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DISPERSION MODEL FOR TVOC EMISSIONS FROM SOLVENT-BASED PAINTS

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ABSTRACT

Indoor Air Quality (IAQ) plays a significant role in building related sicknesses, termed as Sick Building Syndrome (SBS). Several researchers have identified the building materials as sources of indoor pollution during construction and operation. Various types of paints have been studied for IAQ related emissions. This paper covers a study carried out on emissions generated from water based (Emulsion) and solvent based (Enamel) paints and the dispersion pattern of prominent pollutants such as Total Volatile Organic Compound (TVOC), Carbon Monoxide, Carbon Dioxide, Nitrogen Dioxide and particulate matter. A severe impact was observed from TVOC concentration. Therefore TVOC emissions were used to develop a computational model using IAQX software. Since the computational model has not converged well with the experimental dispersion curve, a further attempt was made to develop a mathematical model, which is of an exponential nature. However the computational model was used to predict the variation of peak TVOC concentrations and time of dispersion under different ventilation rates. The mathematical model has been recommended to work out the building flush out period and variation of TVOC concentration with the area of paint application. This model will benefit the building planners to create healthy indoor environments for the occupants.

KEYWORDS: Computational Model, Experimental Model, Mathematical Model, Solvent Based Paint, Water Based Paint

1. INTRODUCTION

The emission from building materials used in construction and maintenance causes a significant impact on indoor air pollution. With the industrial revolution, people prefer to use synthetic building materials rather than conventional building materials considering some of the advantages such as durability, cost effectiveness, better finish and speedy construction. However most of the synthetic building materials could be a main source of indoor air pollution. This can include products like partition boards, carpets, paints, cleaning products, wallpapers, furnisher and air fresheners etc. [1-8]. The most common types of causative agents from the above sources are Total Volatile Organic Compounds (TVOC), Carbon Dioxide (CO_2), Carbon Monoxide (CO), Nitrogen Dioxide (NO_2), Particulate Matter ($PM_{2.5}$ and PM_{10}) and undesirable temperature inside the building [9]. Further modern building operational practices, such as, restricting natural ventilation and use of air conditioners with poor maintenance, has aggravated the situation [10]. This emphasizes that the indoor air quality can influence the health of the occupants since people spend 90 % of their time indoors [11]. If the health condition of occupants is affected due to the indoor environment of any building, it is considered as the sick building syndrome (SBS). “A 1984 World Health Organization (WHO) committee report suggested that up to 30 percent of new and remodeled buildings worldwide may be the subject of excessive complaints related to indoor air quality” [12]. The symptoms due to the sick building syndrome are headache, nausea, irritation of the eyes, mucous membranes, and problems in respiratory system, drowsiness, fatigue and general malaise [13]. Also long term exposure into the pollutants can cause more serious health effects [14].

Meanwhile, growing attention is placed on green building concepts since majority of people understand the importance of better houses on the planet in order to minimize the prevailing environmental issues which are occurred during pre and post construction stages such as energy wastage, unhealthier indoor environment and extensive use of natural resources etc. This in turn has resulted that the green building concepts incorporate environmental considerations into every stage of the building construction. This can be illustrated by the green rating system, LEED (Leadership in Energy and Environmental Design) [15] which concentrated on 6 main aspects, namely sustainable sites, water efficiency, energy and atmosphere, material and resources, indoor environmental quality and LEED innovation credits. Further this rating system assigns 15 points to indoor air quality and from these 15 points, 4pointsare assigned for each of the following;

- Low emitting materials - Adhesives and sealants
- Low emitting materials - Paints and coatings
- Low emitting materials –Flooring systems
- Low emitting materials–Composite wood and agrifiber products [15].

Out of the above four categories of materials, this research has been focused on investigating the variation of indoor environment due to wall paints. There are mainly two types wall paints considered in the study Water based (Emulsion) paint and Solvent based (Enamel) paint.

Water based paint contains polymers which are emulsified in water, hence it is known as emulsion paint. Usually this paint type is used for interior painting since it inherits the quality of super resistance to chalking and chipping due to excellent adhesion of them to most of the substrates. Very little odor and simple water and soap cleanup can be mentioned as some of the physical observations of this paint.

Solvent based paints contain water insoluble polymers; therefore paint must be mixed with organic solvent at required consistency to achieve properties of enamel paint. Several air pollutants are emitted into the indoor environment during evaporation of paints after application on the surface [16]. Frequently this paint is applied on interior surfaces of wood and metal and especially the places which are mostly in wet condition in the designed life. When considering the comparison between these two types, solvent based paint fades away rapidly when exposed to the bright sun light and it has a noticeable prolong odor. Also the painters have to use some organic solvent (Turpentine or Thinner) to clean the brushes and other utensils [17].

This research paper presents the variation of the emissions from water based paint and solvent based paint with time. Based on these results, it is possible to introduce a building flush out period by considering dispersion curves of the paints. This is very important for building designers since they can come up with the entire building flush out period by considering the impact of building materials on indoor air quality. Further above mentioned findings can be used to recommend a desirable paint (Greener version) type depending on the stage of application (construction or maintenance). The material manufactures can rank the paints as high, medium or low emitting sources based on emission data [18]. Also they can improve their products to suit for the building designers' requirements and to meet the green building market by considering occupants' health including environmental pollution. An attempt was made to develop both computational and mathematical models for the emission from solvent based paint so that the building planners can use it for the prediction of dispersion time and the magnitudes of the problem related to IAQ. Since TVOC has been identified as the most significant causative agent based on experimental data, it has been used to develop the models.

2. OBJECTIVES

The main objective of this study is to measure and analyse the concentration of Total Volatile Organic Compounds (TVOC), Carbon Dioxide (CO_2), Carbon Monoxide (CO), Nitrogen Dioxide (NO_2) and Particulate Matter ($PM_{2.5}$) due to the application of water based and solvent based paints under controlled conditions.

The study covered in this paper is aimed at following specific objectives:

- Develop a dispersion model for the solvent based paint
- Find the optimum ventilation rate to have the minimum concentration and dispersion time for the pollutants from the solvent based paint

3. EXPERIMENTAL PROGRAMME

The test chamber was created inside an educational building which was constructed 30 years ago. In order to witness the maximum effect of the paint, the area was made fully enclosed with minimum ventilation of 0.1 ACH (Average air movement rate in test chamber 0.05 m/s and air exchangeable area 0.1 m^2). Since the test chamber is a part of a building which is 30 years old, there were no sink or source materials inside the test chamber. Therefore pollutants generated in the experiment can be entirely from the application of paint.

The layout of the test chamber is shown in Figure 01. The water based paint was applied on the designated wall area (shaded area) and the instruments were operated continuously at the center of the chamber until the pollutant concentration disperses to the ambient condition. Same test procedure was repeated for the solvent based paint and the indoor air quality parameters were recorded with time. The solvent based paint was applied with a sufficient time gap so that no emissions from water based paint mixed up with that of solvent based paint.

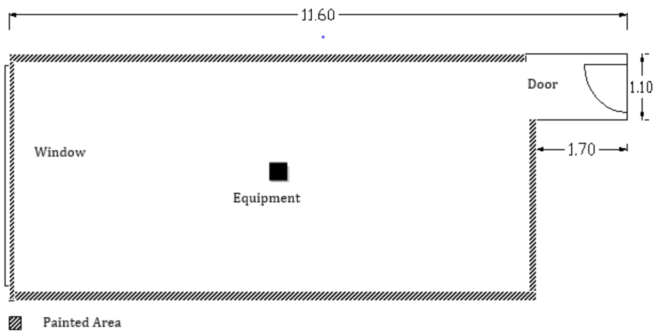

Figure 1: Plan View of the Test Chamber (Dimensions Are in Meters)

The two pieces of equipment used in this study were Indoor Air Quality Monitor (IQM60 Environmental Monitor V5.0 – Figure 02) and Haz-Dust Particulate Air Monitor (Figure 03). Indoor Air Quality Monitor was used to measure the concentrations of Carbon Dioxide (CO_2), Carbon Monoxide (CO), Nitrogen Dioxide (NO_2), Total Volatile Organic Compounds (TVOC), Temperature and Relative Humidity. Haz- Dust Particulate Air Monitor was used to measure the concentration of the particulate matters which are having the diameter less than 2.5μm.

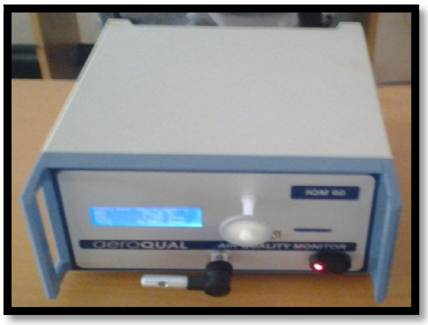

Figure 2: Indoor Air Quality Monitor Figure 3: Haz - Dust Particulate Air Monitor

The equipment was mounted on the center of the chamber at a height of 1 m from the ground level in order to simulate a seated person on a chair. As the base case, the measurements were taken prior to the application of paints with the two pieces of equipment on various causative agents, inside the test chamber. Table 01 shows the average results of the base case obtained from several trials.

Table 1: Concentration of Causative Agents inside the Room (Before Applying the Paint)

Name	Concentration
Carbon Monoxide (CO)	0 ppm
Carbon Dioxide (CO_2)	325 ppm
Total Volatile Organic Compounds (TVOC)	0 ppm
Particulate Matter ($PM_{2.5}$)	0.023 mg/m^3
Temperature (Average)	29^{0}C
Relative Humidity (Average)	77 %

4. RESULTS AND ANALYSIS

The results obtained during the experiment have shown different patterns of concentrations with time. The effect of solvent based paint on indoor air quality is much more significant than that of water based paint.

4.1 Variation of Pollutant Concentration Due to Application of Paints

Charts 1 and 2 show the variation of TVOC concentration with time due to the water based and solvent based paints respectively. The summary of the results is presented in Table 2 with the maximum concentration and dispersion time of TVOC concentration generated from both types of paints.

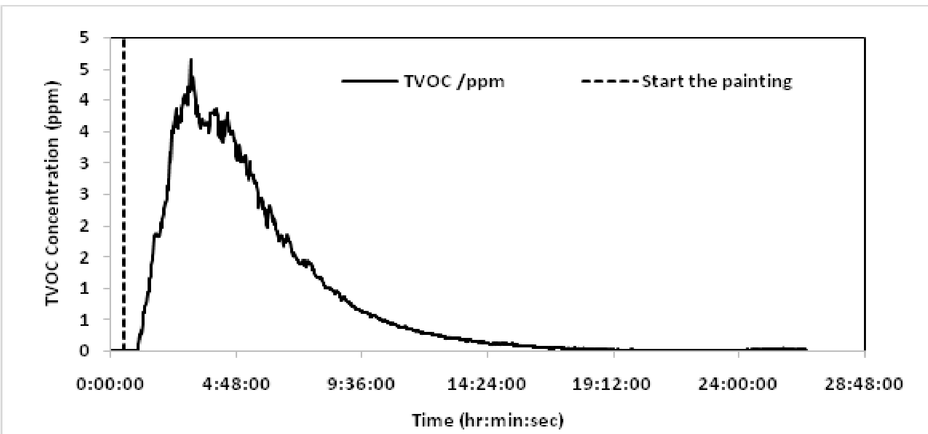

Chart 1: TVOC Variation with Time - Water Based Paint

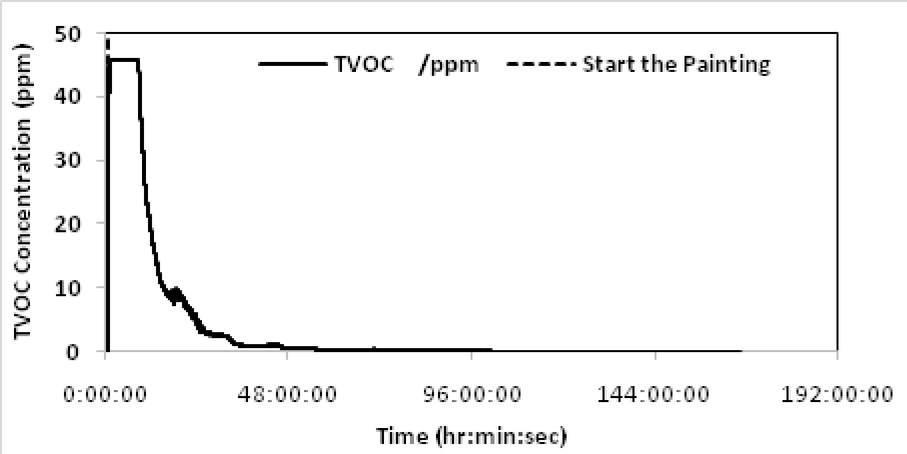

Chart 2: TVOC Variation with Time – Solvent Based Paint

As the Chart 2 illustrates, the concentration of TVOC has drastically increased due to the solvent based paint. Further, maximum concentration of TVOC is beyond the permissible indoor value (0.75 ppm- OSHA) [19] for a considerable period for both the paints. During this period occupants are exposed for this adverse environmental condition, especially during the maintenance or renovation period of a building. Hence it is important to introduce a building flush out period for the paint application depending on the type of paint together with other precautionary measures.

Table 2: Maximum Concentration and Dispersion Time of the Paints

Paint Type	Maximum Concentration	Dispersion Time to the Ambient Condition (0 Ppm)	Dispersion Time to the Threshold Value (0.75 Ppm – OSHA)
Water based paint	4.64 ppm	21 hr	8 hr 40 min
Solvent based paint	45.58 ppm	140 hr	45 hr 30 min

According to the results, the concentrations of CO_2, CO and NO_2 have increased due to the water based and solvent based paint application. However the maximum concentration values are within the threshold value defined for the indoor environment.

The result obtained from the experiment did not show any difference in the variation of $PM_{2.5}$, temperature and relative humidity due to the application of paints. Although the pollutant levels for CO_2, CO and NO_2have been affected with an increase due to the both types of paint application, the most significant impact was made by the TVOC concentration generated from the solvent based paint. Therefore it has been selected for the detailed analysis for the development of computational and mathematical models.

4.2 Computational Model for TVOC Dispersion from the Solvent Based Paint

Since the objective of the research is to develop a dispersion model for the solvent based paint, the software named as IAQX (Simulation Tool Kit for Indoor Air Quality and Inhalation Exposure) was used to develop the computational model [20]. This software was developed by U.S.EPA National Risk Management Research Laboratory. The application of this software is to develop the dispersion model and introduce to the building planners after validating with experimental data. Further this model can be used to find the optimum ventilation rate to have minimum exposure time for the occupants and painters who are exposed to the adverse environmental condition.

The IAQX is comprised of several sub categories which are named as GPS.EXE, VBX.EXE, SPILL.EXE, SLAB.EXE and PM.EXE.

VBX.EXE was used for this experiment since it can predict VOC emission from solvent-based indoor coating materials based on product formulation. The input parameters based on experimental data are presented in Table 03.

Table 3: Inputs for the VBX.EXE Software

Parameter	Value	Parameter	Value
Chamber volume	135.87 m^3	Wet film thickness	83.48 µm
Sink material	0	Coated area	79.315 m^2
Ventilation	0.1 ACH	Room temperature	30 ^{0}C
Analysis type	Bulk Analysis	Air velocity	2 cm/s
TVOC content	819.31 mg/g	Simulation period	170
Product density	0.796 g/cm^3	Output data points	100

TVOC content, product density and wet film thickness were calculated from the laboratory experiments. In order to calculate TVOC content and wet film thickness, pieces of glass were applied with the solvent based paint and measured the weight until it became constant under the same environmental conditions [21]. Headspace gas chromatography was used to find the ingredients of paint with percentage constituent materials (Table 04).

Table 4: Ingredients of Paint with Percentage Constituent Materials

VOC Name	Percentage	VOC Name	Percentage	VOC Name	Percentage
Pentane, 2-methyl	0.64	Octane, 2-methyl	4.08	Heptane, 2,3-dimethyl	0.96
Hexane	1.45	Benzene, 1,3-dimethyl	8.27	Dodecane	5.94
Cyclopentane, methyl	0.55	Octane, 3-methyl	3.96	Ethylbenzene	6.53
Hexane, 3-methyl	0.99	p-Xylene	4.35	Benzene, 4-ethyl-1, 2-dimethyl	1.38
Heptane	2.19	Nonane	9.83	Cyclohexane, ethyl	1.67
Cyclohexane, methyl	1.87	Cyclohexane,propyl	1.20	Benzene, 1,2,3-trimethyl	1.52
Heptane, 2-methyl	2.23	Octane, 3,6-dimethyl	3.08	Octane, 2-methyl	1.22
Toluene	2.14	Benzene, 1-ethyl-2-methyl	1.61	Decane	13.58
Heptane, 3-methyl	1.72	Nonane, 4-methyl	2.42	Octane	3.68
Cyclohexane, 1,2-dimethyl-, trans	1.63	Nonane, 3-methyl	2.47	Benzene, 1,3,5-trimethyl	4.54
Cyclohexane, 1,4-dimethyl-, cis	0.54	Benzene, 1-ethyl-2-methyl	1.78		

The result of the simulation is shown in Chart 03, with a variation of TVOC concentration with time.

In order to find out the optimum ventilation rate, same model was simulated with different ventilation conditions. Results obtained from the software are graphically represented in the Chart 04. TVOC variation has been plotted with time for varying ventilation rates in Chart 04 and the summary of the maximum concentration and dispersion time is presented in Table 05.

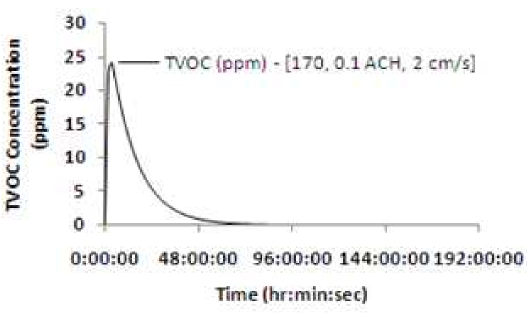

Chart 3: Computational Model of IVOC Dispersion Due to Solvent Based Paint

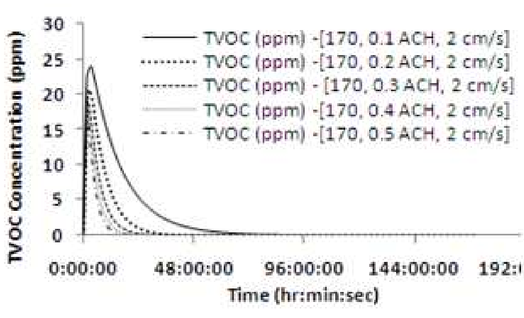

Chart 4: IVOC Variation with Different Ventilation Conditions from the Software Based Results

Table 5: Summary of Dispersion Time with Respect to the Ventilation Rate (ACH)

Ventilation Rate (ACH)	Maximum TVOC Concentration (ppm)	Dispersion Time to the Permissible vaLue (0.75 ppm – OSHA) (hr: min: sec)	Dispersion Time to the Initial Indoor Value (0 ppm)(hr: min: sec)
0.1	24.15	50:29:00	149:36:00
0.2	20.67	26:21:00	78:12:00
0.3	18.87	18:22:00	54:24:00
s0.4	17.27	14:17:00	42:30:00
0.5	15.85	11:54:00	35:42:00

When the ventilation rate increases to 0.5 ACH which was found as the minimum ventilation rate for residential buildings from the several researches [22-24]; the maximum TVOC concentration and dispersion time to the initial indoor value have come down to 15.85 ppm and 1 ½ days respectively. Therefore it is recommended to maintain at least 0.5 ACH ventilation rate in the maintenance cycle of building with a reasonable flush out period so that the occupants are not affected by the indoor pollution due to building renovation. Although the dispersion curve is similar, the peak values of experimental and computational models are not converging (Chart 05). Therefore few more trials are needed for the verification of the computational model.

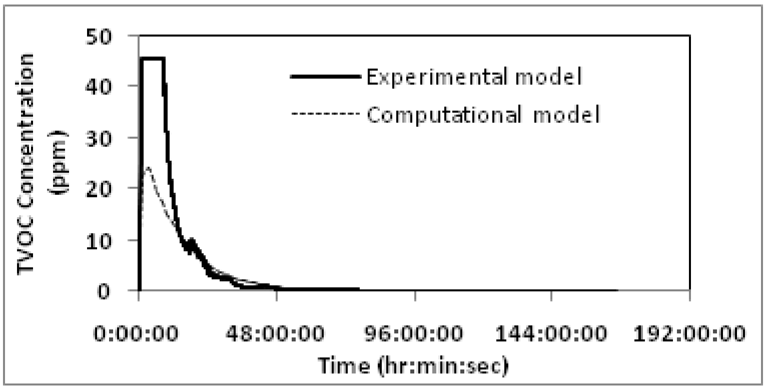

Chart 5: TVOC Variation for Solvent Based Paint from Experimental and Software Based Results

Since the peak concentration values are not converging enough, the computational model could not be confidently used to predict the emission and time of dispersion. Therefore the study has been extended to develop a mathematical model.

4.3 Mathematical Model for TVOC Dispersion from the Solvent Based Paint

Development of mathematical model was carried out in terms of TVOC variation with time and distance from the point of application.

4.3.1 "TVOC Concentration" Variation with Time

Mathematical model for the solvent based paint dispersion was derived with the use of MATLAB software (MATLAB R2014a). The reason for the selection of this software over the other packages is depended on the size of the data set, time for the analysis and model verification with related statistical parameters. The "Time" and "TVOC concentration" obtained from the experiment, were used as the inputs for the MATLAB and the formulae indicated in the table are the outputs of the analysis.

Table 6: Mathematical Models Generated from MATLAB

Equation	Coefficients	Adjusted R^2Value	Sum of Square Error (SSE)	Root Mean Square Error (RMSE)
C(t) = a*exp(b*t) + c*exp(d*t)	a = 3206 b = -0.009692 c = 42.89 d = -0.001559	0.9949	590.5	0.4002
C(t) = a*exp(b*t)	a = 138.2 b = -0.002678	0.9645	4089	1.053
C(t) = a*t^b	a = 5.238e+07 b = -2.26	0.989	1266	0.5859
C(t) = a*t^b+c	a = 4.249e+07 b = -2.227 c = -0.09869	0.9892	1247	0.5815
C(t) = (a) / (t + b)	a = 4809 b = -401.6	0.9572	4933	1.156
C(t) = (a*t + b) / (t + c)	a = -1.382 b = 6919 c = -364.9	0.9878	1410	0.6184

As indicated in Table 06, first form of equation (Exponential function with two terms) has been selected as the most suitable statistical model since it inherits the best fitting parameters as highest R^2 and lowest SSE and RMSE (R^2 = 0.9949, SSE = 590.5 and RMSE = 0.4002) for the experimental data with 95% confidence bounds. This model (equation 1) shows the relationship of TVOC concentration with time.

$$C(t) = 3206\, e^{-0.00969t} + 42.89\, e^{-0.001559t} \quad (1)$$

The statistical hypothesis test called chi squared goodness of fit (χ^2) was used to quantify the deviation of expected values from the statistical model with the observed values from the experimental data. The null hypothesis was made such that the experimental data follows aforementioned distribution which is shown in equation 01.

$$\chi 2 = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$$

Where χ^2 =Pearson's cumulative test statistic

O_i= An observed frequency

E_i= An expected frequency

k= Sample size

According to the chi squared test statistic with degree of freedom of **k-1**,$\chi 2 < \chi 2_{k-1,\alpha}$, with the probability value (α)of 0 .99 ($\chi 2$ = 2239, $\chi 2_{k-1,\alpha}$ = 2522, k-1 = 2690) [25]. Therefore null hypothesis was accepted.

4.3.2 "TVOC Concentration" Variation with Time and Distance

In order to find out the relationship between the TVOC concentration and distance, the data generated by changing the position of equipment from the source (the sample paint application) was used. This set of data was collected under similar environmental conditions as that for the time variation, in the same test chamber. Similar form of equation (1) has been used for the data set which was generated from the sample painted area and obtained the variation of the two coefficients (**a, c**) with the distance which are with the Euler's number (**e**). The relationships for the variation of coefficient with the distance from the source are indicated in equations 2 and 3 which were obtained from the Chart 06.

$$a(x) = 94.78\ e^{-0.24x}\ (R^2 = 0.999) \quad (2)$$

$$c(x) = 15.13e^{-0.18x}\ (R^2 = 0.965) \quad (3)$$

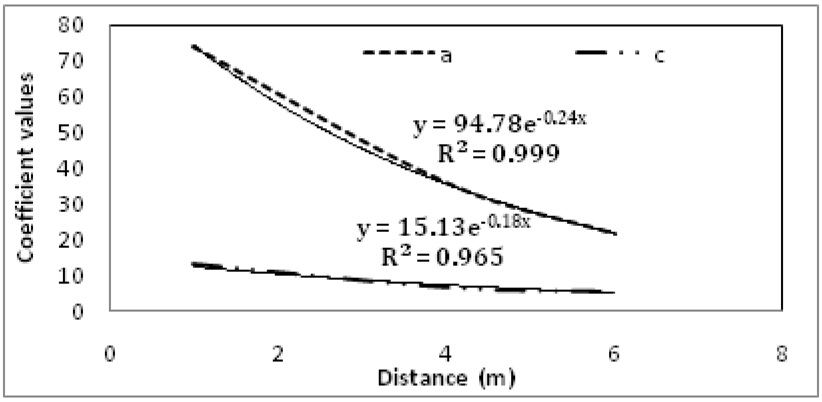

Chart 6: Coefficients (A, C) Variation with the Distance

Further it was observed that the TVOC concentration is proportional to the painted area. Therefore the final outcome is presented as equation 4 which has been derived by combining the above two relationships between TVOC concentration together with time and distance as a function of the painted area.

$$C(x, t) = S\ [1.399\ e^{-(0.24x+0.00969t)} + 0.087\ e^{-(0.18x+0.001559t)}] \ldots\ldots \textit{equation} \quad (4)$$

Where **C(x, t)** = TVOC Concentration (ppm) as a function of distance and time

S = Painted Area ($m^{2)}$

x= Horizontal distance from the source (m)

t = Time relative to starting time of the paint application on surface (min)

The equation 4 can be put forward as the proposed model of TVOC dispersion with time and distance from the source point. This has been expressed as a function of the painted area.

5. CONCLUSIONS

The detailed experimental programme carried out in a test chamber with solvent based and water based paints has shown a significant impact on IAQ with solvent based paint. TVOC has been identified as the most prominent pollutant due to the solvent based paint application with a peak value of 45.58 ppm which has taken more than 5 days to disperse up to the ambient condition.

In order to establish dispersion curves for the TVOC concentration, both computational model and a mathematical model were developed. The mathematical model of exponential nature has been identified as a better dispersion model for the benefit of building planners to work out their planning arrangement with required ventilation rates and building flush out periods during construction and also during renovation periods.

The developed model can be used to predict the building flush out period in new buildings. A safe distance of operation for the occupants from the painted area can also be worked out by the proposed model in the building renovation stage. Building planners can maintain a comfortable and healthy indoor environment using the proposed model with confidence. Further refinement of the proposed model is being carried out with different ventilation rates for the development of a set of curves for the variation of TVOC concentration with time and distance.

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