Modelling the dispersion of a toxic substance at a workplace

P. Kassomenos a,*, A. Karayannis b, I. Panagopoulos b, S. Karakitsios c, M. Petrakis d

a University of Ioannina, Department of Physics, Laboratory of Meteorology, Panepistimioupolis, GR-45110 Ioannina, Greece
b Sybilla Ltd., 16 Ypsilandou Street, Maroussi GR-151 22, Athens, Greece
c University of Ioannina, Department of Biological Applications and Technologies, GR-45110 Ioannina, Greece
d National Observatory of Athens, Institute of Environmental Applications and Sustainable Development, GR-11472 Athens, Greece

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Abstract

The occupational health and safety of the workers in chemical plants are of great importance because they are exposed to concentrations of toxic substances that may exceed institutional limits.

This work presents a methodology of assessing the indoor dispersion of the toxic chemical substance Vinyl Chloride Monomer (VCM) in a Polyvinyl Chloride (PVC) chemical plant using Computational Fluid Dynamics (CFD) techniques. A mathematical model using the CFD Code PHOENICS based on solving the full 3-D Navier–Stokes and scalar conservation equations together with turbulence modelling is used to predict the toxic VCM dispersion in a geometrically complex industrial area. The source emissions, as well as the effect of the geometrical details of the building structure were also studied.

The results showed that the use of a CFD is a promising technique to study the occupational exposure in the known carcinogen VCM and to design the proper ventilation system to reduce the consequences of an accidental release of VCM in a workplace.

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1. Introduction

The use of Polyvinyl Chloride (PVC) has maintained a steady growth and is still one of the three largest-volume plastics despite competition from newer products. PVC is prepared by suspension, emulsion or bulk polymerisation of Vinyl Chloride Monomer (VCM). VCM has been shown to cause liver, brain, and lung cancer, as well as lymphatic and haematopoietic malignancies (such as lymphoma and leukemia) in multiple epidemiologic studies (Kielhorn et al., 2000).

Occupational Safety and Health Administration of USA (OSHA) has adopted a permissible exposure limit of 1 ppm for VCM as an 8-h time-weighted average, with a 5-ppm ceiling for any 15-min period. In order to access the air quality in an indoor workplace environment, an Indoor Air Quality (IAQ) model is needed.

There are three main categories of IAQ models (statistical, mass balance and CFD models). In case that the interest of the application is point concentrations (personal exposure) the most suitable tool is a CFD model. CFD models differ from mass balance models in two major ways. CFD models predict air velocity and pollutant concentration at individual points in a room instead of the average concentration predicted by mass balance models, and also CFD models solve a set of partial differential equations instead of the ordinary differential equations solved by mass balance models.

Prediction of personal exposure is an important use of CFD models (Awbi, 1996; Brohus and Nielsen, 1996). CFD models used for predicting personal exposure can take into account the impact on the person (e.g., thermal effects on the person) on exposure. Rodes et al. (1995) have shown that the person can have a significant impact on personal exposure.
CFD models are especially useful for studying the distribution of air and air movement in rooms and buildings. Kyrabuichi et al. (1989) and Nho and Kim (1996) discuss the use of CFD models for studying airflow in rooms. Nielsen (1995) discusses linking the CFD models of airflow with source emission models to predict source emissions and indoor pollutant concentrations.

Both two- and three-dimensional (2- and 3-D) CFD models are available. The 2-D models have the advantages of speed and ease to use. The 2-D models can provide useful information about many cases of interest. For example, Li and The (1996) demonstrate the usefulness of 2-D models for studying flow through large openings. Yamamoto et al. (1990) present a 2-D CFD model for PCs.

Three-dimensional models provide considerably more information about airflow and pollutant concentrations than do 2-D models. The extra information provided by 3-D models comes at the expense of speed and ease of use. Available 3-D CFD models include VORTEX (Gan and Awbi, 1994) and models built using FLUENT (Fluent, 1995), and FLOVENT (Flomerics, 1994).

Besides these indoor applications, CFD models are used for outdoor applications, like urban air quality (Chu et al., 2005), air fluid dynamics around buildings (Neofytou et al., 2006) and street canyon modelling (Neofytou et al., 2005), and also for several other environmental applications like the analysis of ammonia injection methods to produce chloramines in water containing residual free chlorine (Liu and Ducoste, 2006) or the evaluation of the oil slick spreading and drifting (Tkalich, 2006).

Source and sink models are also important in predicting pollutant concentrations with CFD models. If the source and sink terms are not adequately described, the concentration predictions will be inaccurate, even if the airflow predictions are accurate.

Based on the principles of the above three categories of IAQ models, several computational methods have been developed, like STKi (Guo, 2000), which is a Windows-based Indoor Air Quality (IAQ) simulation software package, or combinational models, like COMIS (Ren and Stewart, 2006), a model capable of predictions of personal exposure to contaminant sources in industrial buildings.

In this work, with the aid of a CFD model (PHOENICS) the VCM concentrations around the blending installations in a PVC-pipe production plant were studied under certain conditions. In particular, the concentrations above two high speed mixers and three ribbon blenders were calculated. The personal exposure of the workers was also estimated. Additionally VCM concentrations were measured. These measurements allowed the development and validation of the model used, describing the distribution of VCM in the major area and the selection of a proper ventilation design.

2. Experimental procedure

The three-dimensional view of the PVC-blending plant, including two high speed mixers and three ribbon blenders is shown schematically in Fig. 1. VCM concentrations were 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 h). In this latter procedure, the NIOSH method (NIOSH, 1978), a known volume of air was drawn through a charcoal tube to trap the VCM present. The charcoal in the tube was then transferred to a small vial containing carbon disulfide, where VCM was desorbed. An aliquot of this sample was injected into a gas chromatographer and the area of the resulting peak was determined and compared with areas obtained from the injection of standards.

The minimum detectable amount of VCM was said to be 0.2 ng per injection at an 1 × 1 attenuation on a gas chromatograph.

The NIOSH method presents numerous advantages. The sampling device is small, portable and involves no liquids. Interferences are minimal and most of them whenever they occur can be eliminated by altering chromatographic conditions. The tubes are analysed by means of a quick, instrumental method. The method is also applicable to the simultaneous analysis of two or more components suspected to be present in the same sample, by simply changing gas chromatographic conditions from isothermal to a temperature-programmed mode of operation.

3. Theoretical model

3.1. The physical problem

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 five VCM sources, five vents just above them, an opening over stacked PVC containers (point F in Fig. 1) 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 were studied, according to the ventilation conditions. 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 Fig. 1 along with the position of the VCM sources (i.e. the high speed mixers and ribbon blenders) and the vents. Some of the geometrical details of the enclosure along with other appropriate, as input to the model, information are given in Table 1.

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.

3.2. Nature of the analysis and the mathematical model

The present analysis was 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 (Fig. 2) was followed by the reduction of the above mentioned equations to their finite domain form using the ‘upwind formulation of the coefficients’. Suitable assumptions were made about the physical processes involved and the boundary conditions corresponding to each case, and were fitted into a computer model which was then incorporated into the general PHOENICS® Ver. 3.6 environment (Spalding, 1981; Markatos, 1982).

The main assumptions that were made are as follows.

a. No outside wind effects were taken into account.
b. The air coming into the cavity was totally free of VCM.
c. The cavity walls were 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 were 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).

3.3. The governing differential equations

The time-dependent equations for continuity, velocity components, temperature and chemical species (where density-fluctuation correlations are ignored) can be expressed in the following general form:

\[ \frac{\partial}{\partial t} (\rho \Phi) + \text{div}[(\rho v \Phi - \Gamma_\Phi \text{grad}\Phi)] = S_\Phi \]  \hspace{1cm} (1)

where \( \rho \), \( v \), \( \Gamma_\Phi \) and \( S_\Phi \) are density, velocity vector, “effective exchange coefficient of \( \Phi \)” and source rate per unit volume, respectively. The source rate and effective exchange coefficient correspond to each conserved property \( \Phi \) solved for this study (i.e. mass/continuity, the three velocity components, energy and concentration).

3.4. The finite domain equations formulation

Finite domain equations were derived by the integration of the above differential equations over finite control volumes, which taken together fully cover the entire domain of interest (Fig. 2). These control volumes are called “cells” or “sub-domains”. Within each cell is a “typical point” (called a ‘grid node’), say P, for which the fluid property values, \( \Phi \), are regarded as representative of the whole cell. It is surrounded by neighbouring nodes which we shall denote by N (North), S (South), E (East), W (West), H (High), L (Low), and T (grid node at earlier time). Cells and nodes for velocity

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**Table 1**

Geometrical details of the enclosure and operating parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enclosure dimensions</td>
<td>20 m × 8 m × 5 m (length × depth × height)</td>
</tr>
<tr>
<td>Inlet area per vent</td>
<td>0.25 m²</td>
</tr>
<tr>
<td>Door inlet area</td>
<td>9.5 m³</td>
</tr>
<tr>
<td>Inlet over stacked PVC containers area</td>
<td>19.5 m²</td>
</tr>
<tr>
<td>Mass flow rate per vent</td>
<td>0.024 kg/s</td>
</tr>
<tr>
<td>Overall vent mass flow rate</td>
<td>0.12 kg/s</td>
</tr>
<tr>
<td>Internal temperature</td>
<td>23 °C (73.4 °F)</td>
</tr>
<tr>
<td>External temperature</td>
<td>11 °C (51.8 °F)</td>
</tr>
</tbody>
</table>
components are ‘staggered’ relative to those for all other variables (Fig. 3). The cells in the situation considered are strictly Cartesian. The computation of the velocity vectors was made in face while the scalars were computed in the middle of the grid cells.

The ‘integration’ involved is different from the usual Taylor series expansion used in the classical finite difference technique, and results in different coefficients of the algebraic equations that are finally obtained, in the general case. This integration allows for injection of physical considerations into the formal mathematical manipulations (e.g. the conservation principle that leads to the differential equations at the first place is satisfied exactly) and permits a fully conservative formulation. Integration entails ‘interpolation assumptions’ about $F$ values and values of $F$ gradients, prevailing at the cell boundaries (Markatos, 1982). Integration leads to finite domain equations (FDEs) having the following form (Markatos, 1982):

$$\alpha_P \Phi_P = \alpha_N \Phi_N + \alpha_S \Phi_S + \alpha_E \Phi_E + \alpha_W \Phi_W + \alpha_H \Phi_H + \alpha_L \Phi_L + \alpha_T \Phi_T + b$$

(2)

where $\alpha_P, \alpha_N,$ etc. are coefficients representing the influence (diffusion and convection) of the neighbouring cells (N, S, E, W, H and L) and time ($T$) to the balance of $\Phi_P$; $b$ is a representation of the source appropriate to $\Phi$ for the cell.

Partial differential equations must satisfy ‘boundary conditions’ of the type:

$$(\Phi, \text{grad}\Phi) = 0$$

at specified points, lines, areas, or volumes. These points, lines, etc., need not be at boundaries, but can be within the flow domain, when such additional information is given.

For a boundary cell the boundary condition is nothing more than a replacement of the unknown $\Phi_n$ value at the corresponding neighbouring cell (which is now missing) by the known value. Therefore, the treatment of boundary cells can be identical to that of any other cell; and the known boundary relations can be expressed again by integration over the cells containing the boundaries. In this manner the boundary (and internal) conditions simply make contributions to the $b$ and $\alpha_P$ of the FDEs (Eq. (2)).

Finally the set of the equations to be solved is closed by auxiliary relations that refer in general to thermodynamic and transport expressions. Buoyancy effects can be inserted in the model this way (Markatos, 1982).

3.5. Method of solution

The sets of FDEs for the various $\Phi$ are solved in an iterative manner. Iteration (as distinct from direct matrix inversion) is essential because the FDEs are in reality non-linear by reason of the $\alpha$ and $b$ being themselves dependent on $\Phi$. There are several procedures for solving sets of linear equations such as Gauss—Seidel, Successive Over-Relaxation (SOR), Alternating Direction Implicit (ADI), Jacobi point by point and the whole-field simultaneous which were used in the present study. This method is similar to Stone’s fully implicit method (Stone, 1968).

The solution technique used to solve the above equations (in fact, the order in which the equations are solved) employs the SIMPLEST algorithm (Markatos, 1989, 1982; Spalding, 1981).

Fig. 2. The computational grid used ($N_X \times N_Y \times N_Z = 20 \times 8 \times 21$).

Fig. 3. Grid note notation for Eq. (2).
3.6. Computational details

The calculations were performed on Pentium IV 2.8 GHz PC running PHOENICS® Ver. 3.6. The sweeps of the computational domain to achieve a prescribed level of convergence for the three cases, along with the time taken for each case and the amount of computer memory occupied for data storage are presented in Table 2.

Grid refinement studies were performed to ensure the grid independence of the solutions. Case 1 was studied with a much finer grid \((25 \times 15 \times 36)\) compared with the one with which the production runs were performed \((20 \times 8 \times 21)\). The results were acceptably close, so they can be regarded as grid independent (see, for instance, Fig. 4 for a comparison of coarse and fine grid results).

The time step used in the transient calculations for Case 3 was 100 s. Time steps (144) were needed to cover the full 4 h of the simulation which was carried out by solving the VCM concentration conservation equation only, based on the ‘frozen’, pre-calculated flow field of Case 1. Although the solution obtained with a time step of 300 s was virtually identical, no computational economy was found in the use of larger time steps (300 or 600 s each) because of the more sweeps of the domain that were required per time step for the same level of convergence. Balance equations for scalar quantities should be closed with an error less than \(10^{-2}\) of inflow.

The boundary conditions were fixed flow rate for the velocity at ventilators and fixed reference pressure in the door and the opening. The boundary condition for VCM concentrations was fixed flux (Tables 1 and 3).

4. Results and discussion

4.1. Experimental results and comparison to safety limits

The results obtained by the experimental procedure, described above, show relatively low concentrations. Specifically the measured VCM concentrations at three ribbon blenders (A, B and C in Fig. 1) were 1.0, 1.5 and 1.0 ppm, respectively, while the concentrations at two high speed blenders (D and E in Fig. 1) were both 0.8 ppm. All measurements were made at height 1.5 m above ground. Table 3 summarises the average concentrations measured above processing machines. More experimental results, for several strategic points inside the cavity, are shown in Fig. 4. Fig. 4a presents along \(x\) axis measured VCM concentrations at \(z\) distance equal to 4 m. It is evident that at height 1.5 m between D and E blenders the recorded value of VCM was 0.3 ppm and after D speed blender was 0.1 ppm. In front of E and after D the measured concentrations were negligible. In addition to Fig. 4a, Fig. 4b presents measurements of VCM along axis \(x\) but at \(z\) distance equal to 8.5 m. Before C blender VCM was measured at 0.7 ppm, between C and B at 0.1 and 0.8 ppm, between B and A at 0.1 and 0.25 ppm and after A at less than 0.1 ppm.

Concerning the occupational exposure to VCM concentrations NIOSH recommends that it must be limited to the lowest feasible concentration. A permissible exposure limit of 1 ppm for VCM has been adopted by OSHA, while for any 15-min period in 8-h this limit could be extended to 5 ppm. OSHA requires medical surveillance, training for workers, use of protective clothing and respirators, warning signs, product labelling, and periodic monitoring for VCM in the workplace in case the limits are exceeded. In our application with the

<table>
<thead>
<tr>
<th>Position (see Fig. 1)</th>
<th>VCM conc. (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ribbon blender</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>1.0</td>
</tr>
<tr>
<td>B</td>
<td>1.5</td>
</tr>
<tr>
<td>C</td>
<td>1.0</td>
</tr>
<tr>
<td>High speed blenders</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>0.8</td>
</tr>
<tr>
<td>E</td>
<td>0.8</td>
</tr>
</tbody>
</table>

Table 2
Computational details

<table>
<thead>
<tr>
<th>Case</th>
<th>Time</th>
<th>Memory occupied</th>
<th>Grid</th>
<th>Sweeps</th>
<th>CPU s/sweep</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>174.4 Kb</td>
<td>20 × 8 × 21</td>
<td>300</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td>No</td>
<td>166.4 Kb</td>
<td>20 × 8 × 21</td>
<td>300</td>
<td>3.5</td>
<td></td>
</tr>
<tr>
<td>Yes</td>
<td>190.4 Kb</td>
<td>20 × 8 × 21</td>
<td>200/time step</td>
<td>0.9</td>
<td></td>
</tr>
<tr>
<td>No</td>
<td>1.081 Mb</td>
<td>25 × 15 × 36</td>
<td>800</td>
<td>21.6</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 4. Grid refinement results and comparison with experiments. (a) Along the line: \(Y = 1.5\) m, \(Z = 4\) m, (b) along the line: \(Y = 1.5\) m, \(Z = 8.5\) m.
exception of B blender the measured VCM concentrations were less than 1 ppm.

4.2. Numerical simulation results

4.2.1. Case 1

Case 1 is characterised by nominal ventilation conditions. The simulations’ results are described in Figs. 5 and 6. Fig. 5 presents a vector plot of the flow field inside the plant. It can be observed that the air flows mainly from the opening over the stacked PVC containers (60%) and then 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. A convergence of the airflow was detected along axis $BB'$ while along axis $AA'$ the flow field seemed very disturbed due to the high velocities of the flow near the open door (Fig. 5a). Except for the velocity vectors from plan view of the enclosure, two sections including the machines and the vents ($xy$ plane) are shown along with the velocity vectors in these planes (Fig. 5b and Fig. 5c, respectively). The lower ventilation (i.e. bad ventilation conditions) was found in blender A (Fig. 5c) then in B and the higher in C (Fig. 5c), E and D (Fig. 5b).

Fig. 6a shows a contour plot of the VCM concentration inside the plant in an $xz$ plane. It can be observed that the predicted value of the concentration is nearly zero in most of the space except very near to 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. Fig. 6b, c shows contour plots of the calculated concentrations of VCM at $AA'$ and $BB'$ axes, respectively (Fig. 1). Concerning axis $AA'$ the calculated VCM concentrations were lower than the limit of 1 ppm, while for $BB'$ axis only around blender B the calculated concentrations were higher than 1 ppm (1.5 ppm).

4.2.2. Case 2

Case 2 is characterised of a ventilation system working at a tenth of its nominal mass outflow rate, simulations’ results are described in Figs. 7 and 8.

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. When the ventilators are
working to the 1/10 of their current capacity the same mass transfer of VCM was detected and consequently the same concentrations throughout the domain were computed. This lead to the conclusion that a subsequent saving of considerable amounts of energy occurred having no negative effect since the concentrations would remain below safety limits.

Fig. 7 represents the flow field at an $xz$ plane while Fig. 7b, c represents the flow fields at $xy$ planes in $AA'$ and $BB'$ axes (Fig. 1). No significant differences were found compared to Case 1. The concentration contour map either in $xz$ plane (Fig. 8a) or in $xy$ plane (Fig. 8b, c) does not show any significant deviation from the results for Case 1. Only over blender B again the calculated concentrations of VCM are higher than the limit of 1 ppm.

4.2.3. Case 3

In Case 3 the nominal ventilation conditions were retained but a hypothetical accident was simulated. An instantaneous release at time step 0 took place. During the first 1000 s after the accident the great part of the installation presented values of $9 - 10$ ppm of VCM. These concentrations are gradually decreased. About 4000 s after the accidental release, the minimum calculated concentrations of VCM ($\sim 4$ ppm) were almost 50% lower than after 1000 s ($\sim 6$ ppm) while after 8000 s the minimum predicted VCM concentrations were lower than 3.5 ppm. The room, initially saturated with VCM vapour, takes about 4 h to be practically free of the contaminant.

The main reason, as it can be easily observed, is the existence of a “dead” space without any air circulation in it. If another auxiliary vent or even another opening (door or window) was employed, the above time would decrease significantly as it can be easily predicted with the present simulation model.

4.3. Evaluation of the results

Fig. 4 presents for Case 1, which is the case with nominal ventilation and ordinary operation of the plant, a comparison between the calculated concentrations and the measurements of VCM.

It is obvious that the simulation results generally agree very well with the experimental values of VCM concentration either for the simulation of a coarse grid ($20 \times 8 \times 21$ m$^3$) or for the simulation of a fine grid ($25 \times 15 \times 36$ m$^3$).

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

a. The PVC processing plant under investigation is generally speaking 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. When the ventilators are designed to work to the 1/10 of their current capacity the same mass transfer of VCM was detected and consequently the same concentrations throughout the domain were computed. This lead to the conclusion that a subsequent saving of considerable amounts of energy occurred having no negative effect since the concentrations would remain below safety limits.

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.

5. Conclusions

In the present study, a CFD model was used to evaluate IAQ in a PVC plant in terms of occupational exposure and the design of its ventilation system. Specifically the dispersion of VCM was studied and the exposure of the workers to this dangerous substance was estimated.

Three different cases during various ventilation conditions (among them a hypothetical accident) were examined with additional results. Measurements were also made and it was found that the computational results are realistic and in good agreement with the experimental measurements.

The realization of the flow field proves extremely useful to the designer of an installation 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 under these situations could provide invaluable information for the correct design of the ventilation system.

Generally, CFD models 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.

References


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