# NUMERICAL SIMULATION OF VOLATILE ORGANIC COMPOUNDS DISPERSION EMITTED FROM FLOORING MATERIALS IN BUILDINGS

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## ABSTRACT

This paper deals with the simulation of VOCs concentration dispersion emitted from flooring material, with the purpose of understanding VOCs emission and dispersion mechanisms. A test chamber is examined, whose flooring material emits a number of VOCs. Given the area specific ventilation rate and considering as boundary conditions experimental data for the examined compounds concentration, the dispersion of the VOCs concentrations is examined, for two cases, steady state conditions and transient state conditions. The model developed is used in conjunction with a general - purpose CFD code, PHOENICS, that can provide detailed information on the flow field as well as pollutants concentrations fields. The results of the above two simulation cases are used as a guide for two other cases, where faster restoration of the air indoor quality was investigated by changing the rate of the ventilation system in the chamber. The simulation results could be used as a base for further analysis for other flooring materials, intending to a proper material selection as well as to a proper ventilation system for a more healthy and comfort environment in a building.

## 1. INTRODUCTION

Until recently, building materials have not been usually suspected as potential sources of health and comfort problems. As a result, they have been specified and certified for other considerations, but not with respect to their impact on health and comfort. However, in recent years, a large number of incidents have been reported where occupants' health and comfort problems have been associated with their homes or with the buildings where they spend part of their time. These problematic cases have normally been attributed to one of two different situations: Sick - Building - Syndrome (SBS) or Building - Related - Illness (BRI). In the case of BRI, it is usually possible to find the cause of illness linked directly to the building, and in many instances, even to the material causing the effect. More recent experience has shown air pollution by volatile organic compounds (VOCs), originating from building materials may be involved in the health and comfort problems of building occupants. Unfortunately, there is currently very little information available for a consumer who wishes to select materials with no, or low pollutant emissions.

Control over the contaminants distribution can only be achieved by regulating the way air flows throughout the buildings. Therefore, the importance of predicting the air flow patterns is obvious. Predictions are often obtained by setting up the flow configuration in a model or full scale room. Flow visualisation and measurements are used to get a picture of the flow. Such investigations are often very expensive in terms of man power and experimental equipment and it can be difficult to alter geometry, and boundary conditions. A numerical computation model of the flow behaviour in the room will therefore make a helpful tool to predict dispersion mechanisms of the VOCs compounds. To alter the flow conditions in the computer model only means to change the boundary conditions.

This paper deals with the simulation of VOCs concentration dispersion emitted from flooring material. A test chamber is simulated, whose flooring material emits a number of VOCs, considering as boundary conditions experimental data for the examined compounds concentration, for two cases: 1) steady state conditions and 2) transient state conditions. The model developed is used in conjunction with a general - purpose CFD code, PHOENICS, that can provide detailed information on the velocities as well as pollutants concentrations fields. Two other simulation cases are also examined decreasing or increasing the specific ventilation rate or the geometry of the ventilation system in the chamber, targeting to the faster restoration of the air indoor quality. The simulation results could be used as a base for further analysis for other flooring materials, intending to a proper material selection as well as to a proper ventilation system for a more healthy and comfort environment in a building.

This study reports on some of the results of the development of a numerical computation procedure for three dimensional turbulent flow. The technique can be used with confidence at least for checking the relative advantages and disadvantages of various design alternatives in construction as well as in instrumentation of these spaces.

Different cases are examined to assess the dispersion of the contaminants inside the chamber targeting to the demonstration of the capabilities of the present model. The program calculates the velocity and the pollutants concentration, throughout the three-dimensional configurations, and the results are presented in the form of velocity and concentration contours. The flooring material which is used is dried birch plank and the emitted pollutants considered, are: hexane, pentanal, 1-pentanol, benzene, hexanal and styrene.

## 2. MATHEMATICAL FORMULATION AND APPLICATION OF THE MODEL

### 2.1 THE DIFFERENTIAL EQUATIONS

For steady flow, the equations for continuity, velocity components, temperature and chemical concentrations can be expressed in the following general conservation form [1]:

$$\frac{\partial}{\partial x_i}(\rho u_i \varphi) \quad \frac{\partial}{\partial x_i}\left(\Gamma_\varphi \frac{\partial \varphi}{\partial x_i}\right) + S_\varphi \tag{1}$$

where $\rho$ is the density, $u_i$ the velocity vector components, $\Gamma_\varphi$ the effective exchange coefficient of $\varphi$ and $S_\varphi$ = source rate per unit volume.

The source rate and the effective exchange coefficient corresponding to each $\varphi$ solved for in this study are given in Table 1.

Table 1 Source rate and effective exchange coefficient for each $\varphi$

| Equation | $\varphi$ | $S_\varphi$ | $\Gamma_\varphi$ |
|---|---|---|---|
| continuity | 1 | 0 | 0 |
| momentum | $u_i$ | $-\frac{\partial p}{\partial x_i}+\left(\rho_{ref}-\frac{p}{RT}\right)g_i$ | $\mu$ |
| energy | h | 0 | $\mu/\delta_h$ |
| kinetic energy of turbulence | k | $G-\rho\varepsilon$ | $\mu/\delta_k$ |
| eddy dissipation rate | $\varepsilon$ | $C_1\frac{\varepsilon}{k}G-C_2\rho\frac{\varepsilon^2}{k}$ | $\mu/\delta_\varepsilon$ |
| concentration | $m_{VOC}{}^k$ | 0 | $\mu/\delta_{voc}{}^k$ |

where $\mu$ the viscosity, $\sigma$ the Prandtl number for $\varphi$ and G $\mu_l\left(\partial u_i/\partial x_j+\partial u_j/\partial x_i\right)\partial u_i/\partial x_j$ the turbulence production rate. The values of the constants $C_l$ and $C_2$ are 1.44 and 1.92, respectively [1].

### 2.2 THE SOLUTION METHOD

To solve the set of the model differential equations together with their boundary conditions, a finite-domain technique is used which combines features of the methods of Patankar and Spalding [2], and Spalding [3] and a whole-field pressure-correction solver [4]. The space dimensions are discretised into finite intervals and the variables are computed at only a finite number of locations, at the so-called "grid points". These variables are connected with each other by algebraic equations derived by their counterparts by integration over the control volumes defined by the above intervals. The pressure-correction equation is deduced from the finite-domain form of the continuity equation. The source terms are linearised. To solve the 3-D flow equations the SIMPLEST practice of Spalding is followed, in which the finite-domain coefficients of the momentum equations contain only diffusion contributions, the convection terms being added to the linearised source term. Hybrid-differencing for convection and harmonic averaging for diffusion are used. The momentum equations are solved by a point-by-point procedure. The present model is implemented in the general computer program PHOENICS [1].

### 2.3 TEST CASES CONSIDERED

The simulation is concerned with the contaminants transfer, emitted by flooring materials, in buildings. Three cases are considered, for steady state conditions, referring to a test chamber, with different area specific ventilation rates $q_e$ of 0.625 $m^3h^{-1}m^{-2}$, 1.25 $m^3h^{-1}m^{-2}$ and 2.5 $m^3h^{-1}m^{-2}$. Another case is also considered, for the same geometry of ventilation system, with 1.25 $m^3h^{-1}m^{-2}$ area specific ventilation rate, for non-steady state conditions

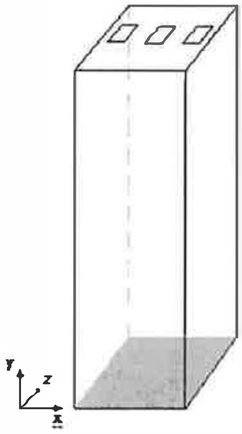

Figure 1: The geometry of the chamber.

The chamber configuration is given at Figure 1. The flooring material that is used is dried birch plank and the values of the emitted VOCs contaminants are given by measurements of European Collaborative Action Indoor Air Quality and its Impact on Man [5]. Other input information are given in Table 2. The program calculates the velocity, temperature and contaminants concentration fields throughout the three-dimensional configurations described above.

Table 2: Input data used in computations

<table>
<tr><th>Data</th><th>Test case 1<br>0.625 $m^3h^{-1}m^{-2}$</th><th colspan="2">Test case 2<br>1.25 $m^3h^{-1}m^{-2}$</th><th colspan="2">Test case 3<br>2.5 $m^3h^{-1}m^{-2}$</th><th>Test case 4<br>1.25 $m^3h^{-1}m^{-2}$</th></tr>
<tr><td>External air temperature (K)</td><td colspan="6">295</td></tr>
<tr><td>Internal air temperature (K)</td><td colspan="6">296</td></tr>
<tr><td>External air velocity (m/s)</td><td>0.1388</td><td colspan="2">0.2777</td><td colspan="2">0.5555</td><td>0.2777</td></tr>
<tr><td>Compounds</td><td>Hexane</td><td>Pentanal</td><td>1-Pentanol</td><td>Benzene</td><td>Hexanal</td><td>Styrene</td></tr>
<tr><td>Concentration ($kg/sm^2$)</td><td>8.333 $10^{-10}$</td><td>2.222 $10^{-9}$</td><td>2.5 $10^{-9}$</td><td>2.5 $10^{-9}$</td><td>6.388 $10^{-9}$</td><td>8.33 $10^{-9}$</td></tr>
</table>

### 2.4 BOUNDARY CONDITIONS

Boundary conditions are specified as follows. At the inlet a fixed mass flow rate is specified as well as the values of velocity and the air temperature. At the walls, wall functions are used to calculate the wall shear stress [2]. The walls are assumed adiabatic. Finally the VOCs concentrations released by the flooring material are added.

### 2.5 GRID DEPENDENCE

The reported results have been obtained using a non - uniform grid consisting initially of 19 cells in the x-direction, 20 cells in the y-direction and 11 cells in the z-direction.

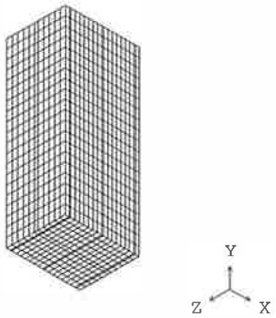

Figure2: A 19x20x11 cells grid.

### 2.6 COMPUTER STORAGE AND TIME REQUIREMENTS

The calculations have been performed on an O2 Workstation (Silicon Graphics), CPU R 10000 processor and main memory 64 Mbytes. A typical CPU time for a run with the 19x20x11grid (4180 cells) is 0.25 hrs for full convergence.

## 3. RESULTS AND DISCUSSION

Some of the results of the study are presented in the next figures in the form of vectors or iso-concentrations.

Figure 3 presents the velocity vectors on the x-y plane passing through the cell 6 (the middle of the examined chamber) for the first steady state case ($q_e$ =1.25 $m^3h^{-1}m^{-2}$). It is seen that the outside air penetrates in the chamber with 0.15 m/s near the inlet and then the velocity values decrease gradually. Near the floor the velocity values are about 0.01 m/s.

Figures 4 and 5 refer to the hexanal and styrene concentration contours respectively on the x-y plane, at the middle of the chamber, for the test case 1. As it is shown in this figures, the pollutants concentrations are increased near the flooring material and then decrease gradually towards the ceiling.

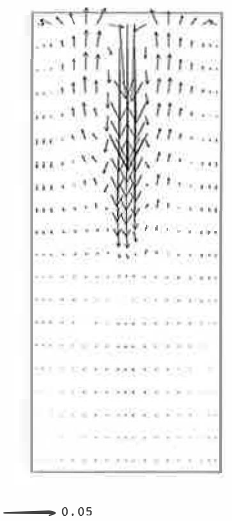

**Figure 3:** Flow field in the middle x-y cross section.

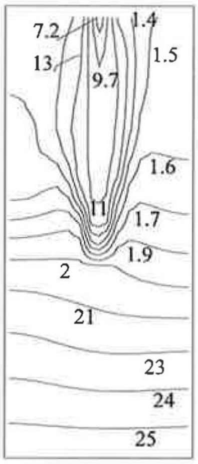

**Figure 4:** Hexanal concentration in the middle x-y cross section.

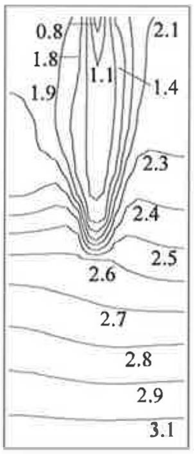

**Figure 5:** Styrene concentration in the middle x-y cross section.

Figure 6 presents the comparison of benzene concentrations, as a function of location position, between the three test case studies (steady state conditions) for the three different area specific ventilation rates. As it is indicated, the ventilation system with the lowest ventilation rate provokes the largest concentration of the benzene inside the chamber.

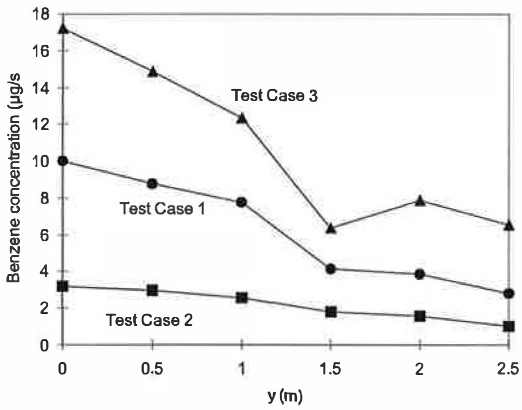

Figure 6: Benzene concentration as a function of ventilation rate and position in the chamber.

Figure 7 represents the the hexane iso-concentrations on the middle x-y plane, for $q_e$ equal to 1.25 $m^3h^{-1}m^{-2}$, for the transient state conditions. As it is observed the concentrations of hexane dicrease gradually as the time increases.

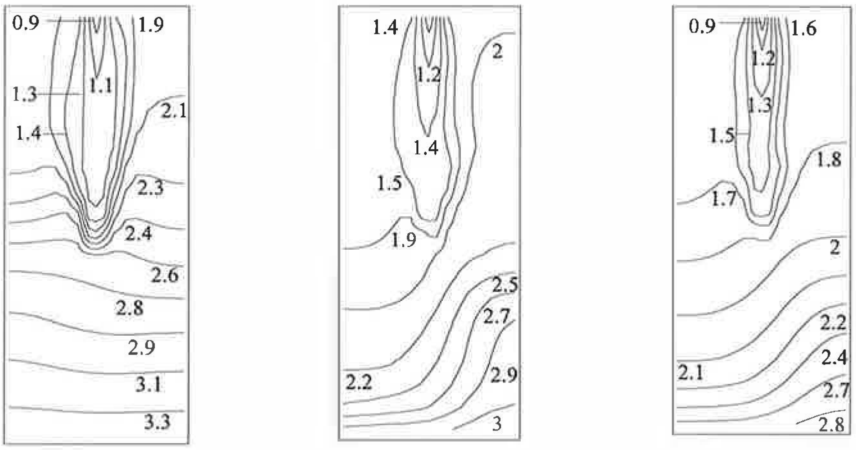

Figure 7: Hexane concentration contours in the middle x-y plane as a function of time
(a) t=0 days (b) t=10 days (c) t=25 days

## 4. CONCLUSIONS

This paper is an attempt to bring the VOCs emission and dispersion from flooring materials to the attention of a wider group of ventilation engineers and environmental scientists, through the description of a computational method. The work demonstrates that numerical solutions for such problems can be obtained quickly and economically. Results have been presented and appear physically plausible. Further work is still required, basically comparisons between predictions and experimental measurements. In the specific case, of volatile organic compounds from building materials emissions, there is much work to be done, if we are to understand how to protect the health of the building occupants. It is intended to contribute to the effort towards designing and instrumenting buildings that provide cleaner and more comfortable environment.

## LIST OF SYMBOLS

### Latin Symbols

| | |
|---|---|
| h | enthalpy, J $kg^{-1}$ |
| k | kinetic energy of turbulence J $kg^{-1}$ |
| P | pressure, Pa |
| R | gas constant, J $mol^{-1}$ $K^{-1}$ |
| $S_\varphi$ | source rate per unit volume |
| T | temperature, K |
| $\vec{u}$ | velocity vector components, m $s^{-1}$ |
| $q_e$ | area specific ventilation rate |

**Greek Symbols**

| | |
|---|---|
| $\Gamma_\varphi$ | effective exchange coefficient of $\varphi$ |
| $\varepsilon$ | eddy dissipation rate, $J\ s^{-1}\ kg^{-1}$ |
| $\mu$ | viscosity, $kg\ m^{-1}\ s^{-1}$ |
| $\rho$ | density, $kg\ m^{-3}$ |
| $\sigma$ | Prandtl number for variable $\varphi$ |

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