of VCM in the major area and the selection of a proper ventilation design.

EXPERIMENTAL PROCEDURE

The three-dimensional view of the PVC blending plant, including two high speed mixers and three ribbon blenders is shown schematically in Figure 1.

VCM concentrations have been measured at a distance of about 50 cm above each machine, using Drager tubes, that can give the concentration over some minutes, as well as by charcoal tubes that allow determination of longer period averages (e.g. over 8 hours). In this latter procedure, the NIOSH method 178, a known volume of air is drawn through a charcoal tube to trap the VCM present. The charcoal in the tube is then transferred to a small vial containing carbon disulfide, where VCM is desorbed. An aliquor of this sample is injected into a gas chromatographer and the area of the resulting peak is determined and compared with areas obtained from the injection of standards.

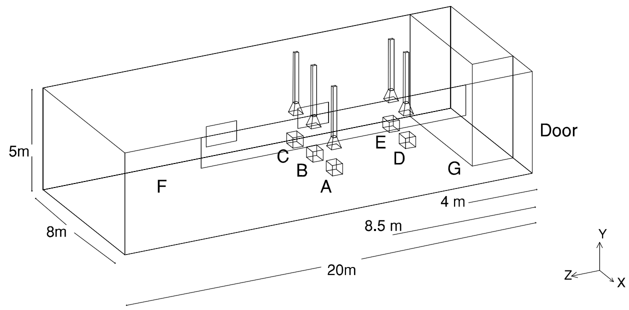


Figure 1.The three-dimensional view of the PVC blending plant

The minimum detectable amount of VCM is said to be 0.2 nanograms per injection at a 1x1 attenuation on a gas chromatograph.

THEORETICAL MODEL

The physical problem concerns the fluid flow and transport of heat and various contaminants inside a general three-dimensional space, that may form part of an industrial building.

To demonstrate and validate the present model a three-dimensional, rectangular enclosure containing 5 VCM sources, 5 vents just above them, an opening over stacked PVC containers and a door was considered. The chosen enclosure is part of a PVC-blending plant of a major Greek plastics Company, located in Athens, Greece. Three separate cases have been studied, according to the ventilation conditions and the VCM emissions. Two of them concern steady-state analysis and the third the transient analysis of a hypothetical accident. The enclosure and its openings are presented in Figure 1 along with the position of the VCM sources (i.e the high speed mixers & ribbon blenders) and the vents. Some of the geometrical details of the enclosure along with other information are given in Table 1 :

Table 1 : Geometrical details of the enclosure & Operating Parameters

Enclosure Dimensions	20m x 8m x 5m (length x depth x height)
Inlet area per vent	0.25 m2
Door Inlet Area	9.5 m2
Inlet over stacked PVC containers Area	19.5 m2
Mass Flow Rate per Vent	0.024 Kg/s
Overall vent mass flow rate	0.12 Kg/s
Internal Temperature	23 oC (73.4 oF)
External Temperature	11 oC (51.8 oF)

The three cases are presented in detail in the following paragraphs.

Case 1.This is a simulation of the real conditions prevailing in the plant. The ventilation system works at its nominal conditions and the VCM sources used are experimentally determined. Flow is dominated by forced convection.

Case 2.Similar to Case 1 except that the ventilation system works at a tenth of its nominal mass outflow rate (probably because of a mechanical malfunction).

Case 3. In this hypothetical case the spread of an initial release of VCM (probably because of an accident) under nominal ventilation conditions is modelled with respect to time.

The present analysis is based on the numerical solution of the set of the partial differential equations that express the conservation principle for mass, momentum, energy and chemical species in steady or transient, three-dimensional, recirculating, flows.

The discretization of the domain (Figure 2) is followed by the reduction of the above mentioned equations to their finite domain form using the ‘upwind formulation of the coefficients‘. Suitable assumptions are made about the physical processes involved and the boundary conditions corresponding to each case ,and are fitted into a computer model which is then incorporated into the general PHOENICS ® ver 3.6 environment.

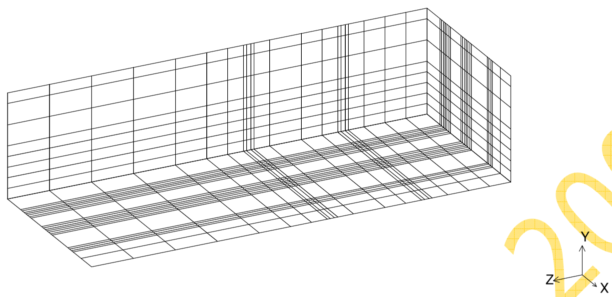


Figure 2. The computational grid used NXXNYXNZ=20X8X21

The main assumptions that are made are :

a. No outside wind effects are taken into account.
b. The air coming into the cavity is totally free of VCM.
c. The cavity walls are considered adiabatic.
d. Since the VCM emission rates cannot be measured (batch process), the internal conditions representing the VCM sources are of the fixed value and not the fixed flux type, and are based on the mean of the experimental measurements, just over the machines.

Computer runs of the resulting model are made and their primary results are the grid-node values of the three velocity components, pressure, temperature and VCM concentration at each time step (when modelling a transient Case).

RESULTS AND DISCUSSION

Case 1. The calculation results for Case 1 are displayed in Figures 3 and 4.

Figure 3 presents a vector plot of the flowfield inside the plant. It can be observed that air flows mainly from the opening over the stacked PVC containers (60%) and from the door (40%). Although high air velocities are observed near the door, there is a great part of the plant, away from the machines and the vents in which the air is nearly stagnant. Except for the velocity vectors from plan view of the enclosure, two sections including the machines and the vents are shown along with the velocity vectors in these planes. This realization of the flowfield proves extremely useful to the designer especially when the geometry of the enclosure is complicated (large Shopping Centres, Underground Stations and Garages etc.). The use of the model described in this work in these situations could provide invaluable information for the correct design of the ventilation system.

Figure 4 shows a contour plot of the VCM concentration inside the plant. It can be observed that the predicted value of the concentration is nearly zero in most of the space except very near the machines. So it follows that when the ventilation system is working at its nominal output the plant is free of VCM and there is no danger for the workers. As it can be easily observed the simulation results generally agree very well with the experimental values of VCM concentration.

Case 2. The calculation results for Case 2 are displayed in Figures 5 and 6.
As it can be easily seen, despite the low performance of the ventilation system the successful positioning of the vents just over the machines gives good results. The concentration contour map does not show any significant deviation from the results for Case 1

CONCLUSIONS.

The evaluation of the results obtained leads to the following conclusions :

a. The PVC processing plant under investigation is safe during operation as far as VCM emission is concerned.

b. The positioning of the ventilation system is the appropriate one and its capacity is sufficiently high.

c. An auxiliary ventilation system would be helpful in case of an emergency (e.g.accidental fire) for fast and effective escape of VCM vapours from the polluted area.

d. General computer programs (like PHOENICS) are very useful tools for evaluation and analysis of existing ventilation equipment. In addition they can dictate new designs for an optimal operation, from the point of view of safety and hygiene.

It is generally concluded that the computational results are realistic and in good agreement with the experimental measurements and that computer simulation is now capable of assisting the designer to optimize ventilation arrangements in Industrial buildings, within practical computer resources.

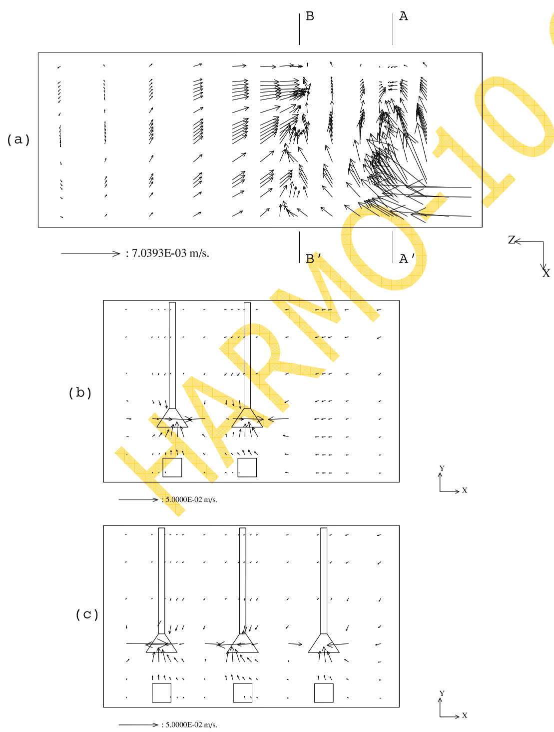


Figure 3. Predicted flowfield for case 1. (a) Plane view 1.5m from the floor, (b) Section AA', (c) Section BB'

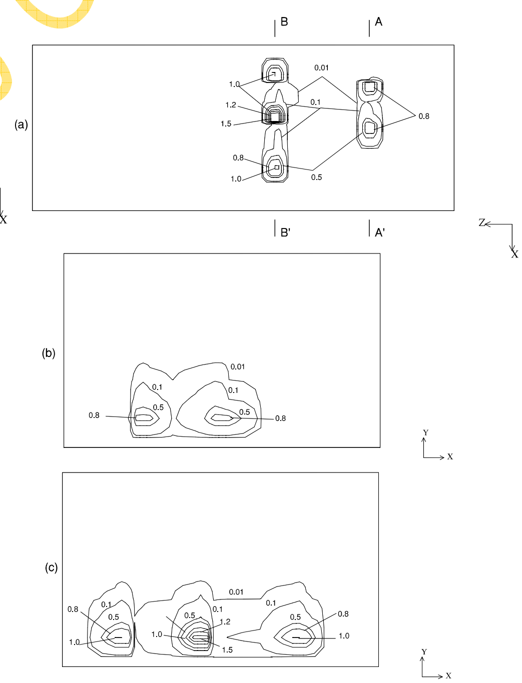
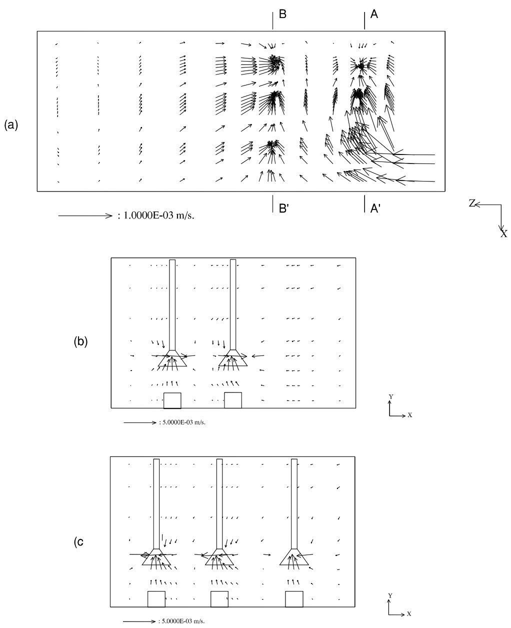


Figure 4. Predicted VCM concentration Contours for case 1. (a) Plane view 1.5m from the floor, (b) Section AA', (c) Section BB'



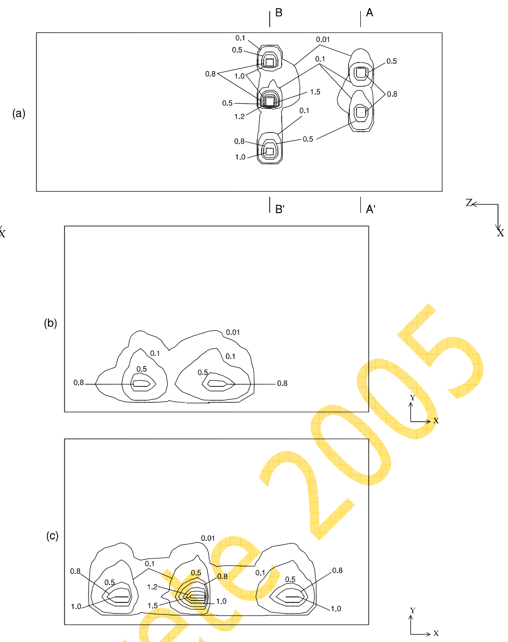


Figure 5. Predicted flowfield for case 2. (a) Plane view 1.5m from the floor, (b) Section AA', (c) Section BB'

Figure 6. Predicted VCM concentration Contours for case 2. (a) Plane view 1.5m from the floor, (b) Section AA', (c) Section BB'