A CFD simulation study of VOC and formaldehyde indoor air pollution dispersion in an apartment as part of an indoor pollution management plan

I. Panagopoulos1*, A. Karayannis1, P. Kassomenos2 and K. Aravossis3

1 Sybilla ltd., 16 Ypsilandou st., Maroussi 151 22, Athens, Greece
2 Department of Physics, University of Ioannina, University Campus 45 110, Ioannina, Greece
3 Sector of Industrial Engineering and Operational Research, School of Mechanical Engineering, National Technical University of Athens, Polytechnioupolis, Zografos 174 54, Athens, Greece

*Corresponding author: E-mail: j.k.panagopoulos@sybilla.gr, Tel: +30 210 8024244, Fax: +30 210 6141245

Abstract
This paper is a preliminary report of an indoor pollution case study in a complex of apartments as a part of an Indoor Pollution Management Plan. It describes the calculation by CFD techniques and presents the predicted air flow and VOCs and Formaldehyde contaminant distribution in an apartment comprised of a full-scale kitchen opened to a living room, ventilated by an exhaust hood. The CFD Code PHOENICS®, which is based on solving the full 3-D Navier Stokes equations for turbulent flow and scalar conservation equations, is used. Major indoor pollution kitchen sources, VOCs and Formaldehyde emitting materials and their emission characteristics were calculated through the use of emission factors. The case of a typical apartment was studied and its detailed geometry was applied. To analyze the characteristics of the indoor environment, different mixing ventilation schemes (different locations of the cooker/oven and air inlets) were chosen as the parameters to investigate the indoor environment. The fields of VOCs and Formaldehyde for several air inlets window positions, and ventilation parameters were calculated and compared. It is concluded that CFD methods can be used as design to aid the rational design of indoor spaces.

Keywords: CDF, Indoor Air Pollution, Numerical Modelling, Turbulence, Indoor Sources

1. INTRODUCTION

Indoor air quality is a major concern to businesses, building managers, tenants, and employees because it can impact the health, comfort, well being, and productivity of building occupants. Most Europeans and Americans spend up to 90% of their time indoors and many spend most of their working hours in an office environment. Studies conducted by the U.S. Environmental Protection Agency (EPA) and others show that indoor environments sometimes can have levels of pollutants that are actually higher than levels found outside [1]. Pollutants in our indoor environment can increase the risk of illness. Several studies by EPA, states, and independent scientific panels have consistently ranked indoor air pollution as an important environmental health problem. While most buildings do not have severe indoor air quality problems, even well-run buildings can sometimes experience episodes of poor indoor air quality [1,2].

Volatile Organic Compounds (VOCs) constitute an important class of indoor air contaminants. Evidence from a variety of non-industrial building investigations and systematic studies found that 60% of VOCs indoor come from building material and furnishings [3]. Various VOCs have been associated with certain symptoms of sick building syndrome and multiple chemical sensitivity, and other health effects.

The emission of formaldehyde from building materials has long been recognized as a significant source of the elevated concentrations of formaldehyde frequently measured in indoor air. Pressed
wood products (i.e., particleboard, MDF and hardwood plywood) are now considered the major sources of residential formaldehyde contamination [4]. Pressed wood products are bonded with UF resin; it is this adhesive portion that is responsible for the emission of formaldehyde into indoor air. Generally, release of formaldehyde is highest from newly made wood products. Emissions then decrease over time, to very low rates, after a period of years [4]. Concentrations of formaldehyde in indoor air are primarily determined by source factors that include source strength, loading factors and the presence of source combinations [4].

Computer models (IAQ models) have been developed and increasingly used for predicting indoor air pollutant concentrations. Five principal factors controlling the generation and ultimate fate of an emission in a room with restricted flow, have been identified: sources, sorption/desorption, mixing volume, air exchange, and removal. In order to account for these factors especially the possible non-uniform VOC distributions in buildings, models based on computational fluid dynamics (CFD) techniques have also been developed. The CFD-based IAQ models solve a set of conservation equations describing the flow, energy, and contaminants in the system.

This paper attempts to develop a CFD-based model for general Indoor Air Quality studies adopting conservative contaminants emissions factors. The new model integrates the effects of airflow and turbulent characteristics associated with the VOC and formaldehyde emission sources to yield the detailed distributions of airflow, temperature, and contaminant in buildings. Such knowledge is needed by engineers and architects for selecting appropriate ventilation systems and control strategies to minimize indoor contaminant exposures. Use of the model is demonstrated by applying it to study IAQ in a room with three different mixing ventilation schemes, and by analyzing the characteristics of air flow and contaminant distribution in a full-scale kitchen opened to a living room, ventilated by an exhaust hood.

2. THE PHYSICAL PROBLEM CONSIDERED

Figure 1 presents the plan view of apartment which area is 98m². The more detail of space with living room and kitchen is shown in Figure 2. As raw material, LNG gas was used and its dimension is 0.3m x 0.3m x 0.1m.

![Figure 1: Plane view of a model apartment.[unit;m]](image-url)
3. CALCULATIONS PERFORMED

3.1 Numerical Model Description

PHOENICS [5] is a general purpose software package which predicts quantitatively how fluids (air, water, oil, etc) flow in and around engines, process equipment, buildings, natural-environment features, and so on, the associated changes of chemical and physical composition, and the associated solids. PHOENICS has been continuously marketed, used and developed since 1981, and is applied by engineers in the design of equipment, architects for the design of buildings, environmental specialists in the prediction, and if possible control, of environmental impact and hazards. PHOENICS [6] has been used in Greece as well for predicting indoor environment to Athletic Halls with HVAC Ventilation, and IAQ in a dentistry clinic [7].

The computer code Code PHOENICS, that was used a development framework, calculates the 3-D (three-dimensional) flow field, energy and pollutant concentrations using the continuity, momentum, energy and pollutant transport equations. The equations of the model used are the cartesian, partial differential equations (PDEs) for the conservation of mass, linear momentum, energy and other fluid-dynamics variables in a steady state and turbulent flow [8-12]. The independent variables of the problem are the three components x, y and z of a Cartesian frame of reference. The dependent variables are the three components of the velocity vector (v), pressure, temperature and concentration of indoor air pollutants contaminants. Under steady-state conditions, the conservation equations for the mean value of every dependent variable, \( \Phi \), can be expressed in the following differential general form:

\[
\text{div}(\rho v \Phi - \Gamma_{\text{eff}} \text{grad}\Phi) = S_\Phi
\]  

(1)

where \( \rho \) is the density, \( \Gamma_{\text{eff}} \) is the “effective” exchange coefficient of variable \( \Phi \) and \( S_\Phi \) is the source term for \( \Phi \) per unit volume. PDEs (1) are integrated over control volumes yielding a set of algebraic equations, the finite-domain equations (FDEs). FDEs are solved using the SIMPLEST algorithm [13]. The difference of this algorithm from the well-known SIMPLE algorithm is that the coefficients of the FDEs for the momentum equations contain only the diffusion terms, while the convection terms are added to the linearized sources of the equations]. More details of the solution algorithm can be found in the literature [12,13].

3.2 Governing equations

The mathematical model for turbulent buoyant flow, heat and mass transfer is based on governing conservation equations of mass, momentum, energy, turbulent kinetic energy equation, turbulent energy dissipation equation, and contaminants, as presented below.
Mass conservation equation:
\[
\frac{\partial}{\partial x_i} (\rho u_i) = 0
\]  
(2)

Momentum conservation equation:
\[
\frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} ((\mu + \mu_t) \frac{\partial u_i}{\partial x_j}) + \rho g_j \beta (T - T_m)
\]  
(3)

Turbulent kinetic energy equation:
\[
\frac{\partial}{\partial x_i} (\rho k) = \frac{\partial}{\partial x_i} (\mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i}) + G_k + G_e - \rho \varepsilon
\]  
(4)

Turbulent kinetic energy dissipation equation:
\[
\frac{\partial}{\partial x_i} (\rho \varepsilon) = \frac{\partial}{\partial x_i} (\mu + \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_i}) + C_k \frac{\varepsilon}{k} (G_k + G_e) - C_\varepsilon \rho \frac{\varepsilon^2}{k}
\]  
(5)

Energy conservation equation:
\[
\frac{\partial}{\partial x_i} (\rho u_i T) = \frac{\partial}{\partial x_i} \left( \left( \mu + \frac{\mu_t}{Pr} \frac{\partial T}{\partial x_i} \right) + S_T \right)
\]  
(6)

Contaminants conservation equation:
\[
\frac{\partial}{\partial x_i} (\rho u_i C) = \frac{\partial}{\partial x_i} \left( \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \frac{\partial C}{\partial x_i} \right) + S_C \right)
\]  
(6)

\[
\mu_t = \rho C_\mu \frac{k^2}{\varepsilon}
\]  
(8)

\[
G_k = \mu_t (\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}) \frac{\partial u_i}{\partial x_i}
\]  
(9)

\[
G_b = -g_j \frac{\mu_t}{\rho \sigma_h} \frac{\partial \rho}{\partial x_j}
\]  
(10)

\[
C_{1\varepsilon} = 1.44, C_{2\varepsilon} = 1.92, C_{3\varepsilon} = 0.09
\]  
(11)

\[
\sigma_k = 1.0, \sigma_\varepsilon = 0.9
\]  
(12)

\[
\sigma_l = 1.0, \sigma_l = 1.0
\]  
(13)

3.3 Boundary conditions
It is assumed that indoor airflow is turbulence with buoyancy force because of the kitchen size and heating source. In Equation (3) \( T_m \) is the reference temperature and in this study it is based on the inlet temperature 20°C of outdoor. Table 1 present the BCs applied for energy and contaminants.
### Table 1. Boundary Conditions for energy and contaminants

<table>
<thead>
<tr>
<th>CONTAMINANT</th>
<th>Parameter</th>
<th>Contamination Source - floor, gas.</th>
<th>Contaminant-Other BC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>KITCHEN</td>
<td>FLOOR</td>
</tr>
<tr>
<td></td>
<td></td>
<td>INLET VALUES</td>
<td>BC – SOLID SURFACES</td>
</tr>
<tr>
<td>CO2</td>
<td>0.394 kg/h</td>
<td>305 ppm/ 600 pg/m²</td>
<td>Zero Gradient</td>
</tr>
<tr>
<td>NO2</td>
<td>50 mg NO₂/KWh</td>
<td>40 μg/m³</td>
<td>Zero Gradient</td>
</tr>
<tr>
<td>VOC</td>
<td>50 mg NO₂/KWh</td>
<td>0.28 μg/m²/s</td>
<td>Zero Gradient</td>
</tr>
<tr>
<td>Formaldehyde</td>
<td>0.08 μg/m²/s</td>
<td>5 μg/m³</td>
<td>Zero Gradient</td>
</tr>
</tbody>
</table>

### ENERGY

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Source of Energy – floor, gas range area</th>
<th>Energy-Other BC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>KITCHEN</td>
<td>FLOOR</td>
</tr>
<tr>
<td></td>
<td>INLET VALUES</td>
<td>BC – SOLID SURFACES</td>
</tr>
<tr>
<td>TEMPERATURE</td>
<td>20 °C</td>
<td>Zero Gradient</td>
</tr>
<tr>
<td>HEAT FLUX</td>
<td>1500 W</td>
<td>No heat source</td>
</tr>
</tbody>
</table>

Uniform velocity is applied at the inlets.

For the wall surfaces the no-slip condition is applied for velocities and “wall functions” for the near-wall values of the dependent variables.

Calculations have been performed for various ventilation scenarios, focusing on the inlet ventilation fan or window and relevant ventilation rates. The cases concerning different inlets (scenario series A, B, C respectively) and operating condition of “medium” ventilation are described at Table 2 which summarizes the different combinations of these cases, describing each scenario.

### Table 2. Ventilation Rates Performed

<table>
<thead>
<tr>
<th>Scenario</th>
<th>VELOCITY (m/s)</th>
<th>VENTILATION (m³/h)</th>
<th>VENTILATION RATE (m³/m²h)¹</th>
<th>ACH²</th>
<th>REMARKS</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.15</td>
<td>324</td>
<td>3.3</td>
<td>3.93</td>
<td>MEDIUM-</td>
</tr>
<tr>
<td>B</td>
<td>2</td>
<td>324</td>
<td>3.3</td>
<td>3.93</td>
<td>MEDIUM-</td>
</tr>
<tr>
<td>C</td>
<td>2</td>
<td>324</td>
<td>3.3</td>
<td>3.93</td>
<td>MEDIUM-</td>
</tr>
</tbody>
</table>

¹ for minimum design ventilation California Title 24 suggests 3 m³/m²h based on ventilation surface (whole apartment)
² for local ventilation, ASHRAE standard 62.2 suggests kitchen exhaust airflow rates 5 ACH based on kitchen volume

### 4. COMPUTATIONAL DOMAIN AND COMPUTATIONAL DETAILS

A rather coarse grid was used in the computations, which covers a computational domain measured 4.96 x 9.78 x 3.00 m. The non-uniform numerical grid consisted of 171990 differential volumes, 63 cells in the x direction, 65 cells in the y direction and 42 cells in the z direction. Almost 3000 iterative sweeps of the domain were necessary to obtain convergence. The computer used is an AMD Anthlon 64 Processor 3200+ 2.0 GHz. Memory RAM used was 512 MB. Execution times per 1000 sweeps for the calculation grid are around 1 hours CPU.

### 5. RESULTS AND DISCUSSION

#### 5.1 Results

Due to the limitation of space in the present article, only few results for the flow field and the indoor pollutants concentrations are presented. These results are shown in Figures 3 to 6.
Observation of the above figures results to the following conclusions:

- The predicted velocities and contaminants fields are physically realistic and plausible.
- Inlet air location is critical since local recirculation and “hot-spots” of stagnant air can appear within the apartment.

5.2 Discussion-Conclusions

This methodology applied provides qualitative and quantitative data in order to evaluate and select measures and techniques that ensure the prevention of adverse indoor environmental impacts and the protection of human health. The mathematical model analysis employed provided the basis in achieving best practice environmental management in the confrontation of indoor air pollution Projects. It can also assist decision-making and provide greater certainty to the construction firms and the community in carrying out planning for Indoor Air Pollution activities.

The method proposed consists a state-of-the-art tool in the direction of employing CFD methodology to improve indoor pollution and ventilation techniques, namely focusing on the optimum sizing and siting of ventilation schemes and provision of practical suggestions as a part of an Indoor Pollution Management System.

References


14. California Title 24 Standards (2001). CCR, Title 24, Part 6, Sec. 121(b) 2