A Systematic Approach to Evaluating Gaseous Filter Models

Vida Safari

A Thesis

in

The Department

of

Building, Civil and Environmental Engineering

Presented in Partial Fulfillment of the Requirements

for the Degree of Master of Applied Science at

Concordia University

Montreal, Quebec, Canada

October 2011

Concordia University

School of Graduate Study

This is to certify that the thesis prepared

By: Vida Safari

Entitled: A Systematic Approach to Evaluating Gaseous Filter Models

And submitted in partial fulfillment of the requirements for the degree of

Master of Applied Science

complies with the regulations of the University and meets the accepted standards with respect to originality and quality.

Signed by the final examining committee:

Dr. M. Elektorowicz Chair

Dr. S. Li Examiner

Dr. Y. Zeng Examiner

Dr. F. Haghighat Supervisor

ABSTRACT

A Systematic Approach to Evaluating Gaseous Filter Models

Vida Safari

Building occupants' health is an important issue for building designers. There are a number of contaminants in an indoor environment. One approach to reduce the level of contaminants from the indoor air is the utilization of gaseous air cleaning devices. These air cleaners are saturated by the contaminants with time. The only deficiency of applying this technology is the lack of knowledge for predicting their lifetime. Although a few models exist for their lifetime prediction, there is no methodology to apply and evaluate their performance.

In this study, a methodology was developed to evaluate the application of existing models. The proposed methodology was applied to study the lifetime of an adsorbent filter containing granular activated carbon as media. Furthermore, the penetration of the contaminants through the filter was investigated under four conditions: dry air containing n-hexane, dry air containing Methyl Ethyl Ketone (MEK), dry air containing n-hexane and MEK, and humid air containing n-hexane and MEK. The lifetime of the filter was evaluated experimentally and modeling was based on the breakthrough of the contaminants under these four conditions. The results of modeling and experiments were compared. The comparison showed that physical properties of the contaminants affect the removal efficiency of the filter. The contaminant with higher molecular weight, n-hexane, had more affinity to be adsorbed on the filter rather than the lighter contaminant MEK.

Also, the results indicated that humidity levels less than 50% do not have much effect on the filter's lifetime.

On the other hand, the proposed methodology was confirmed with this tested filter. The result showed that the selected model could predict the lifetime of the filter for the cases where there is only one contaminant in the air, with less than 10% relative error. Furthermore, the model could predict the breakthrough profile of the lighter contaminant in mixture of contaminants in the air, with 25% relative error.

ACKNOWLEDGMENTS

First and foremost, I would like to express my deepest gratitude to my supervisor, Dr. Fariborz Haghighat, who gave me the chance to benefit from his extensive knowledge, and constructive comments throughout my study. I am grateful for his invaluable advices, and time he devoted me.

I wish to express my warm and sincere thanks to Dr. Chang-Seo Lee for her guidance, invaluable feedbacks, and full cooperation throughout the experimental process. Her wide knowledge has been of a great value for me. Also, I am grateful to Dr. Patrice Blondeau for his constructive suggestions and help. This dissertation owes an enormous intellectual debt to him, as he provided invaluable information and knowledge to me.

I would like to appreciate all my colleagues in our research group who their valuable assistance and friendship means a lot to me. Also, I would like to extend my gratitude to my wonderful friends, who have been like a second family to me; Arash Soleymani, Golnaz Shaverdi, and Parastoo Bastani, who always took the time to listen, even to my complains. Arash Bastani, Carole Elayoubi, and Gilnaz Arzpeyma who taught and helped me a lot, not only in writing my thesis, but also during tough times in my life through these years.

The last, but the most I owe my heartfelt thanks and love to my parents, Akram and Gholamabbas, my trustworthy brothers, Behrouz and Behnam, and my kindhearted sister and friend, Parastoo, for their everlasting support and encouragement. Without them, none of this would have been possible. To my parents, this thesis is dedicated.

TABLE OF CONTENT

LIST OF FIGURES viii

LIST OF TABLES x

LIST OF ABBREVIATIONS xi

LIST OF SYMBOLS xii

CHAPTER 1 INTRODUCTION 1

1.1 BACKGROUND 1

1.2 OBJECTIVES 5

1.3 THESIS OUTLINE 5

CHAPTER 2 LITERATURE REVIEW 7

2.1 INTRODUCTION 7

2.2 MASS TRANSPORT 8

2.2.1 External Diffusion 9

2.2.2 Internal Diffusion 11

2.2.3 Adsorption 15

2. 3 AVAILABLE MODELS FOR GASEOUS FILTERS 24

CHAPTER 3 METHODOLOGY 33

3.1 INTRODUCTION 33

3.2 CHOOSING A MODEL 35

3.2.1 Model Development 36

3.3 FINDING MODEL PARAMETERS 40

3.3.1 Sorption Parameters 40

3.3.2 Filter Design Parameters 44

3.3.3 Environmental Parameters 45

3.4 MODEL VALIDATION 45

3.5 CASE STUDY 47

3.5.1 Langmuir Isotherm Test for Case Study *47*

3.5.2 Validation Tests for the Case Study *48*

3.5.3 Calibration Method for Single Gas Detectors *50*

3.5.4 Calibration Method for Multi-Gas Detectors *52*

CHAPTER 4 RESULTS AND DISCUSSION **54**

4.1 INTRODUCTION 54

4.2 ADSORPTION ISOTHERM 54

4.3 EXPERIMENTAL RESULTS 57

4.3.1. Single Contaminant Injection *57*

4.3.3 Mixture of Contaminants Injection in Humid Air *61*

4.3.4. Comparing the Tests *61*

4.3.5 Repeatability Tests *63*

4.4 MODELING RESULTS 67

4.5 SUMMARY 73

CHAPTER 6 CONCLUSION AND RECOMMENDATIONS FOR FUTURE WORK **76**

6.1 SUMMARY 76

6.2 CONCLUSIONS 78

6.3 RECOMMENDATIONS FOR FUTURE WORK 81

REFERENCES **82**

LIST OF FIGURES

Figure 2- 1. Mass transfer stages in porous material (from Bastani 2008) 9
Figure 2- 2. Collision function for diffusion (from Terybal 1990) 14
Figure 2- 3.Types of equilibrium sorption; C_e=amount sorbed, C_e=amount in solution (from Weber, 1972) 17
Figure 2- 4. Gas concentration profile inside the filter and mass transfer zone (from Noll et al. 1992) 18
Figure 2- 5. Structure of (a) graphite (b) turbostratic carbon (from Noll et al. 1992) 20
Figure 2- 6. Brunauer's classification of adsorption isotherms (from Hines et al. 1993). 23
Figure 2- 7. Schematic representation of discrete filtering medium (from Popescu et al., 2007) 29

Figure 3- 1. Validation Method 34
Figure 3- 2. a) Filter containing sorbent, b) One sorbent pellet 36
Figure 3- 3. Convection inside a filter to one pellet of sorbent media 37
Figure 3- 4. Contaminant's transfer inside a pellet 38
Figure 3- 5. Experimental set up for adsorption isotherm test 42
Figure 3- 6. Experimental set up for model validation 46
Figure 3- 7. Schematic setup for calibration of single gas detectors 50
Figure 3- 8. Calibration curves of single gas detectors for MEK 51
Figure 3- 9. Calibration of single gas detectors for n-hexane 51
Figure 3- 10. Calibration curve of GC/MS for MEK and n-hexane 53

Figure 4- 1. MEK Langmuir Isotherm 55
Figure 4- 2. n-hexane Langmuir Isotherm 55
Figure 4- 3. Moisture Langmuir Isotherm 56
Figure 4- 4. Breakthrough time of 100 *ppm* n-hexane in dry condition 58
Figure 4- 5. Breakthrough time of 100 *ppm* MEK in dry condition 59
Figure 4- 6. Breakthrough curve of MEK and n-hexane in dry condition 60
Figure 4- 7. Breakthrough curve of MEK and n-hexane in humid condition 61

Figure 4- 8. Experimental breakthrough curves of n-hexane in different test conditions 62
Figure 4- 9. Experimental breakthrough curves of MEK in different test conditions 63
Figure 4- 10. Breakthrough curve of 70 *ppm* MEK in dry condition (repeatability test) . 64
Figure 4- 11. Breakthrough curve of 300 *ppm* n-hexane in dry condition (repeatability test).. 65
Figure 4- 12. Breakthrough of curve of 100 *ppm* MEK and n-hexane in dry condition (repeatability test) 66
Figure 4- 13. Breakthrough of curve of 100 *ppm* MEK and n-hexane in humid condition (repeatability test) 66
Figure 4- 14. Breakthrough profile of 100 *ppm* n-hexane in dry condition...................... 68
Figure 4- 15. Breakthrough profile of 100 *ppm* MEK in dry condition 68
Figure 4- 16. Breakthrough profile of MEK and n-hexane in dry air containing two contaminants 69
Figure 4- 17. Breakthrough curve for MEK in humid mixture.. 70
Figure 4- 18. Breakthrough time of n-hexane from modeling and experiments 71
Figure 4- 19. 50% breakthrough time relative error of modeling in different conditions 72
Figure 4- 20. 80% breakthrough time relative error of modeling in different conditions 73

LIST OF TABLES

Table 2- 1. Atomic and molecular volumes (from Treybal 1990) 13
Table 2- 2. Adsorption isotherm models (from Axley 1994) 24

Table 3- 1. Properties of selected pollutants 47
Table 3- 2. Injection rates for MEK 48
Table 3- 3. Injection rates for n-hexane 48
Table 3- 4. Calculated injection rates for each compound and mixture of compounds.... 49

Table 4- 1. Test results and conditions for adsorption isotherm...................................... 56
Table 4- 2. Diffusion Parameters 57
Table 4- 3. Required Parameters... 75

LIST OF ABBREVIATIONS

Abbreviation	**Description**
ASHRAE	American Society of Heating, Refrigerating, and Air-Conditioning Engineers
GAC	Granular Activated Carbon
GC/MS	Gas Chromatograph/Mass Spectrometer
HVAC	Heating, Ventilation, and Air Conditioning
IAQ	Indoor Air Quality
MEK	Methyl Ethyl Ketone
ppm	Parts Per Million
RH	Relative Humidity
TD	Thermal Desorber
UHP	Ultra High Performance
VOC	Volatile Organic Compound

LIST OF SYMBOLS

English symbols	Description
A	adsorbate species
A_p	surface area of particles, $[m^2]$
A_s	exposed surface area of the adsorbent, $[m^2]$
C	adsorbate (contaminant) concentration in gas phase, $[g/g_{air}]$
$C^{'}$	air phase concentration in isotherm function equation, $[g/g_{air}]$
$C^{'}_0$	intercept of the tangent in isotherm function equation, $[g/g_{air}]$
C_0	concentration at the filter's inlet, $[g/g_{air}]$
C^*	air phase concentration at the exposed surface of the sorbent (near surface air phase concentration), $[g/g_{air}]$
C_∞	contaminant concentration in the bulk air, $[g/g_{air}]$
C_{down}	downstream concentration, $[g/g_{air}]$
C_e	equilibrium concentration of adsorbate in gas phase, $[g/g_{air}]$
C_p	pore phase concentration, $[g/g_{air}]$
$\overline{C}_p$	mean air phase concentration within granules of sorbent, $[g/g_{air}]$
C_p	air phase concentration within the pores, $[g/g_{air}]$
C_s	adsorbate concentration in solid phase (sorbed phase concentration) $[g/g_{solid}]$
C_s^*	sorbed phase concentration in equilibrium with air phase, $[g/g_{solid}]$
$\overline{C}_s$	mean sorbed phase concentration, $[g/g_{solid}]$

C_{s0}	temperature independent surface saturation concentration
C_{Se}	equilibrium concentration of adsorbate in solid phase, [g/g_{solid}]
C_{up}	upstream concentration, [g/g_{air}]
D_e	effective diffusivity, [m^2/s]
D_H	hydraulic diameter, [m]
D_k	Knudson diffusivity, [m^2/s]
D_m	molecular diffusivity of the compound in the gas phase, [m^2/s]
D_x	axial dispersion coefficient, [m^2/s]
h_m	convection mass transfer coefficient, [m/s]
I	contaminant injection rate, [ml/min]
k	first order reaction constant, [s^{-1}]
k_b	Boltzman constant
K_h	boundary layer mass transfer rate, [g/s]
K_L	temperature dependent Langmuir constant
K_p	partition coefficient in isotherm model, [g/g]
K_T	tangent slope of the isotherm function equation
M	molecular weight, [g/mol]
M_1,M_2	molecular weights of species 1 and 2 in the mixture, [g/mol]
M_s	mass of the adsorbent, [g]
M_{ai}	mass of air in cell I, [g]
M_{si}	mass of adsorbent in cell I, [g]

m_s	mass of adsorbed contaminants, [g]
P	total pressure, [Pa]
P_p	perimeter of the particles, [m]
Q	volumetric gas flow rate, [m^3/s]
R	first order chemical transformation removal rate, [$g_{sorbate}/s$]
r	radial dimension, [m]
R_o	radius of the activated carbon granules, [m]
R_p	particle's radius, [m]
Re	Reynolds number
S^*	active site on the solid (adsorbent)
Sc	Schmitt number
Sh	Sherwood number
T	temperature, [K]
t	time, [s]
T_b	normal boiling point, [K]
u	air velocity, [m/s]
V_i	volume of compartment I, [m^3]
$\mathrm{V}_{\mathrm{total}}$	total volume, [m^3]
W	contaminant species mass transport rate, [$g_{species}/s$]
w_a	airflow rate passing through the filter, [g_{air}/s]
x	axial dimension, [m]

Greek Symbols	**Description**
ρ_{air}	density of the air, [g/m^3]
ρ_g	density of the gas, [g/m^3]
ρ_s	density of the sorbent, [g/m^3]
ρ_c	density of the contaminant, [g/m^3]
μ_g	dynamic viscosity of the gas, [$Pa.s$]
σ	collision diameter, [$°A$]
ε_p	porosity of the sorbent material (particles)
ε	energy of molecular attraction, [Kj/mol]
ε_r	air recirculation between adjacent cells
τ	tortuosity
ν	molal volume, [cm^3/mol]
λ	mean pore radius, [$°A$]
ΔH	heat of adsorption, [KJ/mol]

CHAPTER 1 INTRODUCTION

1.1 BACKGROUND

In the past few years, indoor air quality (IAQ) has become one of the most challenging issues in the design, construction and operation of buildings. According to (ASHRAE Standard 62.1, 2007) indoor air quality should be sufficiently acceptable in an indoor environment. This means that there should be no harmful contaminant concentration, as determined by cognizant authorities, that could cause the substantial majority of the people (80% or more) who are exposed to such environment feel satisfy.

There are three methods to control the contaminant concentrations in an indoor environment and maintain them at acceptable levels: source control, general ventilation control, and filtration and purification control.

Excluding the contaminant emission source is the most effective and economical way to reach a better indoor air quality. Forbidding smoking inside the buildings, and isolating equipments such as printers and copy machines in a separate room are some practical methods for eliminating the source of contaminants. However, in some cases, the source of contaminants may not be identified easily, rendering the elimination of the source impossible.

Another method to control contaminant level in the indoor air is dilution of the air by increasing the ventilation rate and recirculation of the cleaned air. Outdoor air is used in the air-handling unit as supply air in HVAC systems for recirculation of the air. HVAC systems are used to provide thermal comfort and acceptable indoor air quality. ASHRAE

Standard 2007-b and ASHRAE Standard 55-2004 stated some regulations and standards for adequate IAQ and thermal comfort. There are two procedures that are recommended: Ventilation rate procedure, and IAQ procedure. In ventilation rate procedure, minimum intake rate of outdoor air is applied to achieve adequate IAQ. However, the contaminants in the outdoor air are in a different group and sometimes the outdoor air needs to be conditioned not to contaminate indoor air. The purification of the outdoor air increases the buildings' energy consumption and is not an economical solution. On the other hand, IAQ procedure controls and reduces the level of contaminants using air cleaners.

Air purification and filtration are a promising approach that can be used to control the level of contaminants in the air with a less energy consumption. This method could be considered as an alternative method when the previous two techniques cannot control the IAQ. Based on the ASHRAE Standard (ASHRAE Standard 62.1, 2007), recirculation of the air is allowed only if the contaminant concentration is below a determined criteria. Using air cleaning technology reduces the outside air intake rate equal to the recirculation rate. This rate depends on the air cleaning devices and their removal efficiency. Therefore, air cleaners are the most appropriate way to reach the desired IAQ and save overall energy consumption in buildings. These filters can be used in HVAC systems to remove the pollutants either particulate or gaseous. They have been designed with numerous scrubbers and different characteristics and capabilities that are in use in the current market. The effluence of these filters will be used to re-supply the room. Thus, the effluence has to be perfectly clean. The efficiency and removal performance of these filters are of major importance in the successful design of the appropriate HVAC system. There have been extensive studies on the removal performance of particulate filters in the literature. The evaluation of these filters can be found in the previous studies (ASHRAE Standard 52-1999). However, there is a need to have a standard method for evaluation of air cleaners and a general guideline to quantify the performance of these devices using available models.

As mentioned previously, the most conspicuous gaseous contaminant inside the buildings is VOC. As the concentration level of the contaminant of indoor air is low, there are two technologies that are applied for removing of VOCs. The first method is oxidation technique such as photo-catalysis or cold plasmas (Popescu et al., 2007). In this method, the organic compounds decompose, while the catalyst is deactivated. However this process could possibly generate harmful secondary chemicals, hence it is recommended to opt for other applications when alternative methods can be implemented. The second technology that can be used for air cleaning is the application of adsorption systems. Adsorption technique is the most appropriate technique for controlling the level of VOC using air cleaners (Gupta and Verma, 2002; Mahajan, 1987). There are different sorptive media such as activated carbon, activated alumnia and zeolite that are used in HVAC systems. Commonly, activated carbon has been used as a common scrubber in air cleaner devices in different types and shapes (Henschel 1998). The high usage of activated carbon is due to its high capacity and affinity for VOCs. Furthermore, the qualification and effectiveness of activated carbon have been verified in industrial application (Liu and Huza, 1995). The main deficiency of this technique is the saturation of the sorbent after adsorbing a specific amount of the contaminants. The sorbent will be saturated after a period of time, and it would not be as efficient as it was initially. Therefore, the sorbent should be changed or regenerated periodically. Thus, the lifetime of the filter should be determined. To find the lifetime of the filters some information is needed. Because there are many parameters affecting the removal performance of the filters, it is necessary to have a method that integrates all the required information. This method should be general or should have the capability to be generalized to different applications and conditions. If a general method is available, it will ease determining the efficiency of these air cleaners. This method includes modeling of air cleaners, defining required parameters for the modeling, and validating the proposed model. The efficiency of these cleaners allows determining their life time. By predicting efficiency and lifetime, the filters can be changed or regenerated by building operators, allowing an efficient filter all the time. Therefore, it is necessary to model these air cleaners, as the models will be used to compute the removal efficiency. The removal efficiency is a function of diverse factors. All these factors are important in finding the total contaminant transfer from contaminated air to the air cleaner. Contaminants adsorb to the sorbent in the air cleaner, and diffuse through the air cleaner into the sorbent. Therefore, the adsorption and diffusion phenomena should be modeled. To model the adsorption and diffusion phenomena, the basic mass transfer that occurs in the air cleaners should be defined. Contaminants in the air are transferred from the air to the sorbent. There are different parameters that affect the mass transfer from the air to the filter, and they are: Filter structure and properties, physical and chemical properties of the VOCs in the air, environmental conditions, and sorption parameters (Mahajan, 1987; Popa and Haghighat, 2003). There are various models that could be used for the prediction of air cleaners' removal efficiency. To the best of the author's knowledge, there is not a systematic methodology for verification and validation of these models. All of these concerns claim the necessity for the development of a systematic methodology for predicting the performance of gaseous filters. This method should also consist of the quantification of the required parameters.

1.2 OBJECTIVES

The objectives of this study are:

- To develop a systematic method to evaluating gaseous filter models used for evaluating the removal performance of commercial air cleaners and finding the lifetime of these devices.
- To select a model and establish an experimental set-up to obtain the required parameters and then,
- To validate the selected model against experimental data.

1.3 THESIS OUTLINE

Chapter 2 explains the fundamentals of mass transfer in sorptive gaseous filters. The adsorption process is extensively investigated. The chapter also provides a review of the previous studies that have been done in the removal performance of sorptive gaseous filters, and models development. In addition, the effective parameters of removal performance and lifetime prediction of the filter are presented. Chapter 3 explains the developed method to quantify the required parameters for the available models in gaseous filters. An experimental procedure for evaluation of a filter is presented and explained in details. This case study aims to be used for model validation. Furthermore, the required parameters for the selected model are quantified, and the proposed experimental setup is applied to find the experimental parameters required in the model. In addition, the experimental setup that was established in the methodology is applied to validate the model against experimental data. Chapter 4 reports the calculated results and experimental results stemmed from this research. Finally, Chapter 5 provides the conclusion of this study and recommendations for future work.

CHAPTER 2 LITERATURE REVIEW

2.1 INTRODUCTION

Improving indoor air quality has become a major task in the design and construction of building in today's modern world. There are many sources of pollutants such as tobacco smoke, radon, building materials, combustion products from inside the buildings, outdoor pollutants, and consumer products. However, the major contaminants in indoor air are VOC compounds. Extensive research has been done by the Environmental Protection Agency which stated that most people spend approximately 90 percent of their time in indoor environments. Thus, investing more attention to the air quality in the buildings is necessary to protect building occupant against the contaminants. Poor indoor air quality is a leading cause to many illnesses. Headache, dizziness, nausea, asthma, allergic reactions, cancer, and irritation of eyes, throat, and skin are some of the illnesses which are caused by poor indoor air quality (EPA 2008). Improving the quality of indoor environment will decrease these illnesses. Applying air cleaners is one promising way to ensure a better indoor air quality by reducing the level of contaminants in indoor air. Sorptive filters can remove the pollutants from indoor air by adsorbing the contaminants on the adsorbent in the filter. Activated carbon filter is one of these sorptive filters which only trap gaseous species, especially VOCs. The main problem of this method is that the saturation of the media in the filters (Popescu et al., 2007). Thus, these filters have a limited lifetime and it should be determined prior to using them. The removal performance of the filters has been studied (Axley, 1994; Pei and Zhang, 2010; Pei et al., 2008; Xu et al., 2011). In the previous studies, some models have been proposed. However, all of them are applicable for the case of a single contaminant in the air which is not representative of the real situation in a building. In reality, there exists mixture of compounds in the air. Tsai et al. (1985) have proposed a method with three different adsorption models for adsorbing a mixture of CH_4 and H_2 on activated carbon. Predicted performance of the filter in the three models was not the same and differed from experiments. Furthermore, the behavior of a mixture of common VOCs' adsorption on activated carbon in the air is different from methane and hydrogen. Also, a model is applicable only if it is validated and can be generalized. Despite all the previous studies there exists no general method for validation of these models.

In this chapter, the previous studies on the removal performance of the gaseous filters, and available models for these filters are presented. The required parameters for use in the gaseous filter models have also been introduced. First, however, the fundamentals of the adsorption and mass transfer processes inside gaseous filters have been detailed.

2.2 MASS TRANSPORT

The mass transfer between gas phase and solid phase in a bed containing porous material occurs in three main stages; external diffusion, internal diffusion, and surface adsorption. The contaminants are transferred from the indoor air to the sorbent in the filter by the previously mentioned phenomena. Figure 2- 1 shows the different stages of mass transfer in a porous material.

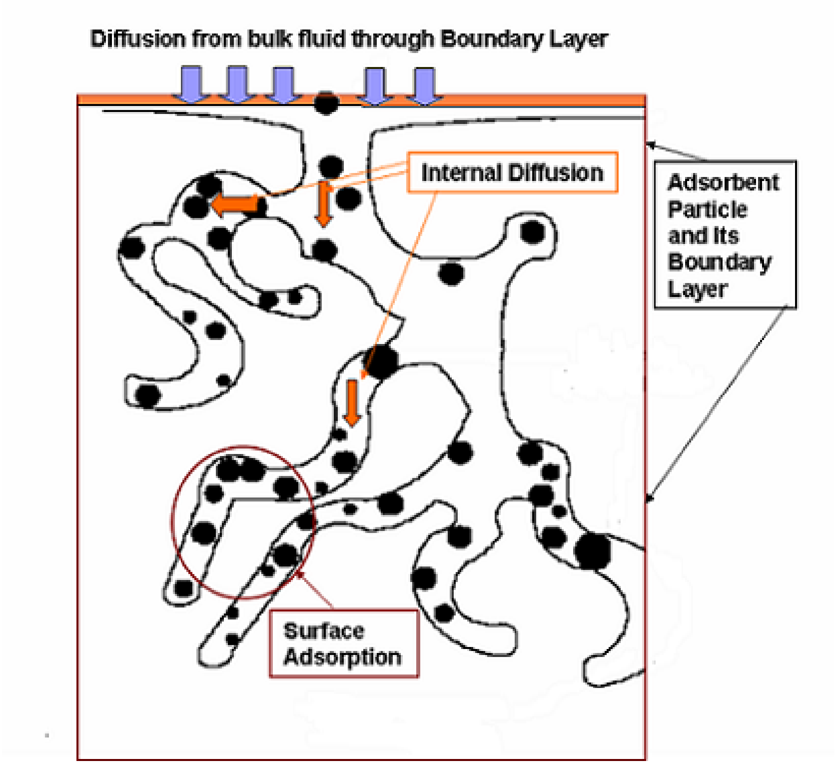


Figure 2- 1. Mass transfer stages in porous material (from Bastani 2008)

2.2.1 External Diffusion

The process of transferring the contaminant's molecules from the gas phase through the boundary layer on the adsorbent surface in the filter is called external diffusion. External diffusion is mostly affected by the external film mass transfer coefficient and contaminant concentration gradient between the bulk air and sorbent's surface (Noll et al., 1992). Therefore, when the adsorbed phase concentration increases, the diffusion rate decreases. Furthermore, when the contaminant concentration in the air phase is low, the diffusion rate is low as well, and it can be neglected. Thus, the external diffusion is negligible in low concentrations (ASHRAE, 2007-a). Thereby, the governing process is adsorption and not diffusion.

The mass transfer is explained by convection mass transfer coefficient, h_m, during external diffusion, which defines the flow through the boundary layer depending on the gradient between gas phase contaminant concentration and concentration of the contaminant on the adsorbent's surface. External mass transfer coefficient is mostly dependent on the compound (in the case of filter, pollutants), and on the airflow rate. Three dimensionless numbers are used to determine the external mass transfer coefficient; Sherwood number, Reynolds number, and Schmitt number that are presented in equations (1) to (3) respectively.

$$Sh = \frac{2h_m.R_p}{D_m} \tag{1}$$

$$\mathrm{Re} = \frac{2R_p u \rho_g}{\mu_g} \tag{2}$$

$$Sc = \frac{\mu_g}{D_m \rho_g} \tag{3}$$

Therefore, the external mass transfer coefficient is determined through different correlations of Sherwood number. Then, the external diffusion rate is obtained after determining the external mass transfer coefficients. However, among the correlations of mass transfer coefficient equations, Ranz and Marshall (equation (4)), Wakao and Funazkri (equation (5)), Petrovic and Thodos (equation (6)), and Williamson et al. (equation (7)) are usually used for packed beds. In general, Wakao and Funazkri correlation yields a higher value for the mass transfer coefficient as compared to the other ones since this correlation considers the axial dispersion effect (Noll et al., 1992). Nevertheless, Ranz and Marshall, and Wakao and Funzkri equations are the two widely used correlation for estimation of the mass transfer coefficients in a porous media in packed beds (Popescu et al., 2007).

$$Sh = \frac{2h_m R_p}{D_m} = 2.0 + 0.6\,\mathrm{Re}^{0.5}\,Sc^{0.33} \tag{4}$$

$$h_m = \frac{D_m}{2R_p}(2.0 + 1.1\,\mathrm{Re}^{0.6}\,Sc^{0.33}) \tag{5}$$

$$h_m = 0.355u(\frac{1-\varepsilon}{\varepsilon})\,\mathrm{Re}^{-0.359}\,Sc^{-0.67} \tag{6}$$

$$h_m = 2.40u\,\mathrm{Re}_p{}^{-0.66}\,Sc^{-0.58} \qquad \mathrm{Re} = 0.08 - 125 \tag{7}$$

$$= 0.442u\,\mathrm{Re}_p{}^{-0.31}\,Sc^{-0.58} \qquad \mathrm{Re} = 125 - 5{,}000$$

Popescu (2008) stated that the Sherwood correlations were developed at different experimental conditions, including temperature and concentration that may have caused different results and added an uncertainty factor to his simulation results.

2.2.2 Internal Diffusion

The transport process of the adsorbate molecules within the pores from the external surface of the adsorbent to the interior of the adsorbent is called internal diffusion. It includes molecular and Knudson diffusion within the gas phase and surface diffusion along the surfaces which surround the pores. Internal diffusion can be considered as Fickian's first law of diffusion with an effective diffusion coefficient (Noll et al., 1992):

$$N_A = D_e \frac{\partial C_p}{\partial r} \tag{8}$$

Intra-particle diffusion involves different mechanisms; ordinary diffusion or molecular diffusion, Knudson diffusion, and surface diffusion. The mechanisms depend on the pore size, the sorbate concentration, and some other conditions. If the pore sizes are high and the solution is dense, then the mechanism can be considered to be molecular diffusion. If the solution is gas which has a low density, or if the pores are small, or both, the collision of the molecules with the pore wall is more than with each other, the Knudson diffusion should be applied. If the transport of the molecules is characterized by a movement over the surface, surface diffusion should be applied.

2.2.2.1 Molecular diffusion

Molecular diffusion coefficient is a basic property of a compound and has been measured for a variety of compounds using different techniques. The value of molecular diffusion for many chemicals is available in handbooks (Lide, 2004; Perry et al., 1963). Molecular diffusion increases with temperature and decreases with viscosity of the medium (Logan, 1999). For a gas-solid system, the effective molecular diffusivity can be calculated by Chapman-Enskog equation correlated with tortuosity, τ , and particle porosity, ε_p (Ruthven, 1984):

$$D_{m,eff} = \frac{\varepsilon_p}{\tau} D_m \tag{9}$$

$$D_m = \frac{BT^{3/2}(\frac{1}{M_1} + \frac{1}{M_2})^{1/2}}{P\sigma_{12}^2\Omega} \tag{10}$$

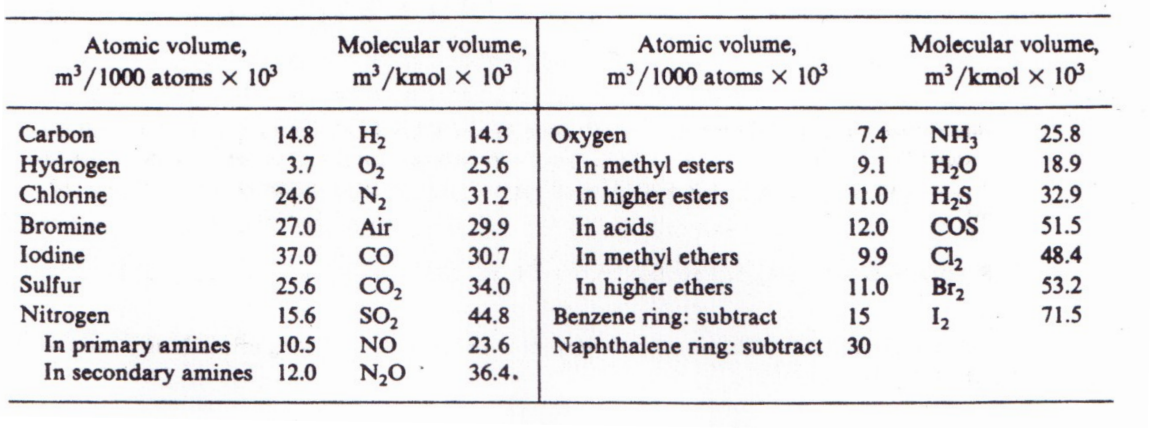
$$B = (10.85 - 2.50\sqrt{1/(1/M_1 + 1/M_2)}) \times 10^{-4} \tag{11}$$

Where, M_1 and M_2 are the molecular weights of species in the mixture, P is the total pressure, $\sigma_{12} = (\sigma_1 + \sigma_2)/2$ is the collision diameter (molecular separation at collision) from Lennard-Jones potential in $\overset{o}{A}$, and Ω is a function of $\varepsilon / k_b T$, $\varepsilon = \varepsilon_1 \varepsilon_2$ is the Lennard-Jones force constant, which is found from collision function curve for diffusion in Figure 2- 2. The values of σ and ε can be calculated from gas properties such as viscosity. If these values are not available, they can be calculated approximately for each compound by the following equation.

$$\sigma = 1.18 \nu^{1/3} \tag{12}$$

$$\frac{\varepsilon}{k_b} = 1.21 T_b \tag{13}$$

Table 2- 1. Atomic and molecular volumes (from Treybal 1990)



Atomic volume, $m^3/1000$ atoms $\times 10^3$		Molecular volume, $m^3/kmol \times 10^3$		Atomic volume, $m^3/1000$ atoms $\times 10^3$		Molecular volume, $m^3/kmol \times 10^3$	
Carbon	14.8	H_2	14.3	Oxygen	7.4	NH_3	25.8
Hydrogen	3.7	O_2	25.6	In methyl esters	9.1	H_2O	18.9
Chlorine	24.6	N_2	31.2	In higher esters	11.0	H_2S	32.9
Bromine	27.0	Air	29.9	In acids	12.0	COS	51.5
Iodine	37.0	CO	30.7	In methyl ethers	9.9	Cl_2	48.4
Sulfur	25.6	CO_2	34.0	In higher ethers	11.0	Br_2	53.2
Nitrogen	15.6	SO_2	44.8	Benzene ring: subtract	15	I_2	71.5
In primary amines	10.5	NO	23.6	Naphthalene ring: subtract	30		
In secondary amines	12.0	N_2O	36.4.				

Where, T_b is boiling point and ν is the molecular volume of liquid at normal boiling point in *$m^3/kmol$* (Table 2- 1). Molecular diffusivity happens when molecule-molecule collision is much more dominant than collision between molecules and the wall. Because this diffusivity depends on the collision between molecules, the molecular diffusivity is a function of temperature, pressure, molecular weight, and other properties of the components. Advanced kinetic theory showed that the composition of the mixture has a small effect on molecular diffusivity. Therefore, the molecular diffusivity of a compound is constant and can be calculated for each compound at the standard condition (Thibodeaux and Mackay, 2010).

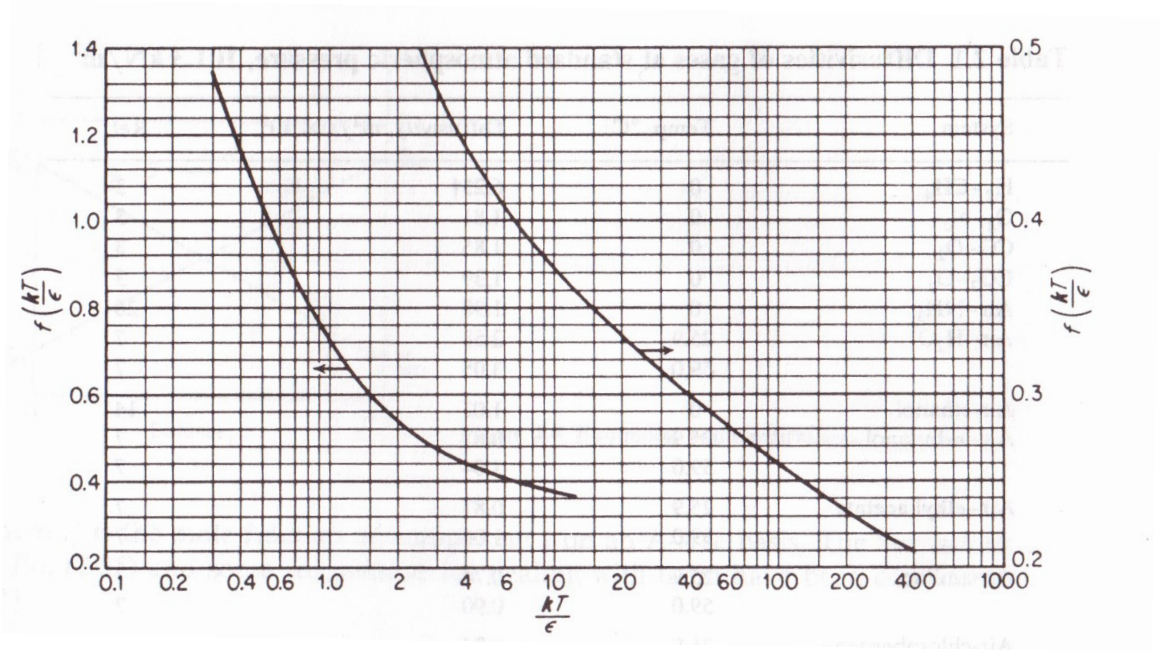


Figure 2- 2. Collision function for diffusion (from Terybal 1990)

2.2.2.2 Knudson Diffusion

The driving force for Knudson transportation is the concentration gradient, and its characteristic parameter is called the Knudson diffusivity $D_{K,i}$ for specie i. Knudson flux depends on the molecular weight (Duong, 1998). Knudson diffusivity can be estimated from (Ruthven, 1984):

$$D_K = 9700\lambda(\frac{T}{M})^{1/2} \qquad (cm^2 s^{-1}) \tag{14}$$

Where, M is the molecular weight of the diffusing species and λ is the mean pore radius. Each species diffuses independently of Knudson regime. Therefore, the Knudson diffusivity does not depend on the composition and concentration of the gas.

2.2.2.3 Surface diffusion

Both Knudson and molecular diffusion occur due to the gas phase flow within the pores. Also, the flux may transport compounds from the physically adsorbed layer on the surface of the macropores. The mobility of this adsorbed phase is much smaller, but the concentration is much higher. Therefore, if the adsorbed layer is thick, the transport from the flux is significant. This transport is called surface diffusion and is the most complicated type of diffusion. It assumes that a surface is flat which contains some sites. If a molecule wants to go from one site to another vacant site (It is assumed that the energy of these sites are larger than the thermal energy of a molecule), the molecule should gain energy (Duong, 1998). Due to the complexity of surface diffusion, and its small effect it has in some cases such as activated carbon, it is usually neglected.

2.2.2.4 Effective diffusion

If the surface diffusion transfer is neglected, the effective diffusion in the adsorption pellets can be determined as:

$$\frac{1}{D_{p,eff}}=\frac{1}{D_{k,eff}}+\frac{1}{D_{m,eff}} \tag{15}$$

2.2.3 Adsorption

Adsorption is a surface physical phenomenon. Mass transfer between two phases where the adsorbents transfer from the gas phase to the solid phase causes relocation of the compounds. This relocation results in the accumulation of the compounds at the surface of the adsorbent or at the interface of the two phases. The adsorption technique is mostly used for removing relatively low concentration of pollutants from a gas phase by trapping the pollutants on a solid. This solid should be able to hold (adsorb) the pollutant with its intermolecular forces. The adsorbent is the phase that is adsorbing on its surface. The material concentrated or adsorbed at the surface of that phase is called the adsorbate. However, absorption is when the transferred material from one phase to another interpenetrates the second phase to form a "solution". Sorption is a general expression used for both adsorption and absorption. There are differences in the sorption processes. C_e and C_{Se} in Figure 2- 3 represent the equilibrium concentration of a substance (pollutant in sorption filters) in each of two phases. In general, C_{Se} is the amount of adsorbate corresponding to a unit weight of solid adsorbent and C_e is the concentration of a compound in the fluid phase. Curves I and III specify the nonlinear correlation of favorable and unfavorable adsorptions respectively. Curve II indicates the linear adsorption characteristics (Slejko, 1985)

Adsorption at a surface is highly influenced by the binding forces between individual atoms, ions, or molecules of an adsorbate and the surface, and all of these forces are the results of electromagnetic interactions. Four main types of adsorption -exchange, physical, chemical, and specific- are identified (Slejko, 1985). Exchange adsorption, or ion exchange, deals with electrostatic attachment of ions to the opposite site charge at the surface of the adsorbent, with displacement of some ions with other ions of higher electrostatic affinity. Physical adsorption involves van der Waals forces which include both London dispersion forces and classical electrostatic forces. In a chemical adsorption, a reaction involves the adsorbate and the adsorbent, and as a result, the chemical form of the adsorbate is changed. Adsorbate molecules attachment on adsorbent surfaces can be an outcome of specific interactions that do not result in adsorbate transformation. The binding energies of "specific adsorptions" cover a wide range of sorption processes; from physical adsorption to the higher chemisorptions.

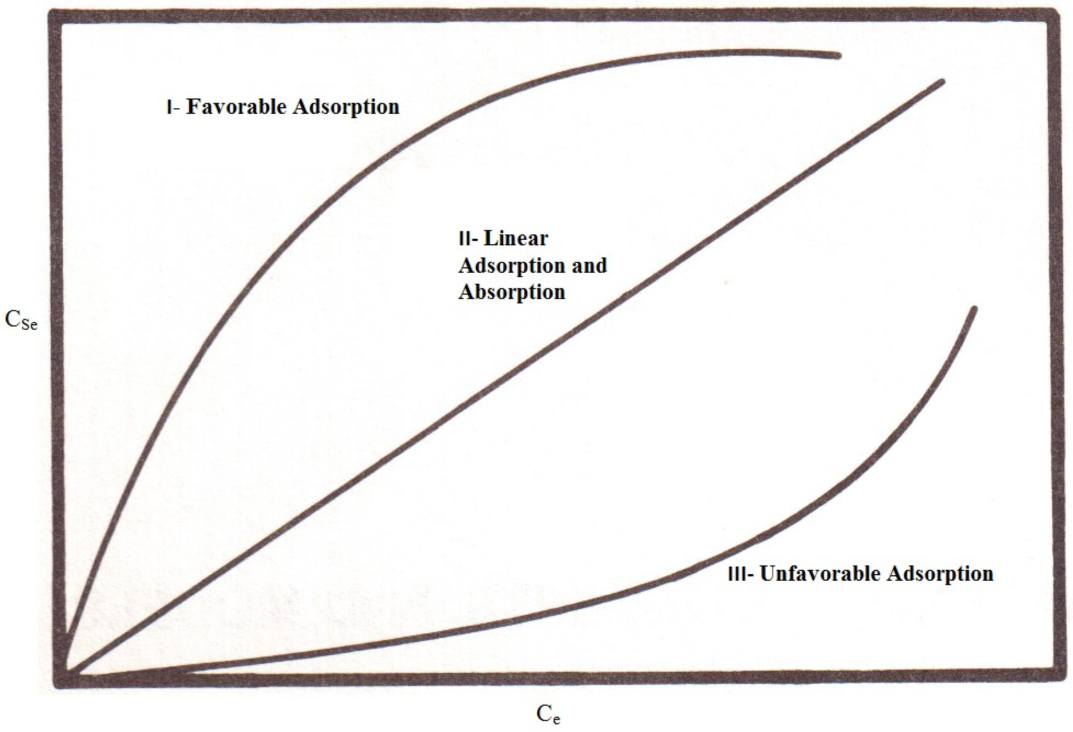


Figure 2- 3.Types of equilibrium sorption; C_e=amount sorbed, C_e=amount in solution (from Weber, 1972)

2.2.3.1 Adsorption gaseous filters

The removal media, size, pore size distribution of the media, removal bed packing density, gas conditions and concentration of the contaminants in the gas, affect the removal efficiency of the gaseous filters. In gaseous filters, the gas with a known concentration passes through the filter that is filled with a sorbent media such as activated carbon. The contaminant concentration decreases due to an airflow that induces a mass transfer from the bulk air to the media. Thus, the concentration of the contaminant in the gas and solid phases is dynamic both in time and space (through filter). The section of the filter in which mass transfer occurs, and the sorbent is filled with the contaminant, is called the mass transfer zone. Figure 2- 4 presents this section.

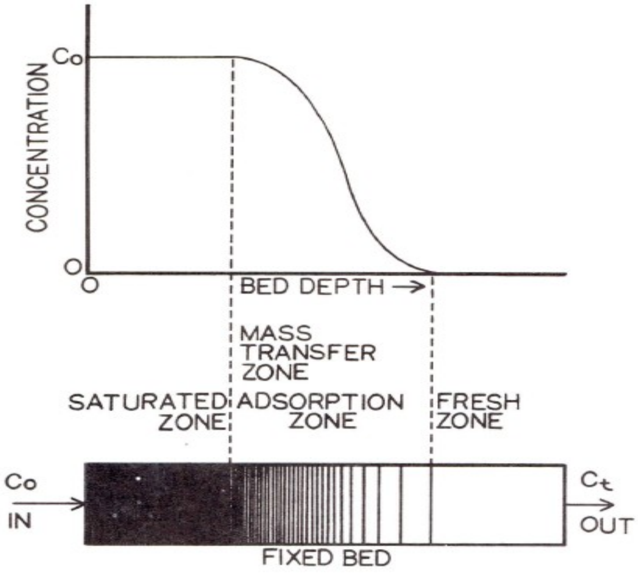


Figure 2- 4. Gas concentration profile inside the filter and mass transfer zone (from Noll et al. 1992)

The filter inlet zone becomes saturated after a period of time. The mass transfer zone moves towards the bed's length. When all the contaminants are removed by the sorbent media in the filter, the contaminant concentration of the filter effluent diminishes to zero and the effluent air is considered clean. At this point, the removal efficiency of the filter is 100%. As the mass transfer zone moves to the end of the filter, the contaminants penetrate the filter, and the removal efficiency of the filter decreases. The time required for the contaminant to reach the effluent of the filter is called the breakthrough time. The penetration profile plotted versus the elapsed time is called the breakthrough curve. Penetration increases while the removal efficiency decreases. The concentrations before and after the filter are equal when the whole mass transfer zone passes the filter. The breakthrough time profile of a filter is important for HVAC designers and has been studied (VanOsdell 1994). Therefore, the present research uses the breakthrough curve as the indicator for discussion.

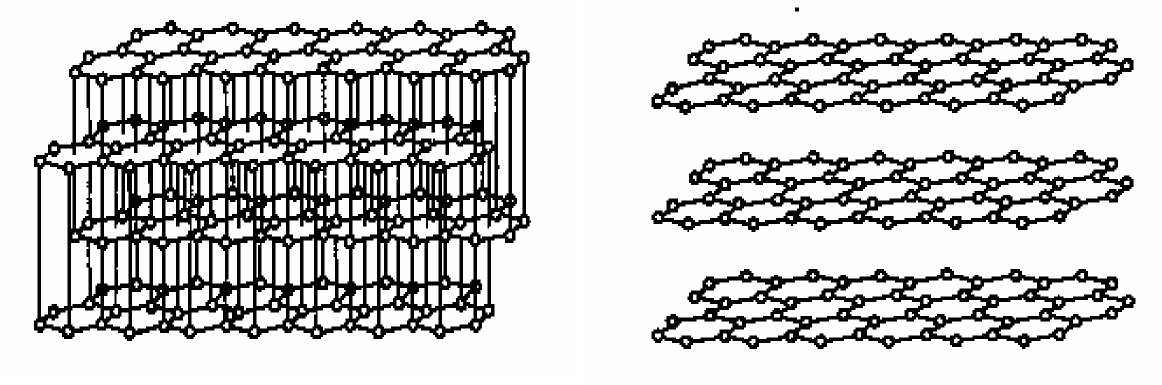
2.2.3.2 Adsorbate Properties

Volatile organic compounds (VOC) are a group of organic gases composed of carbon and hydrogen. Some of the major VOCs found in the air are n-hexane, 2-butanone or methyl ethyl ketone (MEK), i-butanol, toluene, and p-xylene. The VOC concentration indoors is much higher than outdoors (EPA, 2007). VOCs are emitted from different materials in the buildings such as paints and lacquers, paint strippers, cleaning supplies, pesticides, building materials and furnishings, office equipment such as copiers and printers, correction fluids and carbonless copy paper, graphics and craft materials including glues and adhesives, permanent markers, and photographic solutions (EPA, 2008). VOCs may have short or long term adverse health effects on the human body. Eye, nose, and throat irritation, headaches, loss of coordination, nausea, damage to liver and kidney are some adverse health effects that result from exposure to VOCs (EPA, 2008).

2.2.3.3 Adsorbent Properties

Adsorption is a surface phenomenon; practical commercial adsorbents have large surface areas. Most of the adsorbents contain internal surfaces with extensive pores and capillaries of highly porous solids. The pores are either cylindrical, or slit shape (Chiang et al., 2001). For removing VOCs, sorbents that are characterized by a large surface area, no attraction for water adsorption (hydrophobic), thermal stability, no catalytic activity, and easily re-generable are more appropriated (Guo et al., 2006).

Activated carbon, especially granular activated carbon, is commonly used in air cleaning devices (VanOsdell et al., 2006). The solid used in air cleaners as an adsorbent is usually an activated carbon or a crystalline material with high internal porosity. The structure of the pores are macropores (diameters larger than 50 nm), micropores (diameters less than 2 nm), and mesoropores (between 2-50 nm). Noll et al. (1992) studied the structure of graphite and turbostratic carbon. The structure of these sorbents is similar to the activated carbon, as displayed in Figure 2- 5. Activated carbon has micro-crystallites and its width is less than 100 °A. The microcrystallites are connected in different directions as shown in the figure. The connections of microcrystallites form the micropores (Ruthven, 1984). Adsorbed molecules may obstruct the entrance of other molecules to the internal surfaces in micropores's sorbents (Hunter and Oyama, 2000).



(a) (b)

Figure 2- 5. Structure of (a) graphite (b) turbostratic carbon (from Noll et al. 1992)

Activated carbon has hydrophobic and organophilic molecules. The affinity of activated carbon for adsorbing non-polar compounds is much higher than polar compounds.

Pellets or granules of activated carbon are mostly used as adsorbent in the air cleaners in HVAC systems (ASHRAE, 2007-a). The effective removal process for granular activated carbon is verified by determining the contact time between these adsorbents and airflow. The effective contact time ranges between 0.02-0.2 seconds that is known as residence time (Holmberg et al., 1993).

The VOCs removal efficiency from the gaseous phase by adsorption depends: the type of compounds, concentration of the compounds, pressure, temperature, and humidity, pore structure, quantity of the active sites, and characteristics of the adsorbent material.

The molecular size affects the adsorption rates when the adsorption is governed by intra-particle diffusive mass transport in porous adsorbents. The adsorption is faster when the molecule sizes are smaller. However, the adsorption rate dependency on molecular weight is only within a particular chemical class or homologous series. If molecules are large (but from another chemical class), they may be adsorbed more rapidly than smaller molecules of another chemical class (Slejko, 1985).

2.2.3.4 Adsorption isotherm

In adsorption process between gas phase and solid phase, the adsorbate compounds (contaminants) are accumulated on the surface of the sorbent or at the interface of the two phases, and it is generally assumed that the two phases are in equilibrium at a constant temperature. Adsorption isotherm describes the relation between the adsorbed mass in the solid phase and the adsorbate concentration in the gas phase.

$$C_p = f(C_s) \tag{16}$$

Based on Brunauer's classification, below a critical gas temperature, the adsorption isotherm can be classified into five categories as shown in Figure 2- 6. Type I isotherm (Langmuir isotherm) is used in a system with a monolayer molecular adsorption. Adsorption occurs in a micropores solid, where the pore size is not much greater than the adsorbate molecule size. Therefore, the adsorption limit is governed by the micropore volume (Noll et al., 1992). The following isotherm equation represents the type I Langmuir adsorption isotherm (Brunauer et al., 1940):

$$C_s = \frac{K_L . C_{s0} . C}{1 + K_L . C} \tag{17}$$

Where C_s is the equilibrium adsorbate concentration in the sorbed phase (contaminant concentration in solid), C is the adsorbate concentration in the gas phase (contaminant concentration in the air). The constant parameters, C_{s0}, and K_L can only be found experimentally. In the experiment, different gas concentrations are introduced, and the amount of the contaminant that is adsorbed is measured. The constant parameter is determined from the knowledge of gas phase concentrations (C) and the corresponding sorbed phase concentrations (C_s).

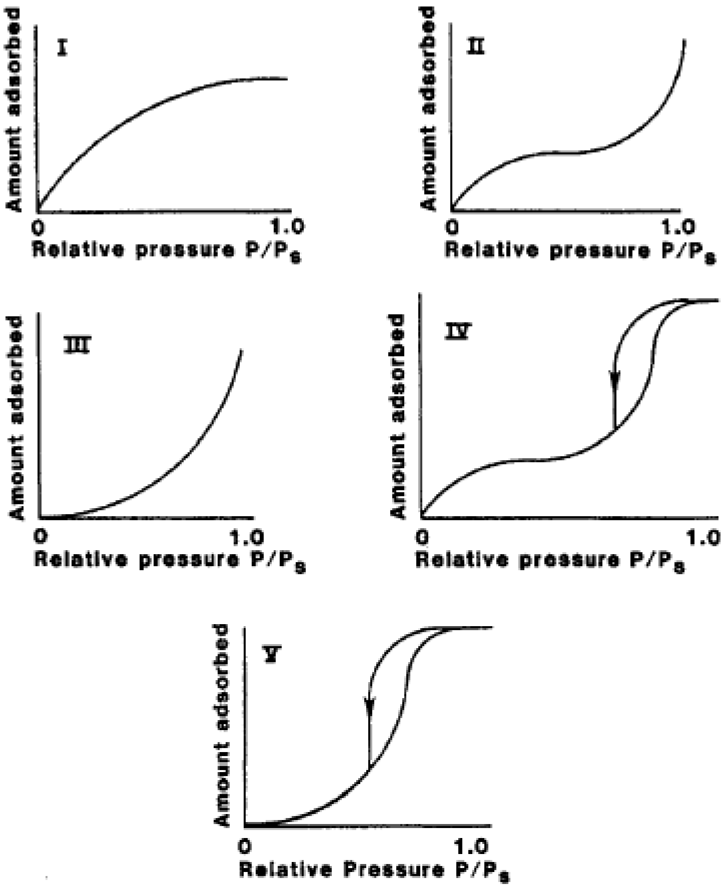


Figure 2- 6. Brunauer's classification of adsorption isotherms (from Hines et al. 1993)

There are various models for adsorption isotherm; Langmuir, Linear, BET, Polanyi, and Freundlich (see Table 2- 2). Axley (1994) mentioned that for sorption of air pollutant in building materials, Langmuir and Linear models are the most appropriate ones. For sorption of any contaminants, if its concentration is within one order of magnitude of its saturated value, the BET model should be used (Axley, 1994). Polanyi and Freundlich models are used for industrial sorbents which show nonlinear equilibrium behavior.

Table 2- 2. Adsorption isotherm models (from Axley 1994)

Model	$C_{se} = f(C_e)$	Model Parameters
Linear	$C_{se} = K_P C_e$	K_P is the Partition Constant.
Langmuir	$C_{se} = \frac{C_{so}K_L C_e}{1 + K_L C_e}$	C_{so} is the molecular mono-layer sorbent concentration. K_L is the Langmuir Constant.
BET	$C_{se} = \frac{C_{so}K_{BET}\hat{C}_e}{(1-\hat{C}_e)(1-\hat{C}_e+K_{BET}\hat{C}_e)}$	K_{BET} is the BET Constant. $\hat{C}_e$ is the ratio of the equilibrium to the saturation concentration C_{sat}.
Polanyi DR	$C_{se} = C'_{so}\exp\left(-D\left[\ln\left(\frac{C_{sat}}{C_e}\right)\right]^2\right)$	D is the Dubinin-Radushkevich parameter. C'_{so} is the sorbed concentration for complete filling of micropores.
Freundlich	$C_{se} = K_F C_e^{(1/n)}$	K_F is the Freundlich constant n is the Freundlich exponent

The other types of adsorption isotherms are intended for the multilayer adsorption occurring on the surface of the adsorbent (Young and Crowell, 1962). Therefore, linear and Langmuir adsorption isotherm are usually assumed to be between the gas phase and the solid phase concentration. A set of experiments is required to obtain the adsorption isotherm constant parameters for the specific contaminants and the specific sorbent.

2. 3 AVAILABLE MODELS FOR GASEOUS FILTERS

The convection diffusion of pollutants in air cleaners like fixed beds of sorbent particles or granules is described through sorption equilibrium-constrained one dimensional convection diffusion equations. Finite element procedures may be used to transform these equations to differential equations that may be later directly integrated with available macroscopic models to simulate the behavior of the whole building/HVAC systems. However, most of the buildings do not employ fixed beds because they need an additional fan power to overcome the large pressure drop. Instead, they use porous media in order to increase mass transfer area and contact time while keeping low pressure drop. Axley (1994) employed a method including tanks that have been connected together in series in order to have a model with a well mixed sorption chamber and plug flow fixed bed devices. This model can be used for the adsorption filters. Sorbent particles and granules can make fixed beds. The mechanism for the sorption is assumed as the sorption of *A* to an active site S^* makes the species bound like A.S* and produces ΔH, which is the heat of adsorption(Axley, 1994).:

$$A + S^* \quad \underset{Desrption}{\overset{Adsorption}{\leftrightarrow}} \quad A.S^* + \Delta\mathrm{H} \tag{18}$$

The rate of adsorption and desorption is instantaneous in comparison with other transport steps. However, for single component sorption under steady state conditions, the rate of adsorption will be equal to the rate of desorption and the concentrations of adsorbate in the air phase, *C* (*g species/ g air*), and sorbed phase, C_s (*g species/g sorbent*), will remain constant in the equilibrium state. If isothermal conditions at atmospheric pressure (general adsorption isotherms) is assumed:

$$C_{se} = f(C_e) \tag{19}$$

This means that the sorbed phase is in equilibrium with the air phase. The function *f* relates the sorbed phase concentration to the air phase concentration. The function is unique for each system of adsorbate-adsorbent.

Furthermore, the following reaction is used for the chemical transformation in filters:

$$A.S^* \xrightarrow{k} products + S^* \tag{20}$$

$$R = k.M_s.C_s \tag{21}$$

Knowing chemical reaction, external diffusion, internal diffusion, and adsorption, the mass transfer inside the filter can be determined. Axley (1994) estimated the external diffusion mass transfer from the boundary layer theory:

$$w = \rho_{air} A_s h_m (C - C^*) \tag{22}$$

However, internal diffusion can be found using Fick's law of diffusion within the granules of sorption filtration, or the linear driving force model which is simpler but less accurate (Weber, 1972; Yang, 1987). Axley (1994) used a linear driving force model like the equation below.

$$w = \frac{15 M_s D_e}{R_p{}^2}(C_s^* - \overline{C}_s) \tag{23}$$

C_s^* is the sorbed phase concentration that can be in equilibrium with air phase concentration at the exposed surface of the sorption granules (C^*). The above equation can be reformulated in terms of air phase concentration;

$$w = \frac{15 M_s D_e}{R_p^2}(f(C^*) - f(\overline{C}_p)). \tag{24}$$

Based on the linear adsorption isotherm, $f(C') \approx K_T C' + C_0'$, where K_T ($g_{air}/g_{sorbate}$) is the tangent slope of the isotherm about the given state of concentration and $C_0{}'$ is the intercept of the tangent. Therefore,

$$w \approx \frac{15 M_s D_e K_T}{R_p^2}(C^* - \overline{C}_p). \tag{25}$$

Three main mass balance equations can be written; One for the bulk air phase, one for the near surface air-phase, and one for the pore air-phase. If C^* from equation 23 is substituted into equations 25 and 22, will result in two equations (Axley, 1994).

$$\begin{bmatrix} \left(w_a + \frac{K_D K_h}{K_D + K_h}\right) & -\frac{K_D K_h}{K_D + K_h} \\ -\frac{K_D K_h}{K_D + K_h} & \frac{K_D K_h}{K_D + K_h} + k M_s f^{\cdot} \end{bmatrix} \begin{Bmatrix} C \\ \overline{C}_p \end{Bmatrix} + \begin{bmatrix} M_a & 0 \\ 0 & M_s K_T \end{bmatrix} \frac{d}{dt} \begin{Bmatrix} C \\ \overline{C}_p \end{Bmatrix} = \begin{Bmatrix} w_a C_{\text{sup}} \\ 0 \end{Bmatrix} \tag{26}$$

To modify Axley's model, Popescu et al. (2007) developed a model based on Yu and Neretnieks (1993) and Axley (1994) for a single, dry and isothermal air conditions. Popescu et al. (2007) considered four elemental transport phenomena: advective transport (airflow passes through the filter and carries the contaminants), diffusion through the boundary layer which separates the bulk air phase from the adsorbent surface, porous diffusion in the adsorbent, and adsorption desorption processes at the pore surfaces. Advection is the transport of the molecules of pollutants by airflow passing through the filter around the adsorbent. During this process, molecules of the pollutants in the gas migrate to the interior pores of the adsorbent by diffusion. This migration is accompanied by the adsorption of some pollutants' molecules which obstruct the surface pores of the adsorbent. Adsorption phenomenon is the basic process that results in air purification by the filter, but the diffusion and the advection processes define the dynamic of the adsorption.

Popescu et al. (2007) considered three terms of mass transfer in the inter-pellet air-phase in equation (27); turbulent axial dispersion, advective transports, and diffusion through the boundary:

$$\frac{dC}{dt} = D_x \frac{d^2C}{dx^2} - \frac{d(uC)}{dx} - \frac{1}{\rho_{air}} h_m A_s (C - C^*) \tag{27}$$

Equation (28) shows the mass balance within the pellet covers the accumulation in the sorbed phase and pore air phase (Popescu et al., 2007).

$$\rho_{air} D_e \left(\frac{d^2 C_p}{dr^2} + \frac{2}{r} \frac{dC_p}{dr} \right) = \rho_s \frac{dC_s}{dt} + \rho_{air} \varepsilon_p \frac{dC_p}{dt} \tag{28}$$

The link between the two equations was given by $C_p(r = R_o) = C^*$. Also Popescu et a. (2007) assumed that C_s and C_p are always in equilibrium, therefore,

$$C_s = f(C_p) \quad or \quad C_p = f^{-1}(C_s) \tag{29}$$

They considered this function a linear adsorption isotherm as follows:

$$C_s = K_p C_p \tag{30}$$

The partition coefficient, K_p, can be determined experimentally from the sorption equilibrium. It is defined as the total mass of gas adsorbed and was calculated by integrating the contaminant masses entering and leaving the filter over time (Popescu et al., 2007):

$$K_p = \frac{C_s}{C_0} = \frac{m_s / M_s}{C_0} = \frac{1}{C_0 M_s} \left(\frac{w_a}{\rho_{air}} C_0 t - \frac{w_a}{\rho_{air}} \int_0^{t_p} C(t) dt \right) \tag{31}$$

Then by decomposing the filter into n elemental cells (as shown in Figure 2- 7), and considering that the concentrations C, C^* and C_p are uniform in the same cell, and also, by using linear driving force (LDF) model, Popescu et al. (2007) transformed equations (27) and (28) into the following equations. The only unknown concentrations in these equations are C_i and C_{si}, which are the inter-pellet air-phase and the sorbed-phase concentrations in each cell, respectively.

$$\left|\begin{aligned}
&M_{a1}\frac{dC_1}{dt} = w_a C_0 - w_a(1+\varepsilon_r)C_1 + w_a\varepsilon_r C_2 - \frac{K_D K_h}{K_D + K_h}[C_1 - f^{-1}(C_{s1})] \\
&M_{ai}\frac{dC_i}{dt} = w_a(1+\varepsilon_r)C_{i-1} - w_a(1+2\varepsilon_r)C_i + w_a\varepsilon_r C_{i+1} - \frac{K_D K_h}{K_D + K_h}[C_i - f^{-1}(C_{si})] \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad for\, i = 2, n-1 \\
&M_{an}\frac{dC_n}{dt} = w_a(1+\varepsilon_r)C_{n-1} - w_a(1+\varepsilon_r)C_n - \frac{K_D K_h}{K_D + K_h}[C_n - f^{-1}(C_{sn})] \\
&M_{si}\frac{dC_{si}}{dt} = \frac{K_D K_h}{K_D + K_h}[C_i - f^{-1}(C_{si})]
\end{aligned}\right. \tag{32}$$

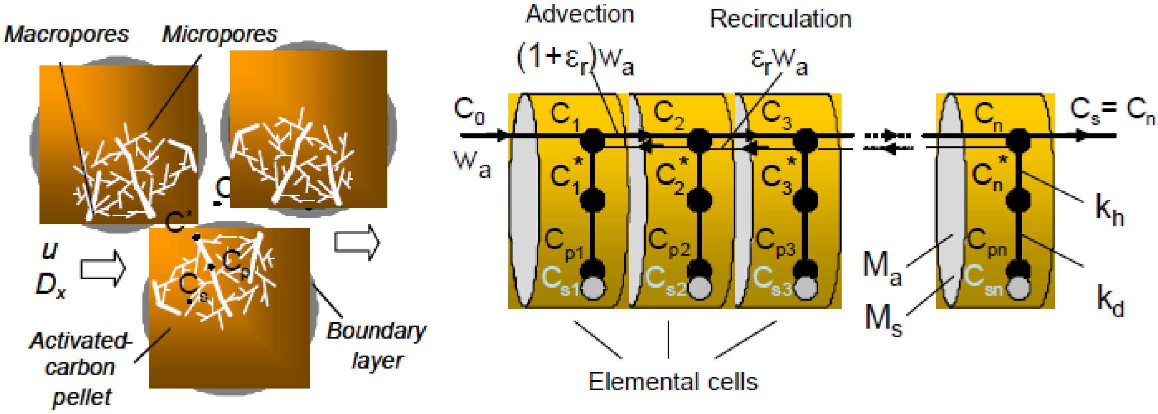


Figure 2- 7. Schematic representation of discrete filtering medium (from Popescu et al., 2007)

ε_r is the air recirculation between adjacent cells which are considered for axial turbulent diffusion and is a number between 0 to infinity; Popescu et al. (2007) defined ε_r as 0. Then, for each mass transport component they implemented the equation using the dynamic system simulation program Matlab/Simulink. The results of the model were conducted within 25% change in K_p because of the uncertainty in the partition coefficient. The developed model was capable of predicting the results for a single contaminant isolated in air within 25% change in K_p, but it is not appropriate for use in the case of a mixture of contaminants in air (Popescu et al., 2007).

As another example of air cleaner modeling, (Yu and Neretnieks, 1993)) proposed a model for a passive sheet containing activated carbon to reduce the concentration of volatile organic compounds in the air. The activated carbon sheet with 5m long, 2m height, and 2mm thick containing activated carbon particles of 1mm in diameter was studied. The porosity of the sheet was 0.4, and the particle density including pore volume was 800 kg/m^3. They provided a mathematical model. The mass balance equation for this filter was:

$$V_i \varepsilon_i \frac{dC_i}{dt} + V_i (1-\varepsilon_i) \frac{dC_{si}}{dt} = \sum_{j \neq i} k_{ij} (C_j - C_i) \tag{33}$$

The first term in the left hand side of the equation represents the mass accumulation in the pores of the compartment i, the second term indicates the accumulation in the sorbed phase and the right hand side represents the mass transfer from/to various compartments in contact with the compartment i (Yu and Neretnieks, 1993). Furthermore, the assumed adsorption isotherm is based on the Henry's Law equation, which means that the sorbed concentration c_{si} is in equilibrium with the gas phase concentration, c_i:

$$C_{si} = K_i C_i \tag{34}$$

Substituting this relation into the mass balance equation, the mass balance equation for the compartment of activated carbon particles becomes:

$$\frac{dC_i}{dt} = \sum_{j \neq i} \frac{k_{ij}}{V_i[\varepsilon_{pi} + (1-\varepsilon_{pi})C_{si'}]}(C_j - C_i) \tag{35}$$

Where, ε_{pi} is the porosity of the sorbent for compartment i. The mathematical model was solved using standard numerical Stiff solver based on Gear's method. This particular solver changes the equation into *n* ordinary differential equations. This model was developed for the filters containing activated carbon sheets. However, this model is not appropriate for filters in HVAC systems in buildings, because the only compartment in contact with the activated carbon sheet is air. This model could be used only for single contaminant in air. The major limitation of this model is that the volume of the compartments could be difficult to determine or could be defined based on a weak estimation.

Xu et al. (2011) developed another model for single contaminant in air neglecting internal diffusion. It was based on the assumption of using one pellet of adsorbent, and then, it was generalized into the bed. Although this assumption simplifies computations for the mass transfers inside the bed, it yields errors and shows low accuracy. They studied applications of dimensionless parameters that are only dependant on the environmental conditions. Therefore, this model is applicable to any environmental condition using dimensionless numbers. The partition coefficient was estimated using the linear assumption. The partition coefficient and diffusion coefficients are very important in this model. However, due to the lack of data about the partition coefficient, further research is required to determine the partition and diffusion coefficient. They applied a mass transfer model for a single porous pellet adsorption process as shown:

$$\frac{\partial (K_p C)}{\partial t} = D\nabla^2 (K_p C) \quad at\ 0 \le r \le R_o,\ t > 0 \tag{36}$$

R_o is the radius of the pellet. The initial condition and boundary conditions are:

$$C = 0\ at\ \ 0 \le r \le R_o,\ t > 0 \tag{37}$$

$$h_m (C_\infty - C) = D\nabla (KC),\ at\ \ r = R_o,\ t > 0 \tag{38}$$

$$D\nabla (K_p C) = 0,\ at\ \ r = 0,\ t > 0 \tag{39}$$

In summary, there are many models that have been developed for gaseous filters. However, no specific methodology has been established yet for obtaining the most accurate results by applying the most appropriate model. Therefore, there exists a need for a universal methodology to evaluate the available models based on their applications. Most of the gaseous filters models are used for single contaminant in the air; a situation that is not realistic for air cleaners. All the available models have been validated for single contaminant. The current study aims to develop a methodology to evaluate the available models for single contaminant cases as well as mixture cases. The proposed method is general and is applicable for different gaseous filters in different environmental conditions.

CHAPTER 3 METHODOLOGY

3.1 INTRODUCTION

Filter performance and active service life are critical information required in order to develop a service and maintenance schedule i.e, changing, charging, or regenerating the filter. Numerous mathematical models have been developed, and can be used to predict the service life of gaseous filters (Axley, 1994; Pei and Zhang, 2010; Popescu et al., 2008; Popescu et al., 2007). The output of the models is the removal performance or penetration of the filters. If the efficiency of the filter over time is provided, a maintenance schedule can be planned to change or regenerate the filter. Prior to using these models, the user must provide a number of input parameters that must be obtained experimentally. Thus, due to the various parameters and procedures that should be implemented to verify those models, the validation technique becomes complicated. Therefore, a systematic approach is needed for validating these models. A methodology is proposed for the validation of gaseous filter models and for quantifying the corresponding input parameters. Figure 3- 1 presents the steps to be followed for determining the required input parameters and validating the model. The proposed methodology is explained in details in this chapter. An existing model is chosen for implementing the suggested methodology, its required parameters are calculated and defined, and the model is validated against the experimental data.

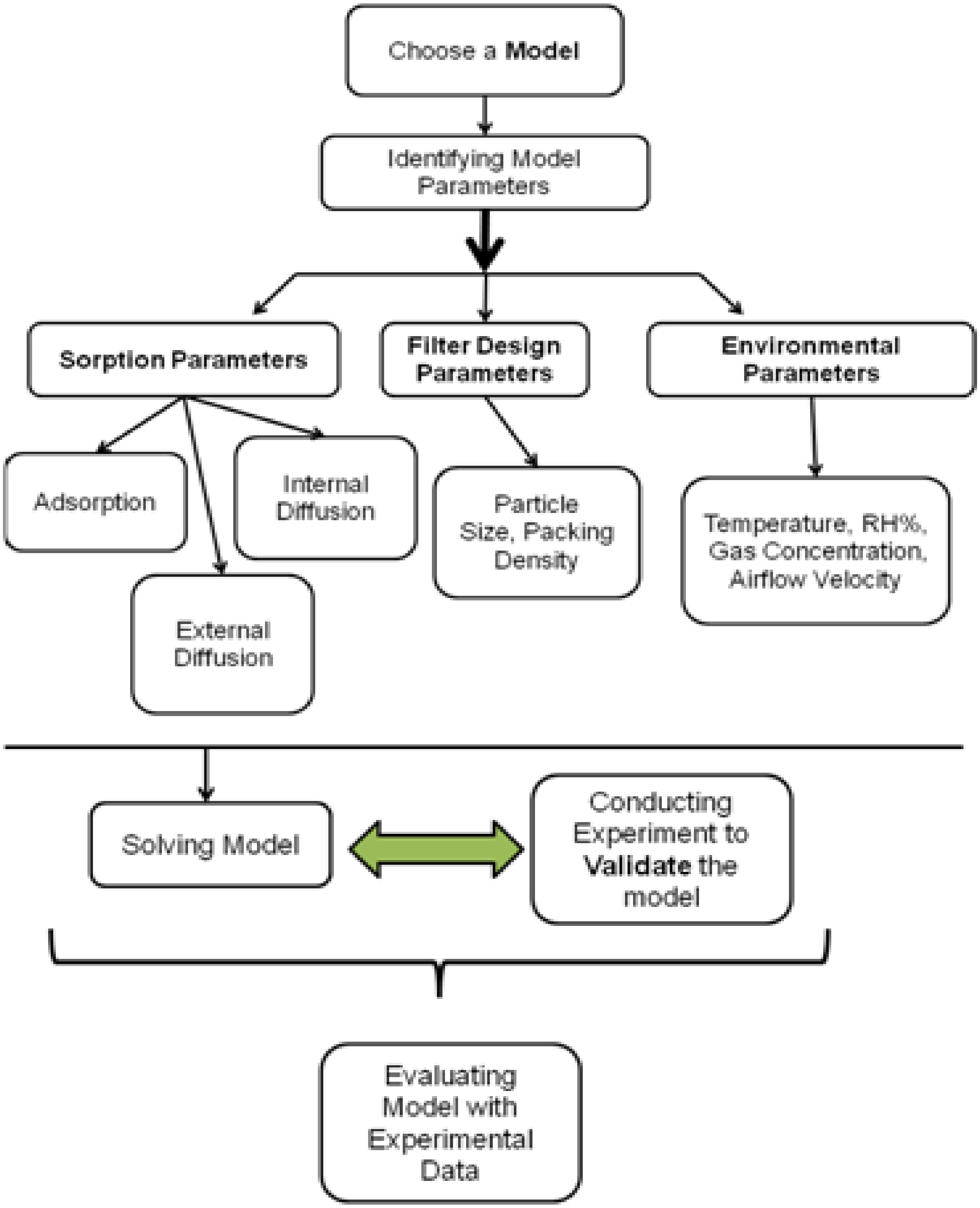


Figure 3- 1. Validation Method

3.2 CHOOSING A MODEL

Several models have been developed to predict the removal efficiency of sorption gaseous filters. The modeling has been implemented based on the physical phenomena occurring in gaseous filters using the fundamentals of mass conservation. As the time passes, the gaseous filter is saturated and its efficiency diminishes. Thus, a contaminant mass balance equation can be written for the filter to describe the transfer of the contaminants from air to the sorbet media in the filter by diffusion and adsorption. The present model is based on the four mentioned elemental transport phenomena: advection, external diffusion, internal diffusion, and adsorption.

Figure 3- 2-a shows a filter containing some media as a sorbent. If a boundary layer is assumed to exist around the filter in the bulk air-phase, a mass balance equation can be written for the contaminants in the air. It is assumed that the incoming air contaminant concentration, or the upstream concentration, is constant. As the contaminants transfer from the air to the sorbent media, the contaminant concentration of the effluent of the filter diminishes, this specific concentration is referred to as the downstream concentration. Thus, a contaminant mass balance equation can be written for the filter. Contaminants going through the filter are adsorbed in the filter or exit as the effluent of the filter. Therefore, the mass balance equation includes the contaminants upstream, downstream and inside the filter.

Figure 3- 2-b displays one pellet of granular filter's sorbent inside the packed-bed in the filter. A hypothetical layer around the pellet is assumed in order to write the contaminant mass balance equation inside the filter. As shown in Figure 3- 2-b, the contaminant is

transferred from the bulk phase to the hypothetical layer and then is adsorbed and diffused in the pellet.

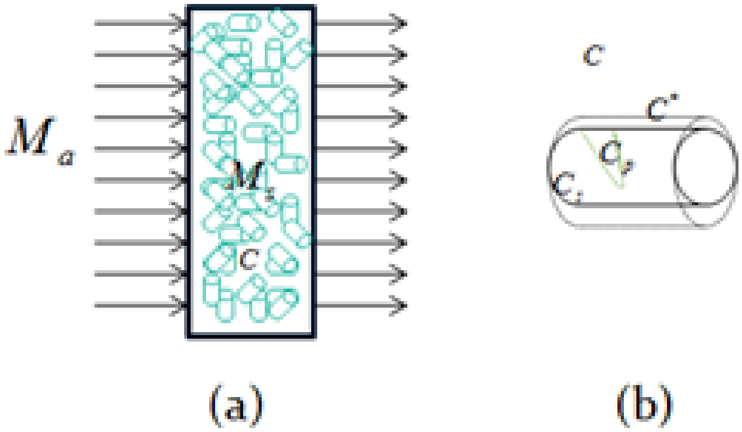


Figure 3- 2. a) Filter containing sorbent, b) One sorbent pellet

The contaminant mass balance around the filter or around the pellets infers that the summation of the inlet, the outlet, the sink, and the source of the contaminant in the filter equals to the concentration change through the filter or inside the pellets in the filter. Or,

In – Out + sink/source = Concentration Change Rate

This mass balance equation can be written for sorbent pellets and for the whole filter. It yields two fundamental equations that forms the basis of the modeling. The output of the model is the concentration change in time and is used to obtain the performance and lifetime of a filter.

3.2.1 Model Development

Figure 3- 3 presents the convective contaminant transfer from the air to the boundary layer of the pellets inside the filter. A hypothetical layer (boundary layer) is assumed

around the pellets of the sorbent media. Therefore, convection is assumed to occur between the bulk air phase inside the filter and the boundary layer of the pellets. Equation (40) presents the mass of transferred contaminants by convection. The total contaminant transfer through the filter and the convection from the bulk air to the adsorbent's boundary layer equals to the rate of concentration change in the filter.

$$w_a C - w_a C_0 + K_h (C - C^*) = -M_a \frac{dC}{dt} \tag{40}$$

where $K_h = \rho_{air} A_s h$ represents the boundary layer mass transfer rate.

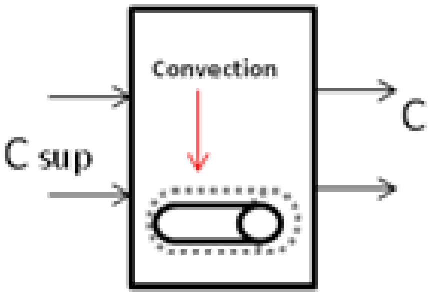


Figure 3- 3. Convection inside a filter to one pellet of sorbent media

To find the hypothetical concentration C^* in equation (40), the contaminant transfer is explained by a mass balance equation for the near surface air-phase. The transferring of a contaminant occurs between the hypothetical layer and inside the pellets. Contaminants diffuse from the hypothetical layer into the pores of the pellets. Therefore, the rate of contaminant concentration change in the pellets (the solid phase) is equal to the rate of contaminant diffusion from the hypothetical layer to the pores. Thus, if no chemical reaction takes place between the solid phase and the fluid phase, the following mass balance equation can be written for the pore phase:

$$K_D(C^* - C_p) - M_s \frac{dC_s}{dt} = 0 \tag{41}$$

Where, C_p is the air phase concentration within the pores of the pellets and is in equilibrium with the sorbed phase concentration (contaminant concentration in the solid phase, C_s), and $K_D = 15M_s D_e K_T / r_p^2$ characterizes the pore diffusion rate (Ruthven, 1984).

A contaminant mass balance is written for a pellet to find the pore phase concentration in the pellets as is shown in Figure 3- 4. The contaminants that have been convected from the bulk to the hypothetical layer are diffused into the pores. Therefore, the diffusion rate from the hypothetical layer to the pores is equal to the convection from the bulk to the hypothetical layer.

$$K_D(C^* - C_p) - K_h(C - C^*) = 0 \tag{42}$$

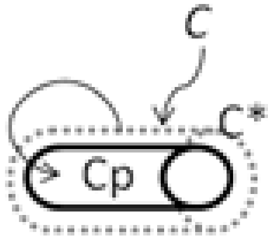


Figure 3- 4. Contaminant's transfer inside a pellet

Directly, after finding C^* from equation (42), and substituting it into equations (40) and (41), the two following equations are obtained:

$$w_a C + \frac{K_h . K_D}{K_h + K_D}(C - C_p) + M_a \frac{dC}{dt} = w_a C_0 \tag{43}$$

$$\frac{K_D K_h}{K_D + K_h}(C - C_p) = M_s \frac{dC_s}{dt} \tag{44}$$

Equations (43) and (44) are the basic mass balance equations for a gaseous filter. The current study objective aims to use the proposed methodology to validate a gaseous filter model experimentally. The inlet or upstream concentration C_0, is required for solving these two equations, which yields outlet concentration, C or C_{down}, as a function of time. The removal efficiency of the filter is then calculated using equation (45).

$$\textit{removal efficiency} \ \ (\%) = \frac{C_{up} - C_{down}}{C_{up}} \times 100 \tag{45}$$

Once the required parameters are obtained for solving equations (43) and (44), a set of experiments is conducted. The experimental results are compared with the results of the numerical model, validating the applicability of the model.

There are three unknown concentrations in equations (43) and (44) namely, the air phase concentration, the sorbed phase concentration, and the pore phase concentration. One more equation is needed to be able to complete and solve the model. Assuming equilibrium between the air phase and the sorbed phase at a constant temperature, adsorption isotherm is considered between the sorbed phase concentration and the air. Therefore, using the appropriate adsorption isotherm from Table 2- 2, allows computing the actual concentrations (C_s) as function of the air phase concentration (C). Therefore, there are two unknown concentrations in two equations (43) and (44) which will be determined by solving the equations using MATLAB SIMULINK.

3.3 FINDING MODEL PARAMETERS

A number of parameters are needed as input to the model and can be classified into three groups. The sorption parameters, the filter design parameters, and the environmental parameters are three types of parameters that affect the removal performance of the filters and as a result, the lifetime of the filter. Therefore, they should be accurately determined to increase the confidence level in the model prediction capability.

3.3.1 Sorption Parameters

3.3.1.1 External diffusion

The contaminant mass transfer (w) through the boundary layer is approximated from boundary layer theory as shown in equation (22). In this equation there are some parameters needed to be identified; the external mass transfer diffusion coefficient, the surface area of the sorbent that is exposed to the contaminated air, and the density of the air. The external mass transfer coefficient is determined using the appropriate correlation of Sherwood number as described in Chapter 2. In the present study, the Wakao-Funzakri correlation was employed (equation 5).

3.3.1.2 Internal diffusion

Knudson, molecular, and effective diffusivity can be estimated from equation (14), (10), and (15), respectively.

3.3.1.3 Adsorption

A set of experiments is carried out to find the constant parameters of adsorption isotherm based on the adsorption isotherm models in Table 2- 2.

3.3.1.3.1 Isotherm Experimental Setup

Figure 3- 5 shows the schematic of the experimental set up for the estimation of the isotherm constant parameters for each gas phase contaminant. The instruments used in this set-up include: two gas detectors, an injector, desiccators, an airflow controller, and a 5-cm diameter cylindrical filter with 2-cm length. The filter was filled with 2 *cm* of granular activated carbon. Activated carbon was chosen as a media for the filter in the present study, because it has a significant ability to adsorb VOCs from the air. As shown in the figure, air is led to the airflow controller. The latter controls the air flow rate at 30 *lit/min*. The residence time for this filter is calculated and found to be 0.08 *s*. In general, the contact time between gas and mediums should range between 0.02 to 0.2 *s* to ensure an effective removal process (Holmberg et al., 1993). Then, air passes through desiccators to be dehumidified and is then mixed with selected gases (contaminants). The contaminants are injected into the dry air with an injector at a constant injection rate. The contaminant concentration is measured by two gas detectors at the downstream and upstream. They were calibrated before initiating the test.

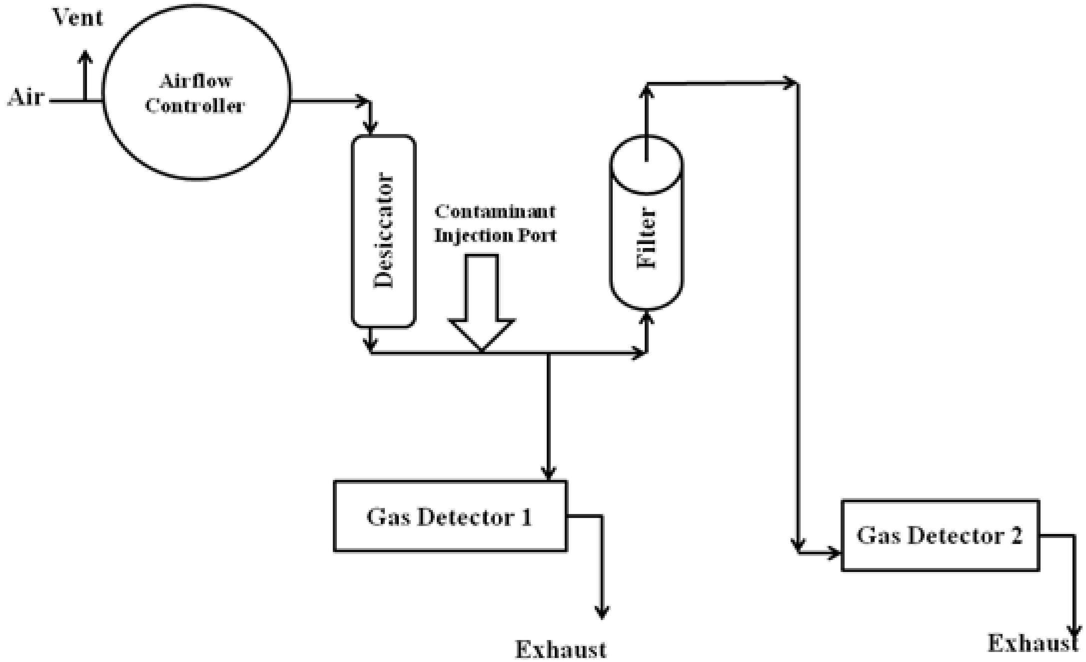


Figure 3- 5. Experimental set up for adsorption isotherm test

Knowing the airflow rate and the density of the pollutant, the injection rate is calculated.

$$\textit{Injection Rate } [\mu l/min] = \textit{Flowrate } [m^3/min] \times \textit{concentration } [mg/m^3] \times (1/\rho)[m^3/mg] \times 10^9$$

Constant upstream concentration is injected continuously until the filter is saturated. When the downstream concentration becomes equal to the upstream concentration, the filter is deemed saturated and the test is stopped. At this point, the removal efficiency of the filter is zero. The removal efficiency is calculated at all times during the test using equation (45).

Now, the maximum capacity of the filter is determined by measuring the amount of contaminants adsorbed on the filter. Therefore, the adsorption isotherm constant parameters for the pollutants are calculated.

Similarly, moisture exists in the air that is adsorbed to the filter's media, and usually affects the removal performance of the filter. Accordingly, the maximum amount of moisture that a filter can adsorb should also be determined experimentally following the same procedure as that implemented for the contaminants. The only difference is that instead of injecting different contaminant concentrations into the air, different humidity levels are introduced. For this purpose, the air passes through a bottle of water, and a valve is connected to the tubes to control the moisture level. In other words, it is assumed that moisture is another contaminant in the air. The gas detectors can monitor the concentration of the moisture based on the dew point temperature of the humid air. Psychrometric chart provides relative humidity and concentration of the moisture based on its dew point temperature (ASHRAE 2005).

The contaminant concentration is related to the removal capacity of the filter. Removal capacity is a parameter used for evaluating the effectiveness of the filter. Removal capacity is the percentile fraction of the total adsorbed mass of the contaminants over the total sorbent media weight (Haghighat et al., 2008). The capacity that is used as a contaminant concentration in a solid, C_s, is calculated using equation (46). This equation represents the ratio of the total mass of the contaminant that is adsorbed on the sorbent to the total mass of activated carbon, which was used in the filter. The capacity is calculated at each time step, and the total capacity is calculated by integrating over the duration of the experiment. This capacity represents the contaminant concentration in the sorbed phase.

$$C_s = \frac{\int_0^t (C_{up} - C_{down}) \times Q \times dt}{M_s} \tag{46}$$

C and C_s allow computing the isotherm parameters. Using Langmuir isotherm, for example, equation (17) is rewritten into a linear equation as equation (47) , then the experimental results are substituted into equation (47), and the Langmuir isotherm constant parameters, C_{S0} and K_L, are calculated.

$$\frac{1}{C_S} = \frac{1}{K_L.C_{S0}.C} + \frac{1}{C_{S0}} \tag{47}$$

Isotherm constant parameters are calculated individually for each contaminant. However, air contains a mixture of contaminants. The extended Langmuir isotherm equation is used to find the Langmuir isotherm constants for a mixture of contaminants. Equation (48) is written for each component of the mixture. *i* represents the specific contaminant , and *j* represents all the pollutants in the air.

$$C_{si} = \frac{K_i.C_{s0i}.C_{pi}}{1 + \sum_{j=1}^{n} K_j.C_{pj}} \tag{48}$$

3.3.2 Filter Design Parameters

The next step consists of determining the geometric parameters of the filters and the sorbent exposed surface area. Relevant geometric parameters include particle size and packing density. Particles used as media in the filter can be spherical, cylindrical, or unshaped. Therefore, a hydraulic diameter is used for the non spherical particle shapes. The hydraulic diameter is defined as:

$$D_H = \frac{4A_p}{P_p} \tag{49}$$

The particle diameter is used to compute the surface area. However, the exposed surface area of the sorbent is different from the total surface area. Packing density needs to be determined in order to find the actual exposed surface area. The packing density is defined as the ratio of total mass of the sorbent (m_{total}) to the volume of the filter (V_{total}). The total area of the sorbent that is exposed to the bulk contaminated air can be calculated using the number of particles, the area of one pellet, and the number of particles as follows:

$$total\ \ \exp osed\ \ surface\ \ Area = \frac{(\frac{m_{total}}{V_{total}})}{sorbent's\ density} \times No.\ of\ \ pellets \times Area\ \ of\ \ one\ \ pellet$$

3.3.3 Environmental Parameters

Relevant environmental parameters that affect the filter's performance include air temperature, relative humidity, contaminant type and concentration, and airflow velocity. The indoor air temperature and relative humidity depend on the season and the operation of the air-handling units.

3.4 MODEL VALIDATION

It is necessary to validate the model against experimental data. A set of experiments are required for model validation. Figure 3- 6 shows a schematic diagram of the proposed test set up. This test is almost the same as the ones conducted for the isotherm constant estimation, but in the model validation test, air passes through a humidifier. A multi-gas detector, GC/MS, was used to monitor the downstream and the upstream concentration.

These values were used to determine removal efficiency of the filter using equation (45). Breakthrough time is also another factor used in model validation. Penetration or breakthrough is calculated as the ratio of the downstream concentration to the upstream one.

$$P_t = \frac{C_{down,t}}{C_{up,t}} \tag{50}$$

The model validation is done by comparing the measured penetration or breakthrough time with the one predicted with the model.

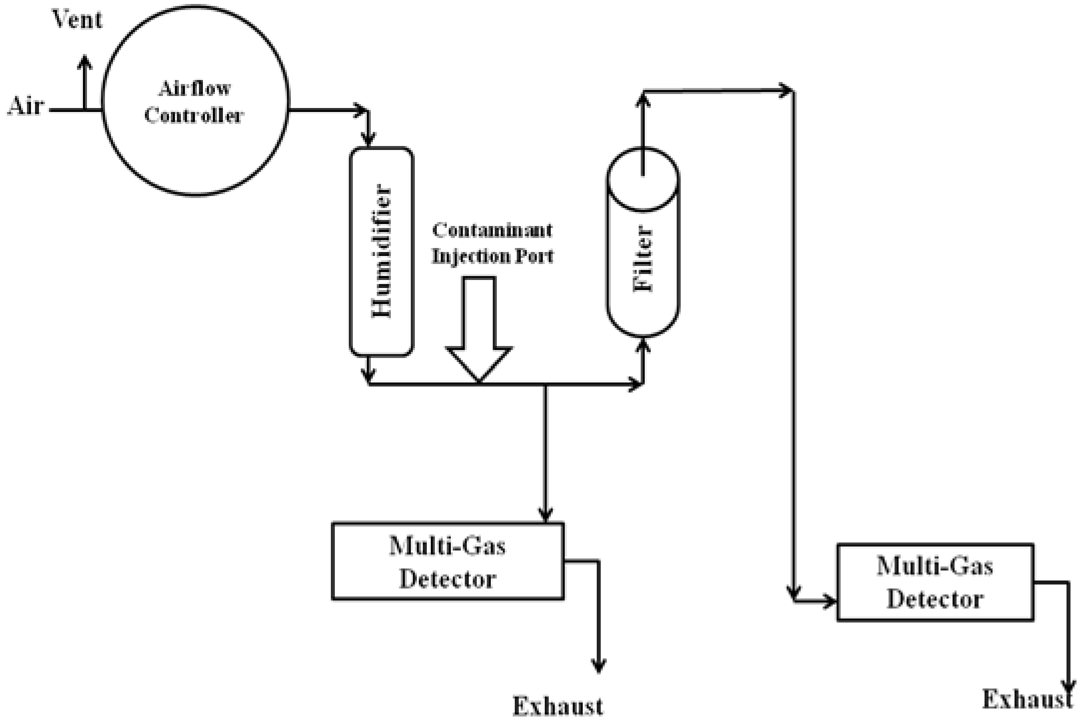


Figure 3- 6. Experimental set up for model validation

3.5 CASE STUDY

As a case study, the application of the proposed methodology was verified for an available model. Herein, the granular activated carbon as the adsorbent. The filter was a cylinder with a 2 inch diameter filled with 25 g of cylindrical granular activated carbon. On the other hand, two compounds were considered as the gaseous pollutants; Methyl Ethyl Ketone, and n-hexane. Their properties are presented in Table 3-1.

Table 3- 1. Properties of selected pollutants

Chemical Category	Chemical Name	Molecular Formula	M.W	BP (C)	VP at 20 (mmHg)	Solubility in water at 20 C (g/l)	Polarity
Alcane	n-hexane	C_6H_{14}	86.2	69	132	Insoluble	Non-Polar
Ketone	MEK	C_4H_8O	72.1	80	78	290	Polar

3.5.1 Langmuir Isotherm Test for Case Study

The Langmuir adsorption isotherm constant parameters of MEK and n-hexane were measured experimentally. The tests were conducted with an experimental setup as shown in Figure 3- 5. Five different concentrations of MEK between 15-100 *ppm* (15, 30, 50, 70, and 100 *ppm*) and n-hexane between 30-300 *ppm* (30, 60, 100, 200, and 300 *ppm*) were introduced to the clean dry air (upstream line) at a flow rate of 30 *lit/min* at 23±1˚*C*. The injection rates for MEK and n-hexane are presented in Table 3- 2 and Table 3- 3. For each concentration, the test was carried out until the filter was saturated. Consequently, the maximum amount of a contaminant that a filter could adsorb was determined and corresponded to the filter saturation and contaminant concentration. This amount divided by the mass of the filter's media represents the concentration of the contaminant in the solid phase (sorbent's media). This amount presents C_s in the equation (46). Thus, five different C_s corresponding to the C (15, 30, 50, 70, 100 *ppm* for MEK and 30, 60, 100, 200, 300 *ppm* for n-hexane) were calculated.

Table 3- 2. Injection rates for MEK

Conc. (*ppm*)	Conc. (*mg/m*^{3})	density (*g/ml*)	airflow rate (*lit/min*)	Mass flow rate (*g/min*)	Volume flow rate (*µl/min*)
15	44.35	0.805	30	0.0013	1.6531
30	88.70	0.805	30	0.0027	3.3061
50	147.84	0.805	30	0.0044	5.5102
70	206.97	0.805	30	0.0062	7.7143
100	295.68	0.805	30	0.0089	11.0204

Table 3- 3. Injection rates for n-hexane

Conc. (*ppm*)	Conc. (*mg/m*^{3})	density (*g/ml*)	airflow rate (*lit/min*)	mass flow rate (*g/min*)	volume flow rate (*µl/min*)
30	105.90	0.655	30	0.0032	4.8519
60	211.80	0.655	30	0.0064	9.7037
100	353.00	0.655	30	0.0106	16.1729
200	706.00	0.655	30	0.0212	32.3458
300	1059.00	0.655	30	0.0318	48.5186

3.5.2 Validation Tests for the Case Study

The experiments described previously were carried out at four conditions. For the first two conditions, only one contaminant was present in the dry air. In the first phase, 100 *ppm* of MEK, and the in the second phase, 100 *ppm* of n-hexane was injected in the dry air. The downstream concentration was measured by a photo-acoustic gas detector, INNOVA. The upstream concentration was monitored by another photo-acoustic gas detector, B&K.

In the third and fourth phases, both MEK and n-hexane were injected at concentration of 100 *ppm*. The mass balance equation between liquid phase and gas phase was written to convert the volume of the injected liquid (contaminant in liquid phase) to the contaminant concentration in gas phase:

$$\frac{I \times \rho_c}{Q} = C = ppm \times M \times \frac{P}{8.314 \times (273.15 + T)} \tag{51}$$

Table 3- 4 shows the calculated injection rate for each contaminant in the single-contaminant tests (case 1 and 2), and the total injection rate in the mixture-of-contaminants tests (case 3 and 4), at 30 *lit/min* airflow rate.

Table 3- 4. Calculated injection rates for each compound and mixture of compounds

VOC	Conc (*ppm*)	Conc (*mg/m³*)	Mass injection rate (*g/min*)	Density (*g/ml*)	Volume injection rate (*µl/min*)
MEK	100	295.71	0.0012	0.81	1.47
n-hexane	100	353.54	0.0014	0.65	2.16
Total	100	649.25	0.0026	-	3.63

Therefore, for 20 *ml* of contaminant mixture, the required calculated amount of MEK and n-hexane are:

Volume of MEK needed (*ml*) = 20 *ml* × (1.47 *µl/min*) / (3.63 *µl/min*)

Volume of n-hexane needed (*ml*) = 20 *ml* × (2.16 *µl/min*) / (3.63 *µl/min*)

The mixture was injected at rate of 3.63 *µl/min*. The third test was conducted with dry carrier gas, and the fourth one was done in 50% relative humidity. The downstream and upstream concentrations were monitored with a multi-gas detector, gas chromatography mass spectrometry (GC/MS). The breakthrough profiles of these four phases were estimated both experimentally and numerically.

3.5.3 Calibration Method for Single Gas Detectors

The schematic setup of the calibration is presented in Figure 3- 7. Both gas analyzers were calibrated separately for MEK and n-hexane. Gas detectors were calibrated for MEK approximately between 0-80 *ppm*, and for n-hexane between 0-200 *ppm*. Dry air was used as carrier gas and the airflow rate was adjusted at 30 *lit/min*. Contaminants were injected into the air stream with a syringe pump. The injection rates for each concentration of the contaminants were calculated using equation (51). The single gas detectors readings were used to derive their calibration curves for each compound. The curves and their equations are presented in Figure 3- 8 and Figure 3- 9.

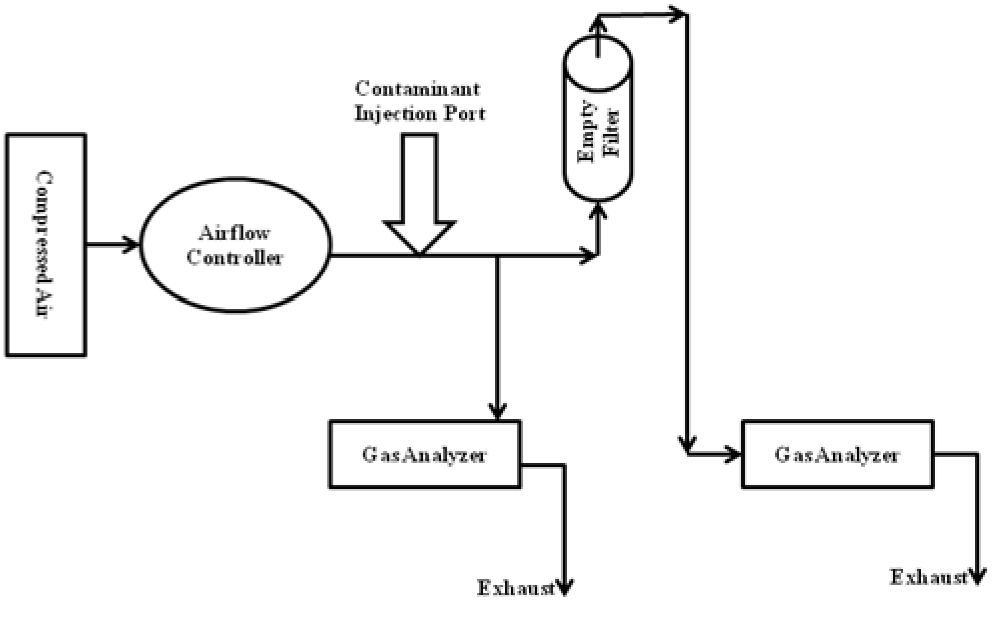


Figure 3- 7. Schematic setup for calibration of single gas detectors

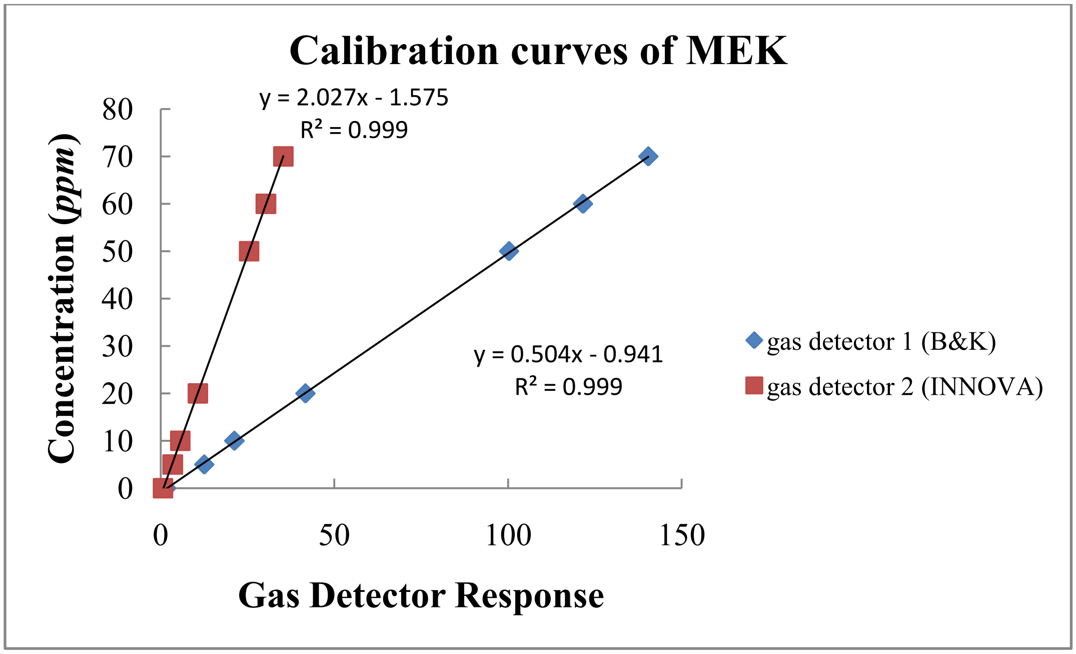


Figure 3- 8. Calibration curves of single gas detectors for MEK

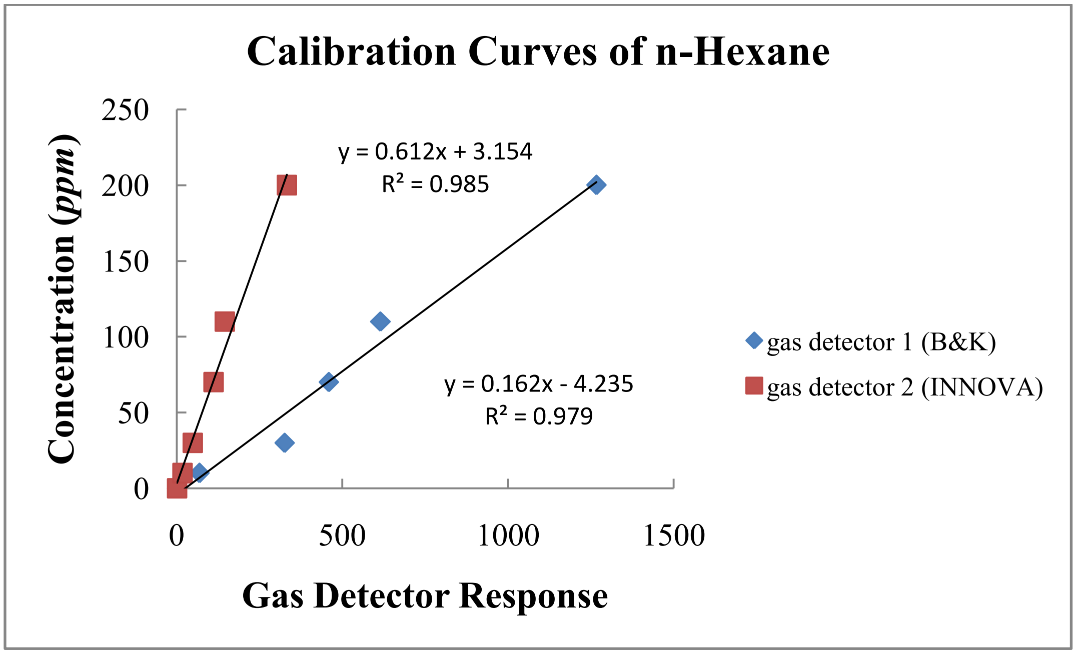


Figure 3- 9. Calibration of single gas detectors for n-hexane

3.5.4 Calibration Method for Multi-Gas Detectors

A gas chromatograph/Mass spectrometer (GC/MS) coupled with a Thermal Desorber (Perkin Elmer model TurboMatrix 350) was used for analyzing the contaminants concentration. The Thermal Desorber (TD) collects gas samples, and GC/MS analyzes the samples. Sampling is done using sampling tubes (Air Toxics stainless steel sampling tubes). Before starting the calibration, sampling tubes were preconditioned by passing a flow of 50 *ml/min* of helium (UHP 5.0) through the sampling tubes for 30 minutes at 300°C. Besides, Turbo Mass software was used to control the GC/MS and TD system on a laboratory personal computer. A method was developed for TD to collect upstream and downstream samples. Then, GC/MS analyzed the samples to determine the contaminants and the concentration of contaminants for each pollutant in the air.

Based on Figure 3- 7, the mixture of contaminants with concentrations ranging between 0-150 *ppm* for each compound was injected into the upstream line and the response of GC/MS (gas analyzer) was read. Both upstream and downstream sampling analyzing were conducted by GC/MS. The calibration result is given in Figure 3- 10.

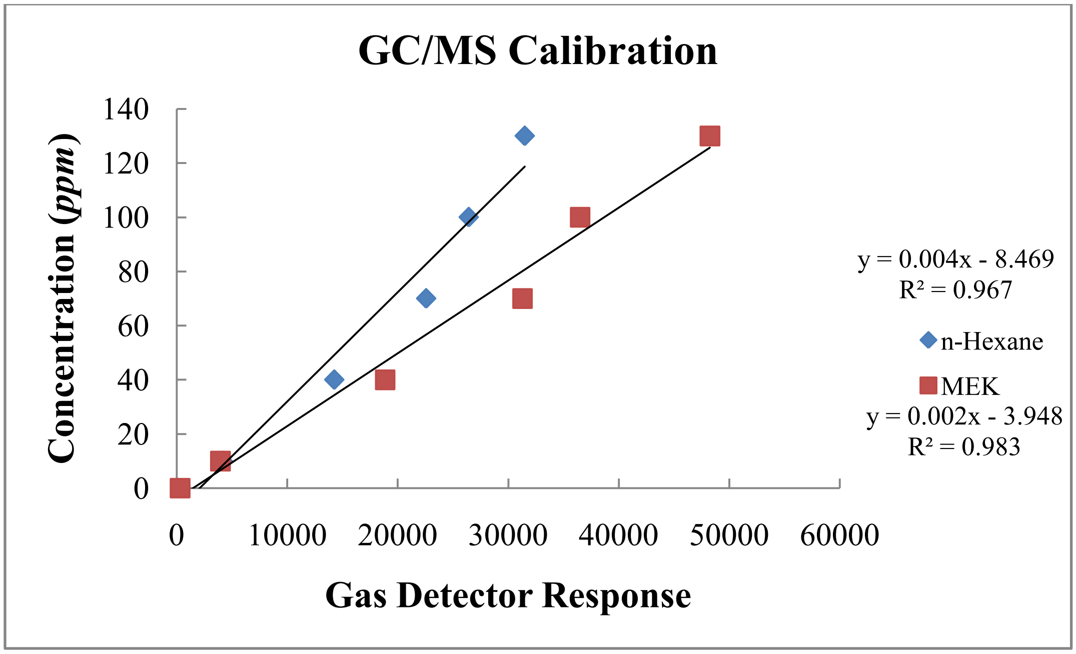


Figure 3- 10. Calibration curve of GC/MS for MEK and n-hexane

CHAPTER 4 RESULTS AND DISCUSSION

4.1 INTRODUCTION

In this chapter, the quantified parameters for the case study are presented. Furthermore, the breakthrough profile of the contaminants used in the case has been compared based on the results of the modeling and the experiment. Therefore, the model has been evaluated for the four mentioned conditions: single contaminant (MEK) in dry air, single contaminant (n-hexane) in dry air, mixture of MEK and n-hexane in dry air, mixture of MEK and n-hexane in air with 50% relative humidity.

4.2 ADSORPTION ISOTHERM

4.2.1.1 Langmuir isotherm constants

For each injected concentration in Table 3- 2 and Table 3- 3, the corresponding sorbed phase concentration (capacity, C_s) was calculated by equation (46), and the maximum capacities were fitted to the Langmuir isotherm model (equation (17)). Then, the isotherm constants were determined by regression (equation (47)). The results are shown in Figure 4- 1 and Figure 4- 2.

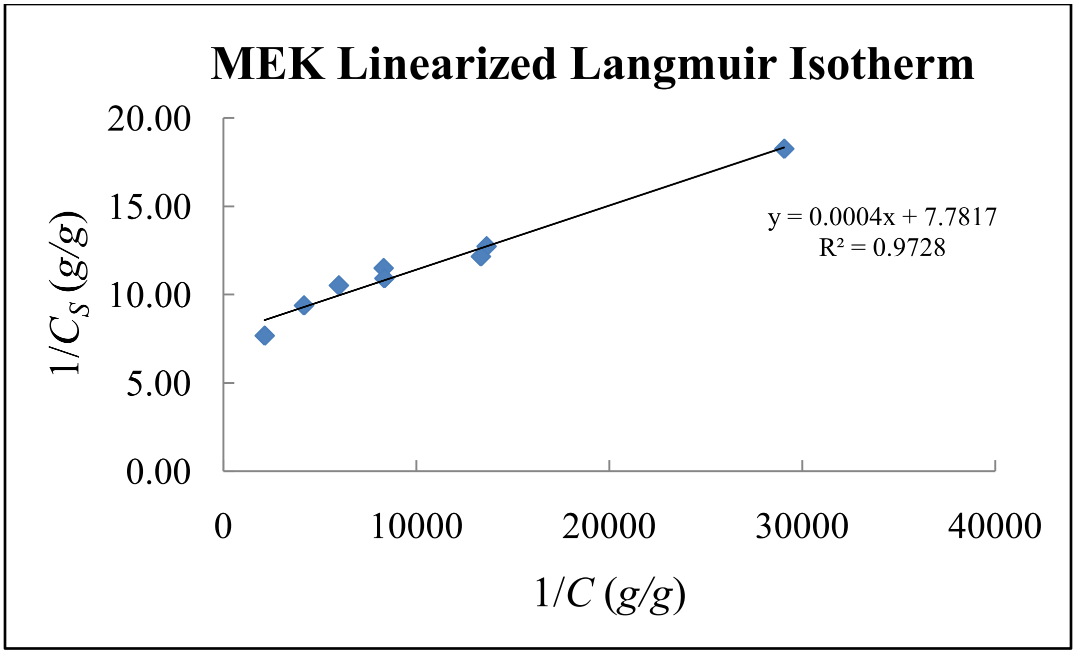


Figure 4- 1. MEK Langmuir Isotherm

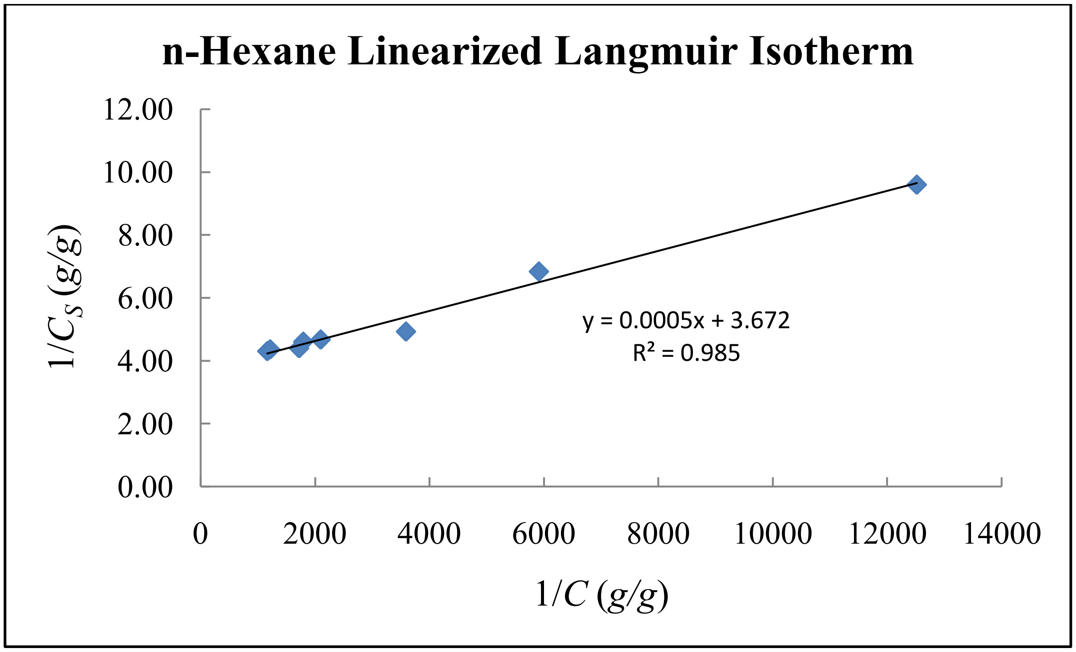


Figure 4- 2. n-hexane Langmuir Isotherm

Besides, Langmuir isotherm constants for water vapor were calculated as displays in Figure 4- 3.

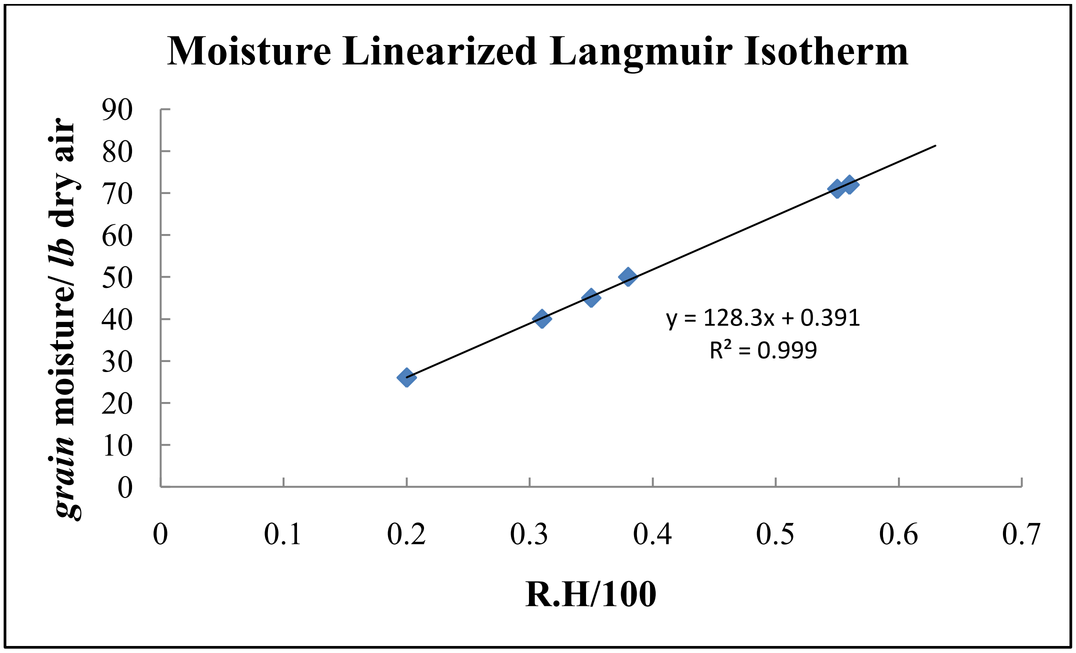


Figure 4- 3. Moisture Langmuir Isotherm

The calculated Langmuir isotherm constants, K_L and C_{s0} for MEK, n-hexane, and moisture are presented in Table 4- 1.

Table 4- 1. Test results and conditions for adsorption isotherm

Pollutant	K_L *(g/g)*	C_{S0} *(g/g)*	Media	Airflow Rate (*lit/min)*
MEK	19531	0.128	25 *g* A.C	30
n-hexane	7407	0.272	25 *g* A.C	30
moisture	0.013	10000	25 g A.C	30

4.2.1.2 Diffusion parameters

For internal diffusion, the Knudson diffusivity was calculated using equation (14) for each compound, and the molecular diffusivity was extracted from the literature (Kwon et al., 2003). The molecular diffusion and Knudson diffusion and effective diffusivity were employed to calculate equation (15) for each compound. The results are shown in Table 4- 2.

For external diffusion, the external mass transfer coefficient (convection coefficient) is calculated using a Sherwood correlation, equation (15). The mass transfer coefficients obtained for both MEK and n-hexane are tabulated in Table 4- 2.

Table 4- 2. Diffusion Parameters

Compound	$D_m\ (m^2/s)$	$D_k\ (m^2/s)$	$D_e (m^2/s)$	$G (kg/m^2.s)$	R_p (mm)	h (m/s)
MEK	$8.210e^{-6}$	$3.09e^{-4}$	$1.97e^{-6}$	0.3	1.25	0.047
n-hexane	$8.1e^{-6}$	$2.83e^{-4}$	$2e^{-6}$	0.3	1.25	0.046

Using the obtained input, the simulation was carried out using MATLAB SIMULINK.

4.3 EXPERIMENTAL RESULTS

4.3.1. Single Contaminant Injection

Figure 4- 4 shows the experimental breakthrough curve of 100 *ppm* n-hexane, in dry air condition. The filter reached 50% breakthrough in 8.56 hours and reached 80% breakthrough in 10.88 hours.

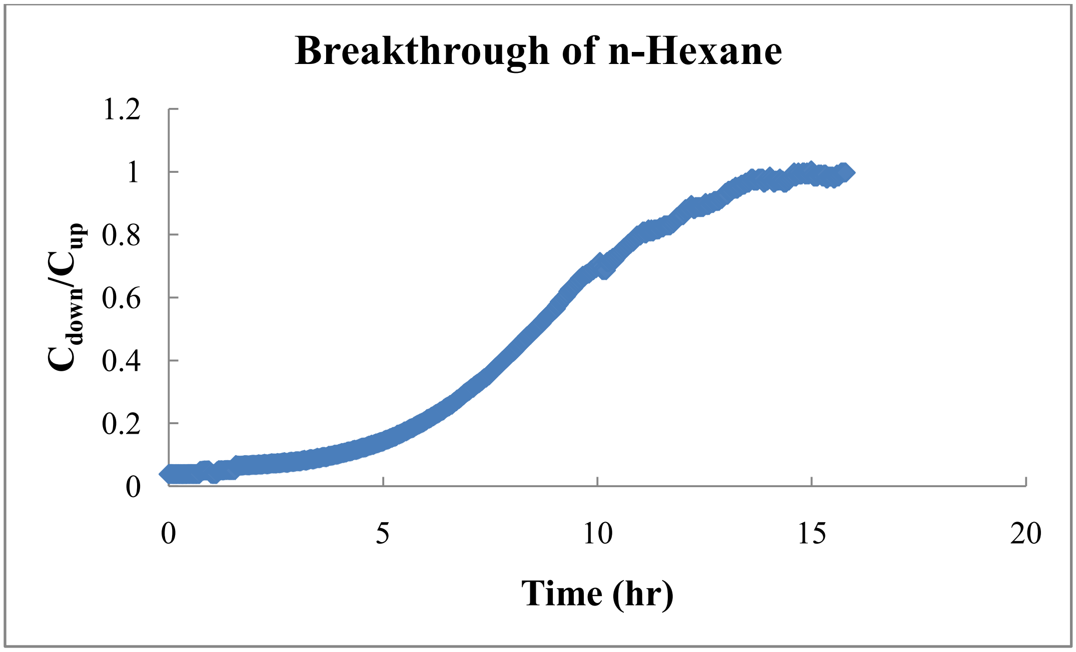


Figure 4- 4. Breakthrough time of 100 *ppm* n-hexane in dry condition

Figure 4- 5 presents the breakthrough curve of 100 *ppm* MEK in dry air condition. The filter reached 50% and 80% breakthrough in 5.25 hours and 7.3 hours, respectively.

Figure 4- 4 demonstrates that it took 15.5 hours for the filter to be saturated when it was challenged with 100 *ppm* n-hexane, while Figure 4- 5 shows that it took 12.5 hours when the filter was challenged with 100 *ppm* MEK. This is because the heavier compound (n-hexane) had more affinity to be adsorbed on the activated carbon rather than the lighter one (MEK), and the carbon had a stronger bond with n-hexane rather than MEK. As presented in Table 3- 1, n-hexane has a molecular weight of 86.2, while MEK has a molecular weight of 72.1. Therefore, the lifetime of a filter is longer for pollutants with higher molecular weight.

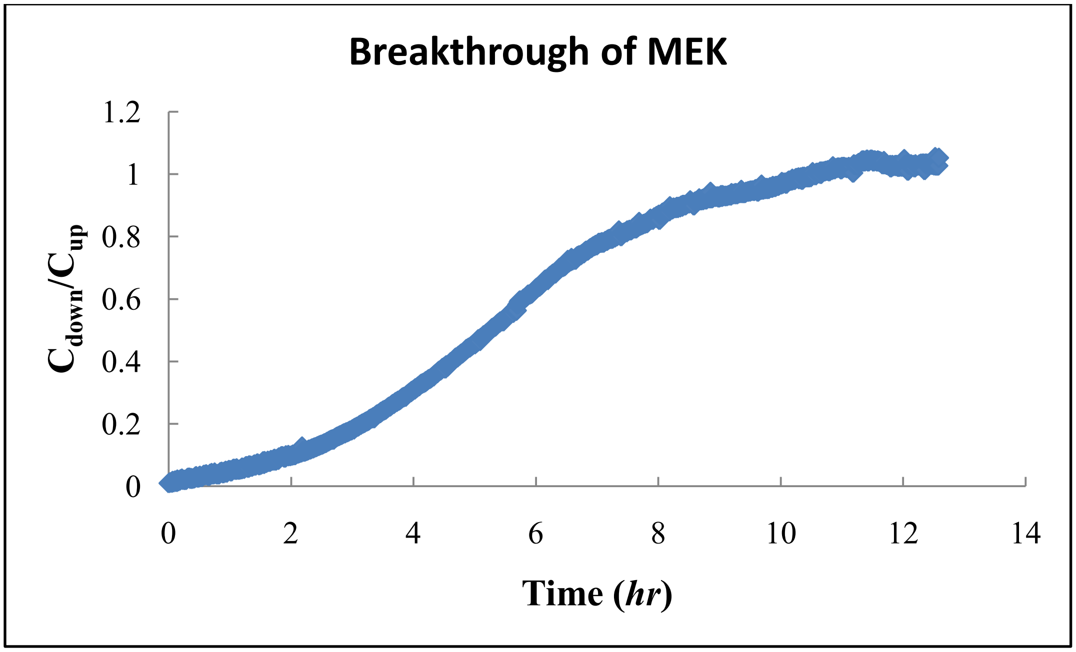


Figure 4- 5. Breakthrough time of 100 *ppm* MEK in dry condition

The impact of a mixture of pollutants was investigated by injecting a mixture of contaminants in the air. The tests were conducted at two different conditions; dry air, and humid air. Furthermore, the tests were carried out at the same condition twice to assure their repeatability. Taking Figure 4-6 into account, the relative error for the two tests at the same condition in dry air at 50% breakthrough and 80% breakthrough was less than 5%.

Figure 4-6 presents the breakthrough profile of MEK and n-hexane when a mixture of contaminants was injected. This figure demonstrates that the downstream concentration of the lighter compound increased quickly and exceeded the upstream concentration, and finally decreased to the upstream concentration. On the other hand, the breakthrough of the heavier compound increased slowly. Afterward, the downstream concentrations of

MEK and n-hexane reached the same level as their upstream concentrations and remained stable until the end of the adsorption of the heavier compound.

The results of the mixture tests (Figure 4-6 and Figure 4-7) indicate that when the filter is challenged with a mixture of contaminants, the compounds compete to be adsorbed on the sorbent. Here, n-hexane is heavier than MEK and has a higher affinity to be adsorbed on the filter. Therefore the lighter compound (MEK) reached its 100% breakthrough faster than n-hexane. Meanwhile, the heavier compound replaced the adsorbed lighter compound, resulting in the forced-desorption of MEK. Therefore, the MEK concentration downstream exceeded its upstream one due to the contribution of the displaced adsorbed MEK by n-hexane.

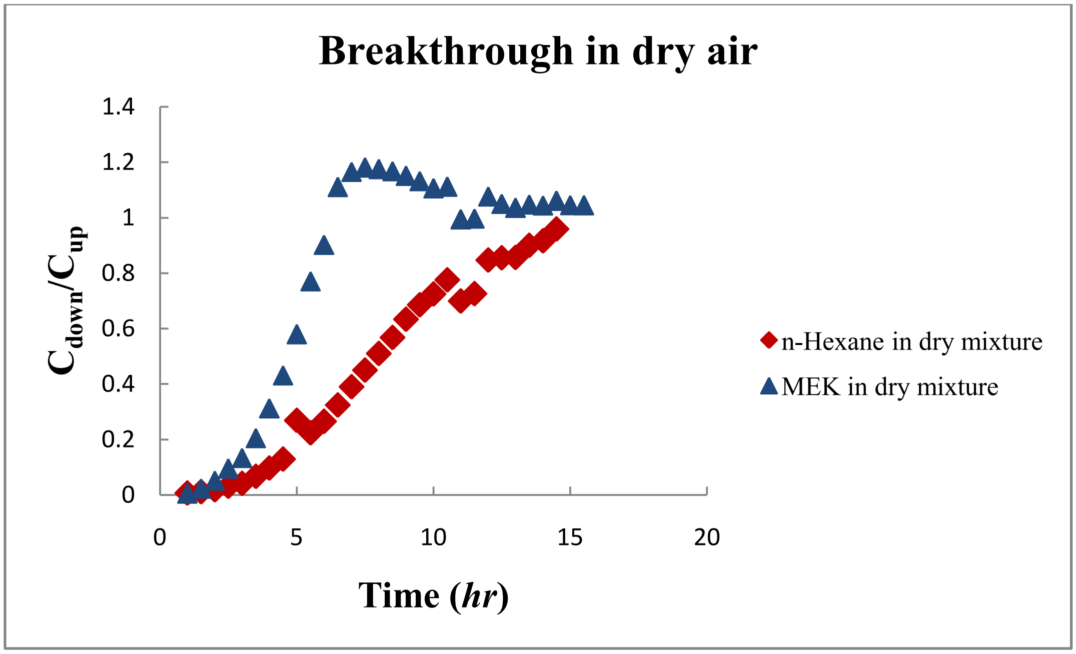


Figure 4- 6. Breakthrough curve of MEK and n-hexane in dry condition

4.3.3 Mixture of Contaminants Injection in Humid Air

Figure 4-7 shows the breakthrough profile of MEK and n-hexane when the filter was challenged with a mixture at 50% relative humidity.

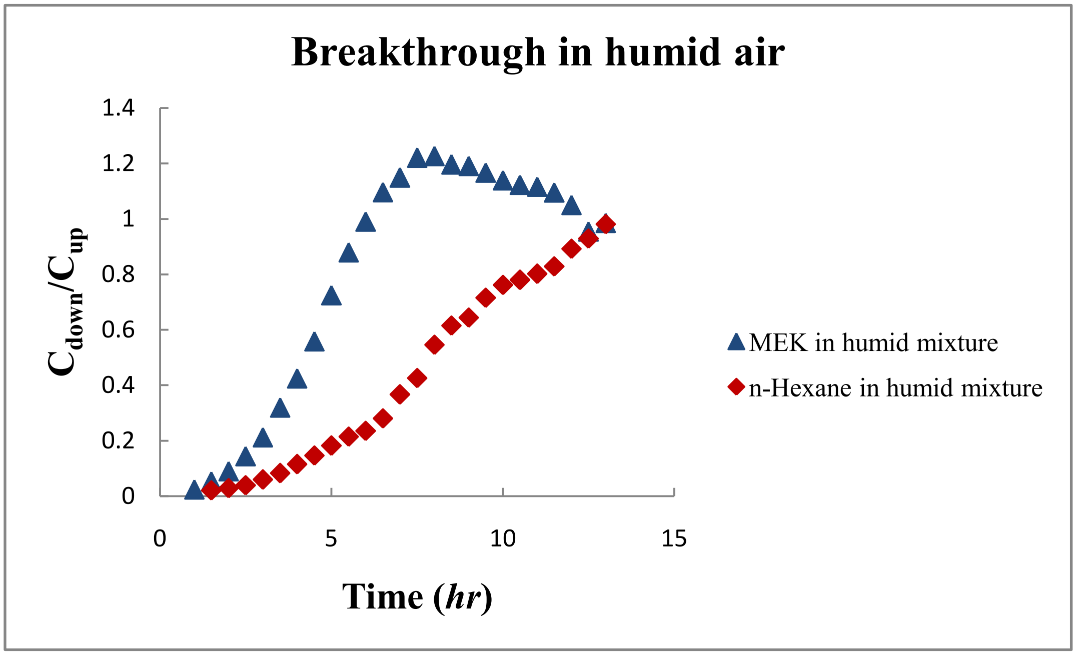


Figure 4- 7. Breakthrough curve of MEK and n-hexane in humid condition

Figure 4-7 shows the same trend for the MEK breakthrough profile as Figure 4-6 when the filter is challenged with a contaminant mixture of 100 *ppm* (MEK and n-hexane). Therefore, it is concluded that humidity did not have much effect on the adsorption of either MEK or n-hexane.

4.3.4. Comparing the Tests

Figure 4-8 compares the experimental breakthrough profiles of n-hexane in dry air, MEK in dry air, and MEK in humid air. In all three experiments, n-hexane had a concentration of 100 *ppm*. It was observed that the breakthrough curve of n-hexane was the same in all experiments and the existence of MEK or water vapor did not affect the removal performance of the filter for n-hexane. 50% and 80% breakthrough time of n-hexane either as a single contaminant or accompanied with MEK or water vapor was almost the same.

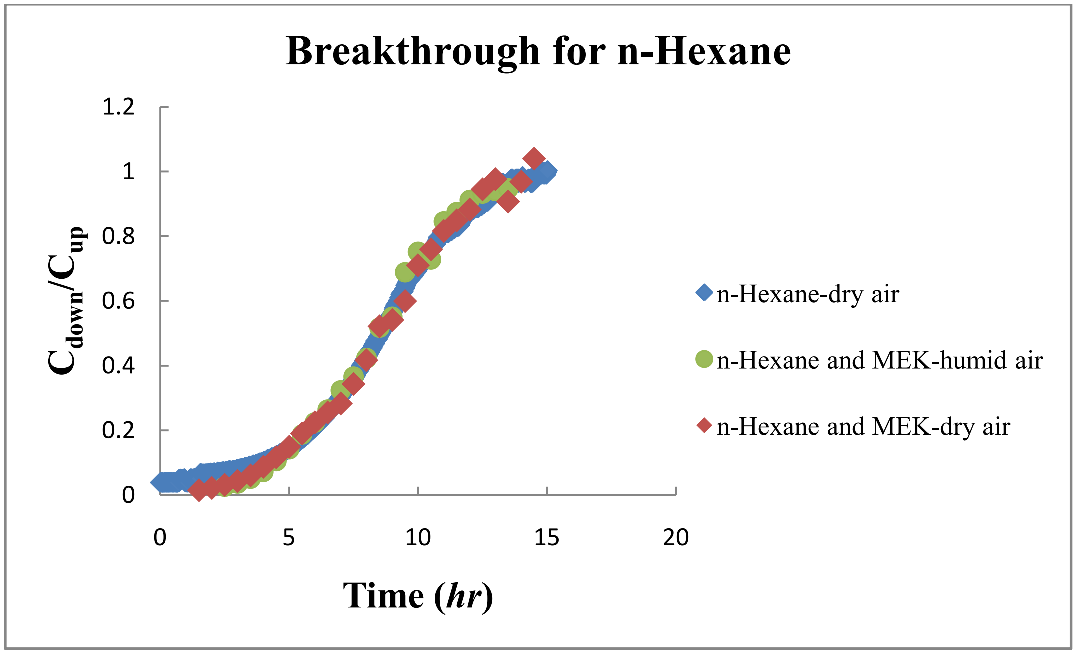


Figure 4- 8. Experimental breakthrough curves of n-hexane in different test conditions

Figure 4-9 shows that MEK has completely different behavior when it is injected as a single gas or as a mixture. When there was only one contaminant in the air (MEK), the breakthrough of MEK increased as time elapsed until the filter became saturated. Complete saturation of the filter occurs when the removal efficiency is zero or the breakthrough time is 100%. However, when both n-hexane and MEK were injected in the air, the penetration of MEK changed due to the interaction between the contaminants' molecules. The molecules of n-hexane interfered with the adsorption process of MEK. Therefore, when more than one contaminant was present in the air, the heavier compounds were adsorbed more on the filter because of their high affinity in adsorption on activated carbon. Figure 4-9 depicts that penetration of MEK increased quickly, reached to 1.2% of its complete breakthrough, and then decreased to the complete breakthrough when n-hexane was in the air in addition to MEK. However, the discrepancy of breakthrough time of MEK in dry and humid air is negligible.

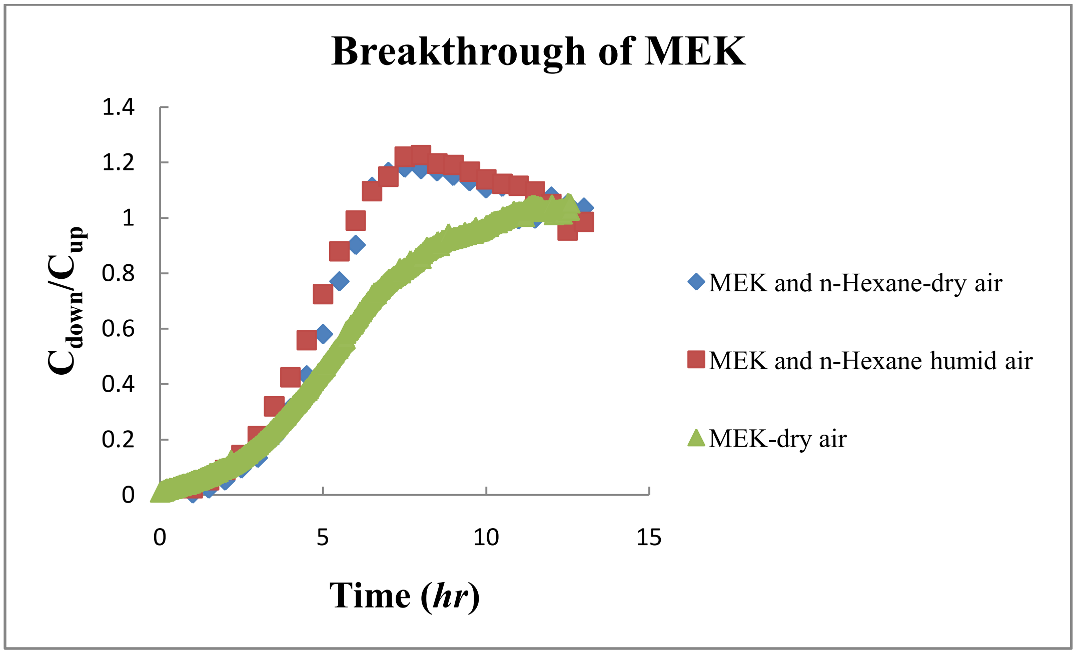


Figure 4- 9. Experimental breakthrough curves of MEK in different test conditions

4.3.5 Repeatability Tests

Some tests were repeated twice to confirm the reliability of the developed test procedure and measurement technique. The breakthrough results of 300 *ppm* of n-hexane, and 70 *ppm* of MEK for the isotherm tests, and 100 *ppm* of mixture (MEK and n-hexane) at dry and humid air condition for the verification tests is presented in Figure 4-10, Figure 4-11, Figure 4-12, and Figure 4-13, respectively.

Figure 4-10 shows the breakthrough profile of 70 *ppm* MEK for two tests (experiment 1 and experiment 2) that have been conducted at the same conditions. The results confirm the repeatability of the tests. The relative error between two tests is 1.6% in 50% breakthrough and 5% in 80% breakthrough time. Figure 4-11 presents the breakthrough profile of 300 *ppm* n-hexane. The relative error between the two tests (experiment 1 and experiment 2) in 50% breakthrough is 3% and in 80% breakthrough is less than 1%.

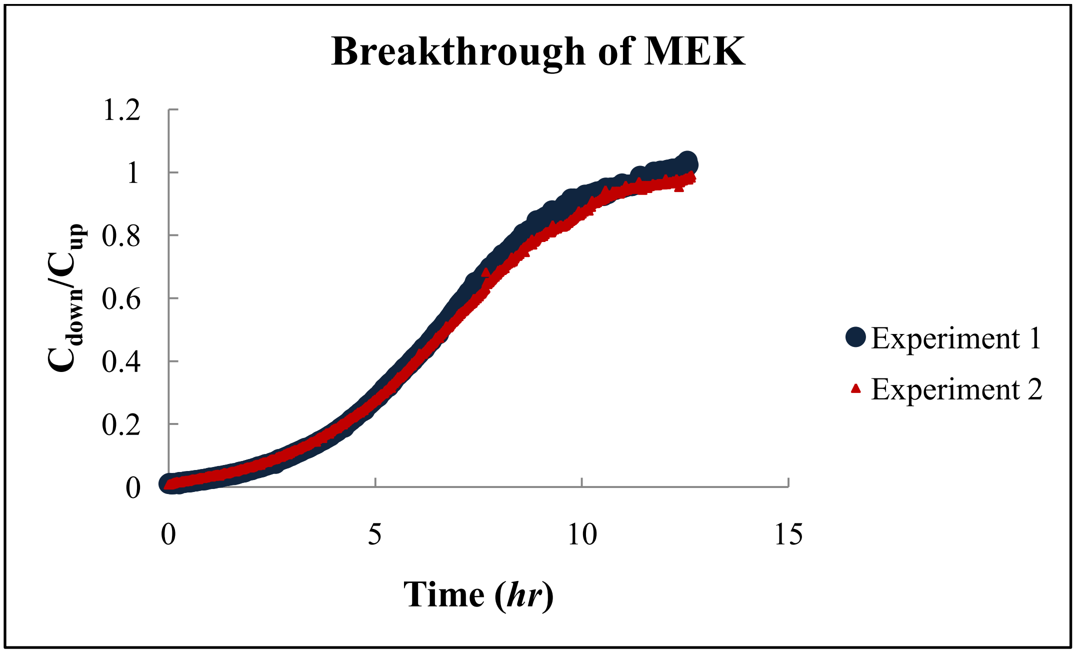


Figure 4- 10. Breakthrough curve of 70 *ppm* MEK in dry condition (repeatability test)

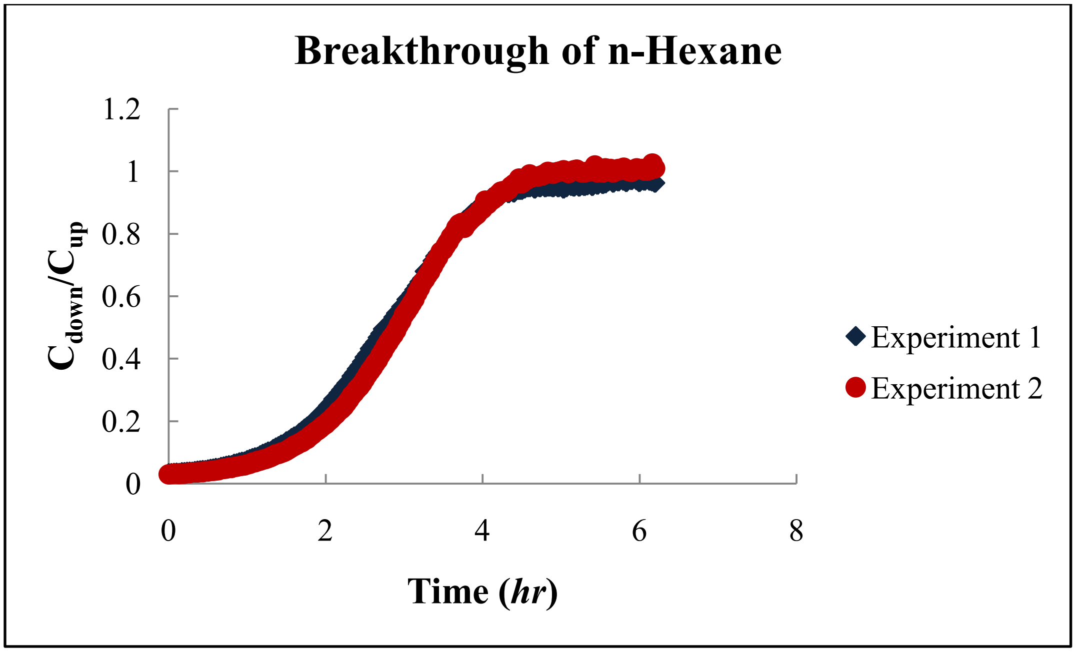


Figure 4- 11. Breakthrough curve of 300 *ppm* n-hexane in dry condition (repeatability test)

The breakthrough profiles for the repeatability tests for mixture of contaminants (100 *ppm* MEK and 100 *ppm* n-hexane at dry and humid air condition) depict less than 6% relative error in 50% and 80% breakthrough time. Figure 4-12 shows the results of two experiments for a case when the filter was challenged with a mixture of 100 *ppm* MEK and 100 *ppm* n-hexane. While Figure 4-13 presents the breakthrough profile of the same compounds at 50% relative humidity. These results indicate that the experiments were carried out correctly.

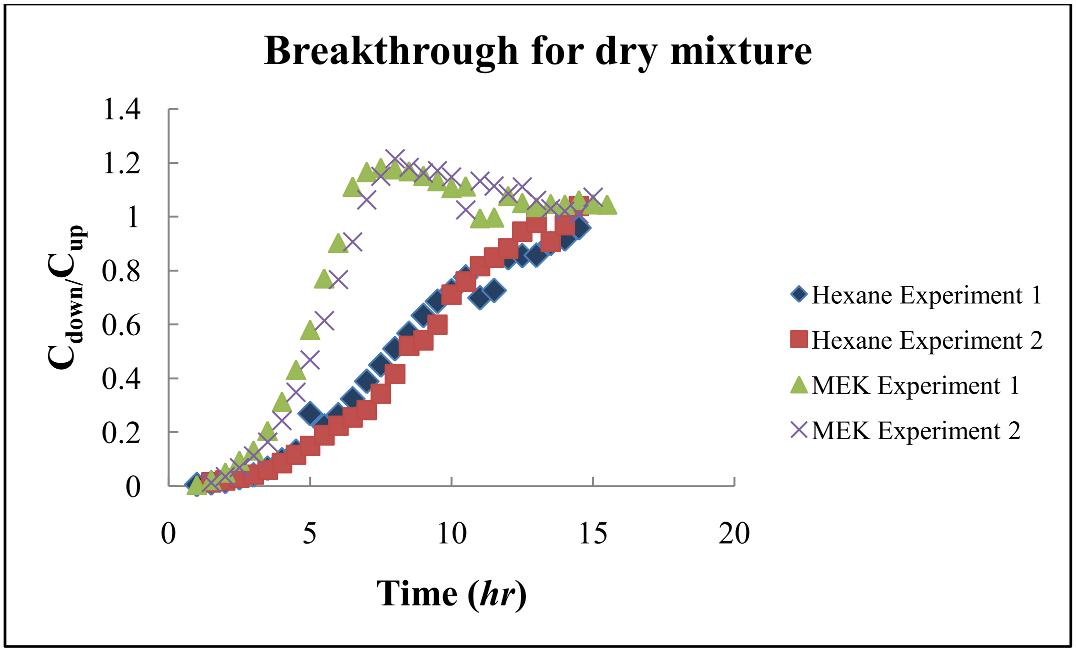


Figure 4- 12. Breakthrough of curve of 100 *ppm* MEK and n-hexane in dry condition (repeatability test)

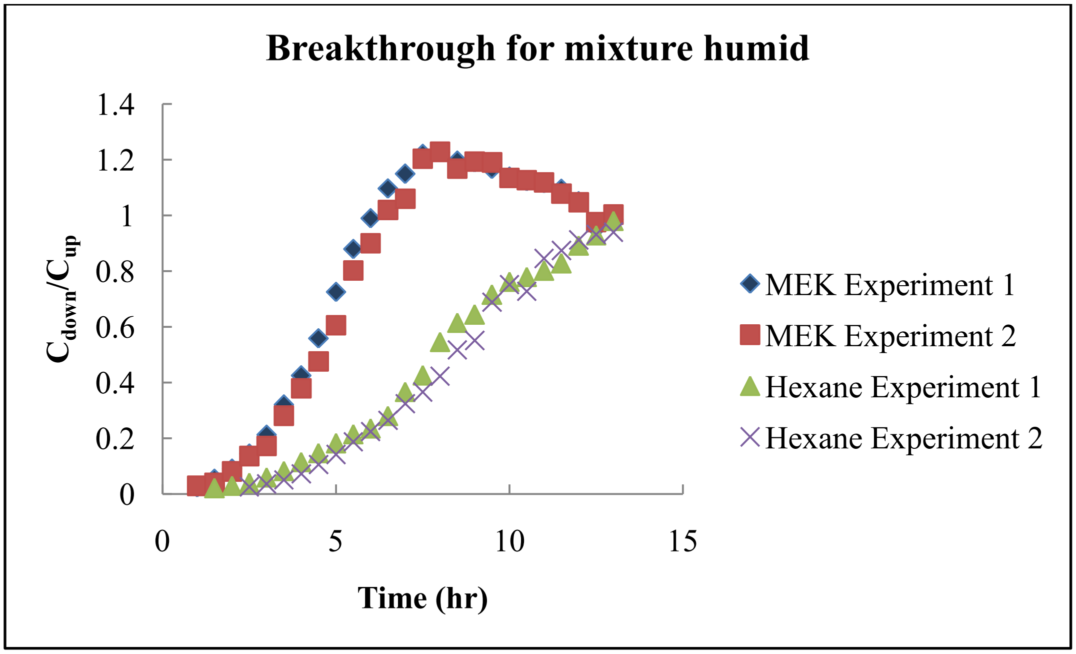


Figure 4- 13. Breakthrough of curve of 100 *ppm* MEK and n-hexane in humid condition (repeatability test)

4.4 MODELING RESULTS

The simulation was carried out after determining all the required inputs either experimentally or using the existing formulate. The simulation was carried out by solving two ordinary differential equations (43) and (44) using MATLAB SIMULINK. The simulations were performed at the same conditions as the experiment, i.e, in 30 *lit/min* airflow rate, and $23^{\circ}C$ temperature for 100 *ppm* upstream concentration for four different conditions: single contaminant (MEK) at dry condition, single contaminant (n-hexane) at dry condition, mixture of contaminants (MEK and n-hexane) at dry condition, and mixture of contaminants (MEK and n-hexane) at humid condition. Then, the prediction made by the model was compared with experimental data.

Figure 4-14 presents the breakthrough profile of 100 *ppm* n-hexane at dry air condition obtained from the simulation and experiment. The relative error between the model prediction and the experiment at 50% breakthrough time was 9.7% and, at 80% breakthrough time was 7.7%.

Figure 4-15 displays the model prediction and experimental breakthrough time of MEK for dry air condition. The error of predicting the 50% and 80% breakthrough time of MEK as a single contaminant was 1.6% and 2.8%, respectively.

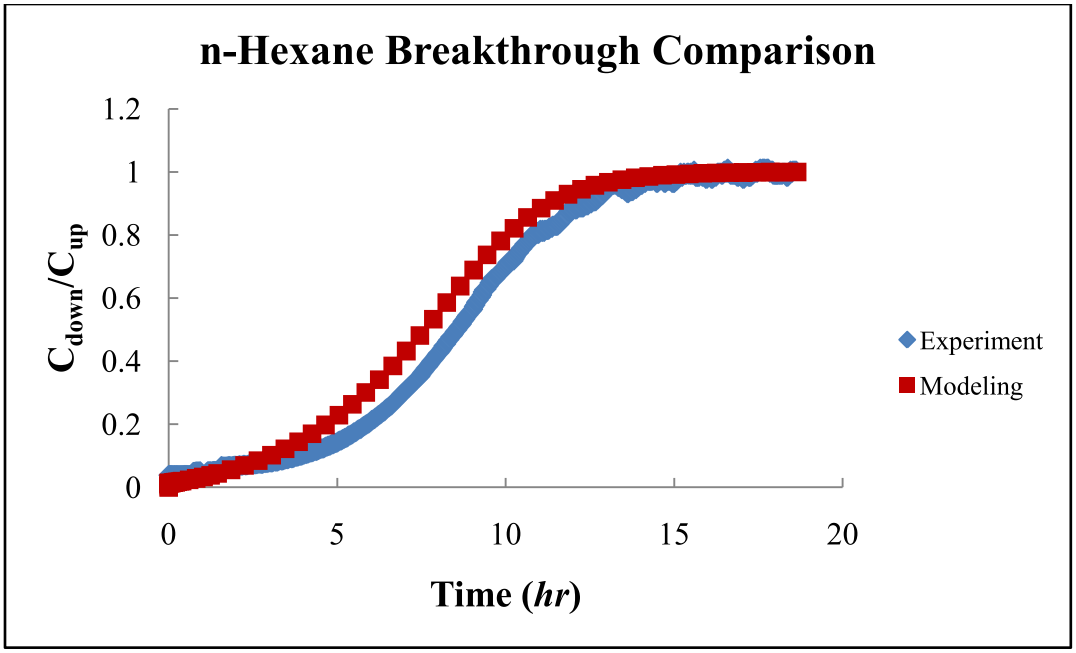


Figure 4- 14. Breakthrough profile of 100 *ppm* n-hexane in dry condition

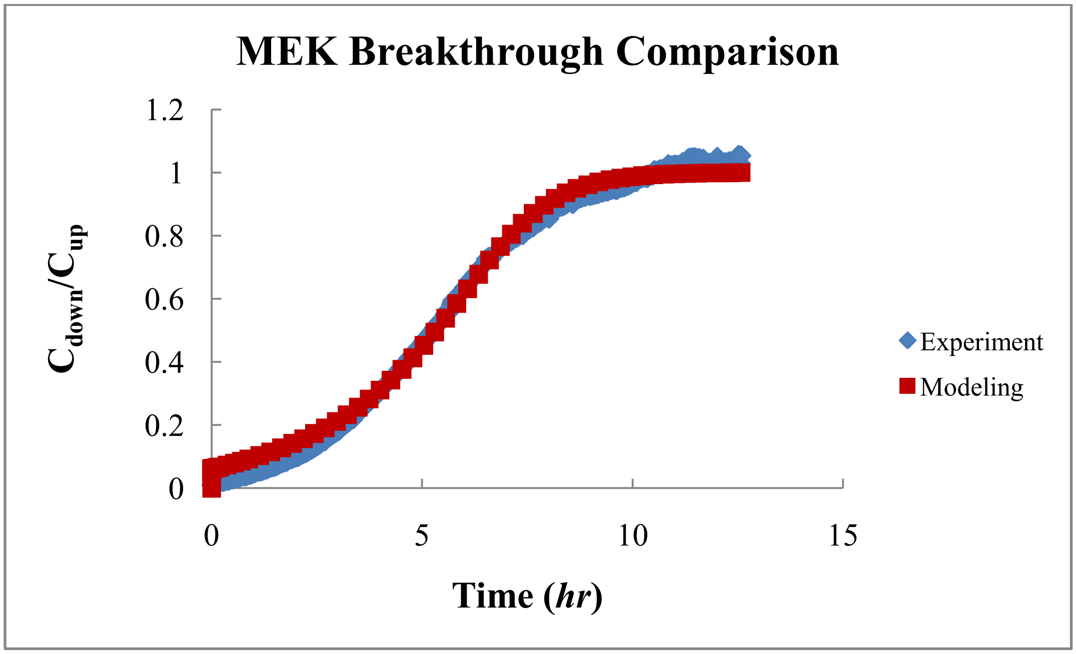


Figure 4- 15. Breakthrough profile of 100 *ppm* MEK in dry condition

It therefore could be concluded that the model is able to predict the performance of a gas-phase filter when it is challenged with a single compound. For example, the model was able to predict the penetration of both MEK and n-hexane at 50% and 80% breakthrough time with an error of less than 10%.

Figure 4-16 compares the experimental results for a contaminant mixture (100 *ppm* MEK and 100 *ppm* n-hexane) in dry air with the model prediction. The model predicts the removal performance of the filter for the lighter compound (MEK) with a less accuracy. It predicts the 50% breakthrough time with an error of 25% and 80% breakthrough time with an error of 26%. However, the model failed to predict the removal performance of the filter for n-hexane.

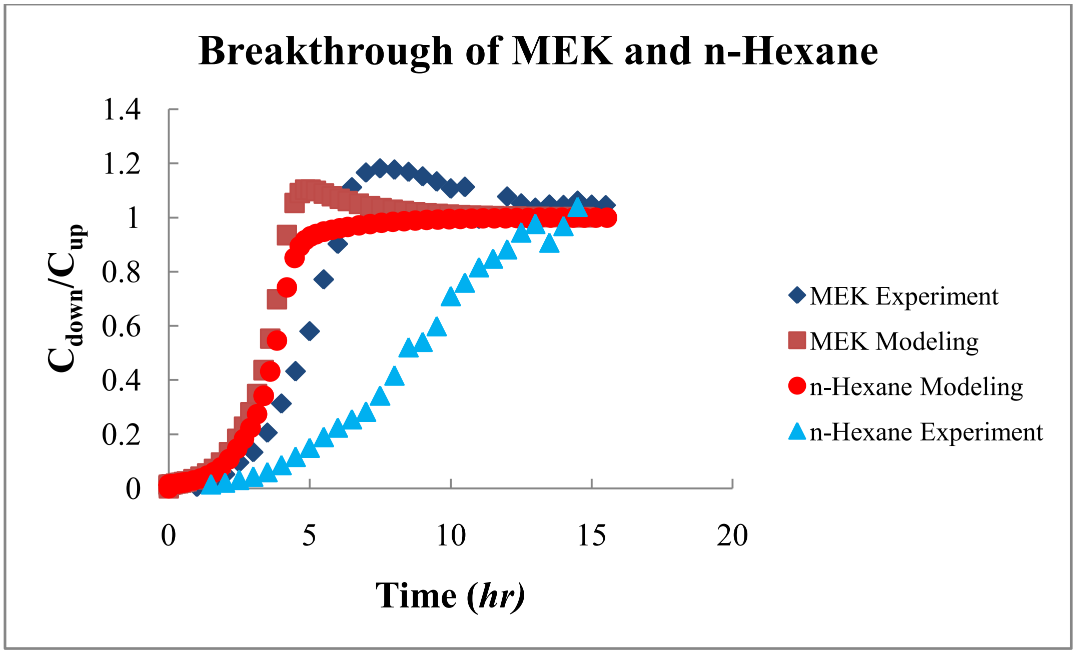


Figure 4- 16. Breakthrough profile of MEK and n-hexane in dry air containing two contaminants

Figure 4-17 compares the breakthrough profile of MEK and n-hexane (100 *ppm* MEK and 100 *ppm* n-hexane) in dry air and 50% relative humidity predicted by the model and obtained experimentally. The relative error for the penetration of MEK extracted from modeling in 50% breakthrough time was 18% and in 80% breakthrough was 23%. However, the relative error for breakthrough prediction from modeling is high (80%) for n-hexane. Therefore, it is concluded that the model applied for a mixture of contaminants in humid condition could predict the breakthrough of MEK with 25% relative error, but with 80% relative error for n-hexane.

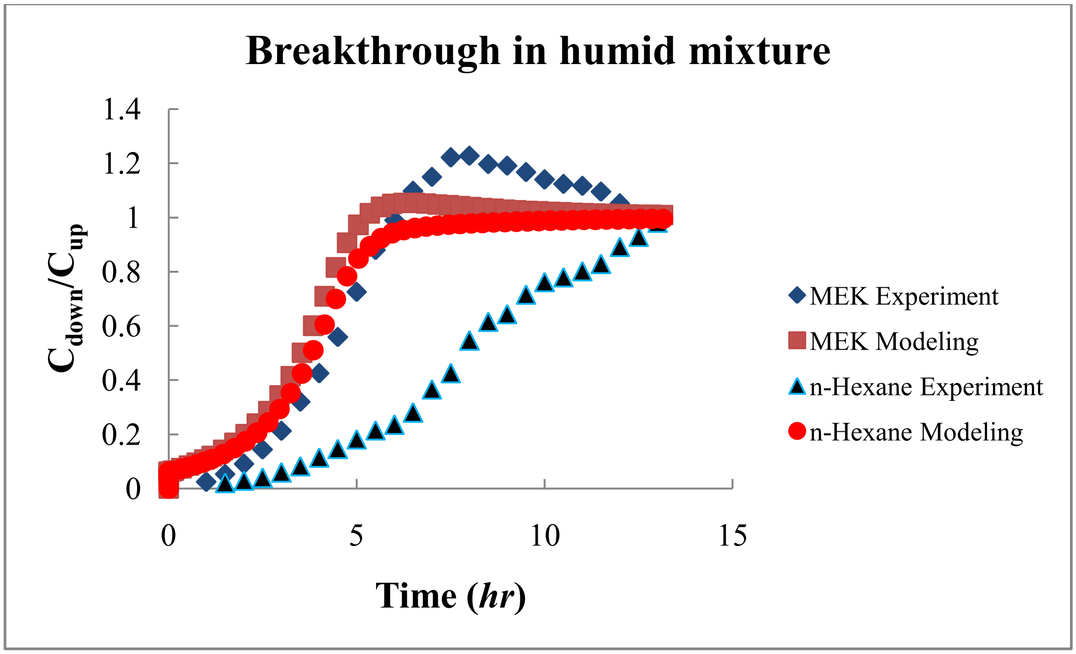


Figure 4- 17. Breakthrough curve for MEK in humid mixture

However, n-hexane showed almost the same breakthrough profile for different test conditions as it is presented in Figure 4-8. Therefore, if Figure 4-8 and Figure 4-14 are merged together as in Figure 4-18, it was concluded that single contaminant model can predict the penetration of n-hexane, because its breakthrough profile does not change whether it is the only contaminant in the air, or it is accompanied with another contaminant in dry or humid air conditions.

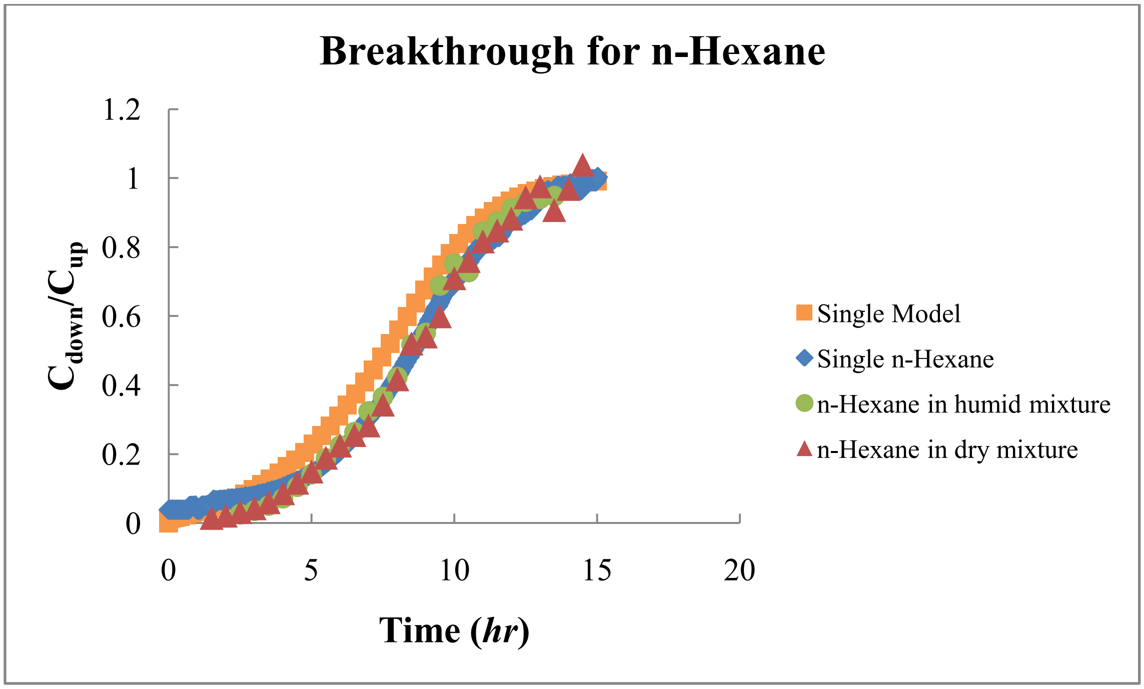


Figure 4- 18. Breakthrough time of n-hexane from modeling and experiments

Figure 4-19 shows the relative error of MEK and n-hexane in 50% breakthrough time between the prediction made by model and experimental result for the previously mentioned four conditions; single contaminant, mixture of contaminants in dry condition, and mixture of contaminants in humid condition for MEK and n-hexane. The results show that there is excellent agreement between the prediction made by the model and experimental results. Although the model cannot predict the breakthrough time of contaminants for the case of mixture as accurately as it can predict the breakthrough time for a single one, the error obtained for a lighter compound in the mixture is less than 25% while the error in modeling the heavier compound in mixture is significant.

Figure 4-16 and Figure 4-17 display a very little difference between dry air and humid air for adsorption. As it was mentioned, MEK reached 50% breakthrough in 4.3 hours in humid air containing a mixture of MEK and n-hexane, and in 4.7 hours in dry air. The effect of different relative humidity levels has been studied in the previous literatures (Owen et al., 1995). It has been concluded that water vapor adsorption on granular activated carbon filters is not significant for 50% relative humidity or lower (Khazraei Vizhemehr et al., 2011). The present study also confirms the effect of humidity on adsorption is insignificant for cases less than 50% relative humidity.

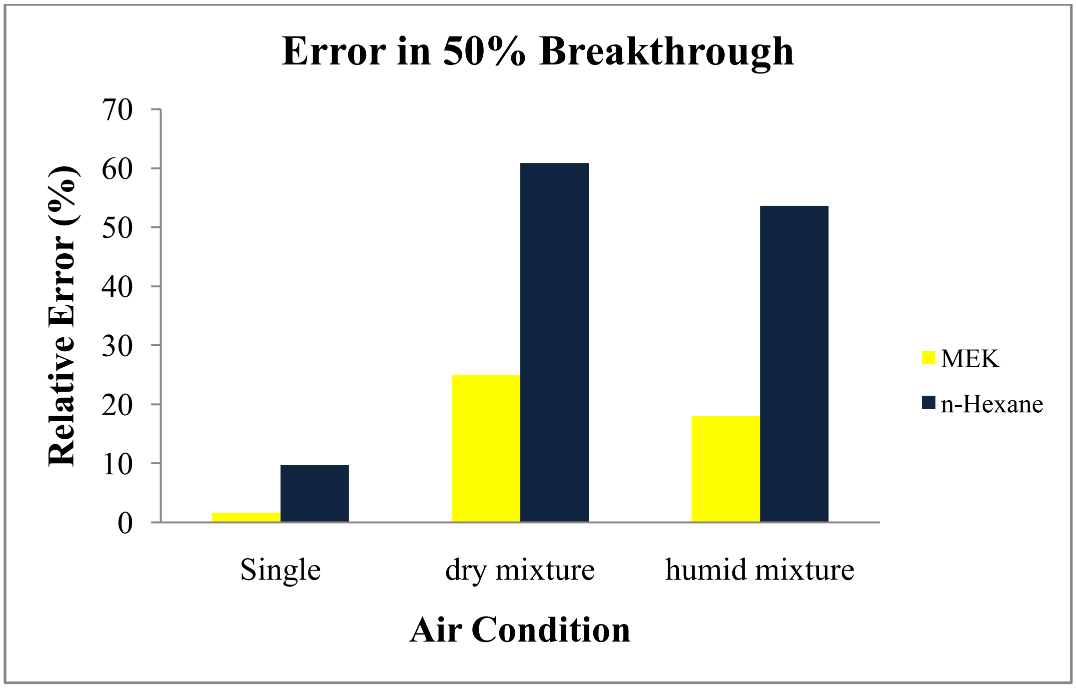


Figure 4- 19. 50% breakthrough time relative error of modeling in different conditions

The error in predicting the penetration of MEK and n-hexane at 80% breakthrough time in the air containing a single contaminant or a mixture of contaminants, for dry and humid conditions is shown in Figure 4-20. This also confirms that the model is accurate for predicting the performance of a filter when it is challenged with a single contaminant. The model, however, cannot predict accurately when it is applied to a mixture of contaminants. Modeling results are deemed acceptable for the n-hexane (heavier contaminant), but almost acceptable for MEK (the lighter contaminant).

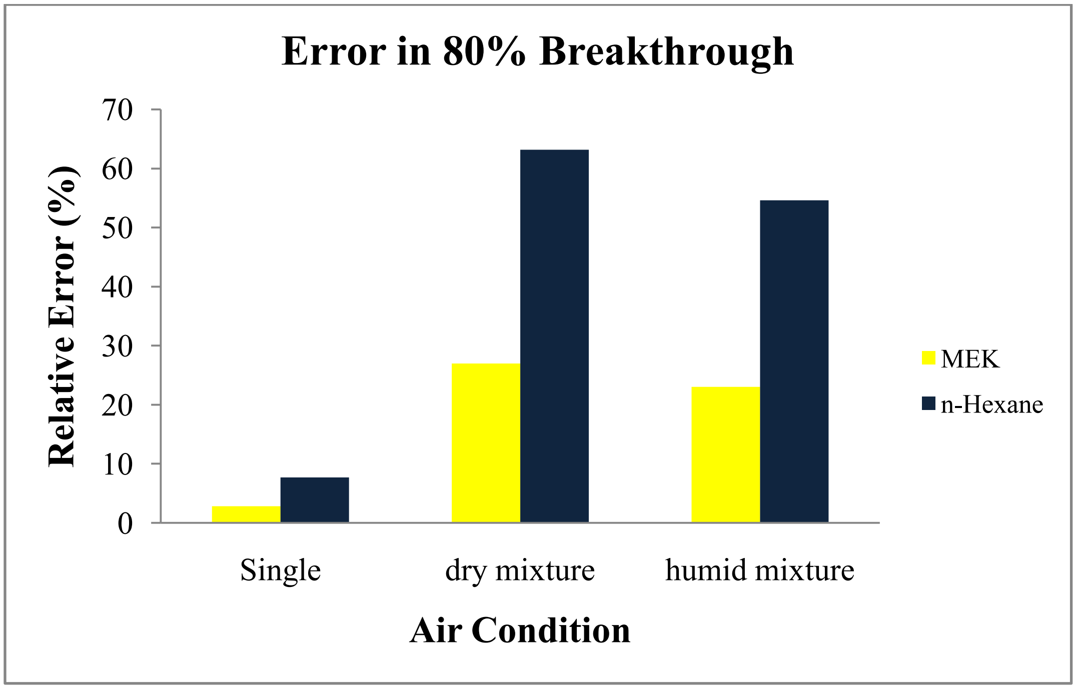


Figure 4- 20. 80% breakthrough time relative error of modeling in different conditions

4.5 SUMMARY

In summary, a specific case study was investigated in order to evaluate the validity of a methodology to evaluate gas phase models. The proposed methodology was evaluated through a case study. The methodology was applied to validate the selected model. The required parameter for the model were extracted from the literature or obtained experimentally. The parameters are presented in Table 4- 3.

Then, the model was verified against the experimental results. The model exhibited a very good capability in predicting the performance of the filter when it was exposed to a single contaminant. In fact, the error for single contaminant was less than 10%. However, when it was applied to a mixture of contaminants, the model could not predict the behavior of the heavier compound. It could predict the breakthrough profile of the lighter compound with an error of less than 26% for dry air and 23% for humid air. The heavier compound could be predicted by single model, because there was no significant discrepancy between the behavior of the heavier compound in single-pollutant contaminated dry air, mixture of pollutants in dry air, and mixture of pollutant in humid air.

Table 4- 3. Required Parameters

<table>
<tr><th colspan="5">Sorption Parameters</th></tr>
<tr><td>Compound</td><td>h_m (<i>m/s</i>)</td><td>D_e (m/s^2)</td><td><i>K</i> (<i>g/g</i>)</td><td>C_{s0} (<i>g/g</i>)</td></tr>
<tr><td>n-hexane</td><td>0.046</td><td>$1.97e^{-6}$</td><td>0.0272</td><td>7407</td></tr>
<tr><td>MEK</td><td>0.047</td><td>$2e^{-6}$</td><td>0.0128</td><td>19531</td></tr>
<tr><th colspan="5">Filter Design Parameters</th></tr>
<tr><td>Filter's Media</td><td>Particle Size (<i>mm</i>)</td><td colspan="2">Packing Density (kg/m^3)</td><td>A_s (m^2)</td></tr>
<tr><td>G.A.C</td><td>2.5, 6</td><td colspan="2">411</td><td>0.35</td></tr>
<tr><th colspan="5">Environmental Parameters</th></tr>
<tr><td>Pollutants</td><td>Concentration (<i>ppm</i>)</td><td>Flow Velocity (<i>lit/min</i>)</td><td>Relative Humidity (<i>%</i>)</td><td>Temperature (<i>℃</i>)</td></tr>
<tr><td>n-hexane</td><td>100</td><td>30</td><td>0 and 50 *</td><td>23±1</td></tr>
<tr><td>MEK</td><td>100</td><td>30</td><td>0 and 50 *</td><td>23±1</td></tr>
</table>

* Experimental tests and models have been done in both dry air condition and 50% R.H

CHAPTER 6 CONCLUSION AND RECOMMENDATIONS FOR FUTURE WORK

6.1 SUMMARY

The objective of the present research was developing a systematic methodology to evaluate the performance of existing models of gaseous air cleaners for application in building mechanical ventilation systems. The study focused on models of filters that remove pollutants such as VOC from the air by the process of adsorption. The proposed methodology is of great help to HVAC designers for estimating the lifetime of filters using the selected model, prior to its production.

The objectives of the current study were achieved by; first, selection of the most comprehensive model available for predicting the penetration of the contaminants on an adsorbent. The model could be generalized for diverse adsorbent media in the filters for any mixture of contaminants in the air. Furthermore, this model:

- predicted the penetration profile for each contaminant in the air.
- was applied to more than one contaminant in the air.
- provided penetration data in the presence of moisture in the air.

The model is based on the basic mass transfer phenomena occurring during the adsorption process. These consist of adsorption, external diffusion, and internal diffusion. Therefore, the parameters required for solving the model and determining the rate of mass transfer by the three phenomena listed above were quantified. Some parameters were calculated based on previous studies, some were environmental parameters that were adjusted based on ASHRAE standards, and some were filter design parameters that were assumed. The method used to obtain the required parameters is general and could be used for any case. However, a case study selected, and investigated. The corresponding required parameters were determined.

- The external mass transfer coefficient was defined based on the Wakao-Funzakri correlation of Sherwood number. The external mass transfer coefficient provided the convection mass transfer rate.
- The relative humidity was set to 50% since it is the most usual humidity level in Canada.
- The airflow rate was adjusted to 30 *lit/min* based on the calculations for residence time needed between the media and air.
- The filter's adsorbent was selected as granular activated carbon with 2.5 *mm* diameter and 6 *mm* length.

Finally, some parameters were quantified using extensive experimental tests. These tests were carried out at the conditions mentioned above for simulation. The parameters included the adsorption isotherm constant parameters. Tests were conducted for MEK, n-hexane, and moisture. The experimental results were regressed with the Langmuir isotherm equation and the constant parameters of the Langmuir equation were quantified.

After collecting all the required parameters, the simulations were performed for four different scenarios. The four experiments corresponding to the four scenarios were carried out to study the filter performance in term of breakthrough time. The four experiments include:

- Case 1: injecting 100 *ppm* n-hexane to the air at dry condition.

- Case 2: injecting 100 *ppm* MEK to the air at dry condition.
- Case 3: injecting 100 *ppm* n-hexane and 100 *ppm* MEK to the air at dry condition.
- Case 4: injecting 100 *ppm* n-hexane and 100 *ppm* MEK to the air at 50% relative humidity level.

Then, the results obtained from the model prediction were compared to the results extracted from the experiments.

6.2 CONCLUSIONS

In conclusion, the applicability of the proposed methodology was validated based on the case study. The proposed approach was followed systematically for the case, and its generality was confirmed. Furthermore, the selected model was verified experimentally. It was concluded that lifetime prediction based on the single model was acceptable, with less than 10% calculated relative error. However, lifetime prediction in the mixture model had more relative error. The obtained error of the model for MEK breakthrough profile was less than 30% and n-Hexane breakthrough profile was almost 80%. Therefore,

- The selected model was capable of predicting the lifetime of the filter with less than 10% error for case 1, and within 3% relative error for case 2. This discrepancy could be due to the simplifying assumptions included in the model, e.g neglecting intra-particle diffusion coefficient, linear driving force assumption for convection rate, and adsorption isotherm assumption. Furthermore, the error could come from experimental mishaps such as variations in temperature, pressure drop, air leakage, etc.

- The selected model was capable of predicting the penetration profile of MEK with less than 26% relative error in case 3 and 4, but it was not able to predict the penetration profile of n-hexane in phase 3 and 4. Therefore, when a mixture of pollutants is present, the model failed to predict the breakthrough profile of the heavier contaminant, but succeeded in predicting for the lighter one.
- Because the breakthrough profile of n-hexane did not change in case 1, 3, and 4, the simulation results of case 1 could be used to predict the performance of a filter for case 3 and 4.

According to the breakthrough profiles of MEK and n-hexane extracted from the model and the experiments, other conclusions have been made:

- The concentration of n-hexane in the downstream (in case 1) increased with time and reached half of the upstream concentration in about 8.56 hours.
- The concentration of MEK in the downstream (in case 2) increased as the removal efficiency decreased. MEK showed the same breakthrough profile as n-hexane. However, MEK reached 50% breakthrough time in 5.25 hours.
- n-hexane had more affinity to be adsorbed on activated carbon than MEK because of its molecular weight. The removal efficiency of the filter reached zero in 16 hours for n-hexane in the first case, and in 13 hours for MEK in the second case. Therefore, the filter (activated carbon) is capable of removing heavy contaminants more efficiently than light contaminants.
- Case 3 of the experiments demonstrated that when there is more than one pollutant in the air, the breakthrough profile of the lighter contaminant changes. The lighter contaminant downstream concentration (MEK) increased and

exceeded its upstream concentration. This is due to the displacement of lighter compound molecules (MEK) by the heavier compound molecules (n-hexane) because of the existing competition between these two kinds of molecules. The breakthrough value of n-hexane reached unity 9 hours after the MEK breakthrough reached unity.

- Case 4 of the experiment presented almost the same results of case 3. This comparison showed that 50% relative humidity has insignificant effect on the removal performance of the filter.
- The removal efficiency of the filter in removing multiple VOCs was higher for n-hexane than MEK. This is due to the fact that the removal efficiency of a filter (breakthrough value of the contaminants on the filter) is affected by the physical properties of VOCs. Among different physical properties, the molecular weight of the pollutants is the most significant factor that affects the filter's performance based on previous researches. The current study also confirmed that the pollutants with higher molecular weight had more affinity to be adsorbed by activated carbon and resulted in more removal from the air.
- Comparing case 1, 3, and 4, it was found that the breakthrough profile of n-hexane (heavier compound) did not change whether it was the only pollutant in the air, or was accompanied with a lighter contaminant, or even if the air is dry or humid.
- The selected model MEK penetration profile prediction did not change for cases 3 and 4 and confirmed the outcomes of conducted experiments. Besides, it confirmed that humidity did not have much effect on the filter performance.

6.3 RECOMMENDATIONS FOR FUTURE WORK

Based on the achievements of the present study, further work is recommended as follows:

- The present method has the ability to assess the lifetime of other adsorbents such as activated carbon cloth and bonded carbon panel with other groups of VOC gases. The effect of other adsorbent and other adsorbates could be investigated using this method. The polarity of the VOCs on the removal performance of the filter should also be investigated.
- This method should be applied to evaluate the model performance for different upstream concentration levels. Its applicability should be tested for ppb level as well as for high *ppm* levels.
- The method should be applied for other available models, and the outcome of other models should be compared with the present one.
- The developed methodology should be applied to investigate the effect of environmental parameters such as temperature, relative humidity, and airflow velocities. The lifetime of the filter is a function of environmental conditions. Relative humidity effect is low for humidity levels below 50% based on Owen et al (1995) study. However, the removal efficiency of the filters may decrease with increasing relative humidity for more than 50%.

REFERENCES

ASHRAE. 1999. ANSI/ASHRAE Standard 52.2-1999: method of testing general ventilation air-cleaning devices for removal efficiency by particle size, American Society of Heating, Refrigerating, and Air-Conditioning Engineers, Inc., Atlanta.

ASHRAE. 2004. ANSI/ASHRAE Standard 55-2004: thermal environmental conditions for human occupancy, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta.

ASHRAE. 2005. ASHRAE Handbook Fundamentals, SI Edition, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., 1791 Tullie Circle, N.E., Atlanta.

ASHRAE. (2007-a) ASHRAE Handbook-HVAC Applications (SI), control of gaseous indoor air contaminants, American Society of Heating, Referigerating and Air Conditioning Engineers, Inc, Atlanta.

ASHRAE Standard 62.1. (2007-b) ventilation for acceptable indoor air quality, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta.

Axley J.W. (1994) Tools for the analysis of gas-phase air-cleaning systems in buildings, Proceedings of the ASHRAE Annual Meeting, June 25, 1994 - June 29, 1994, ASHRAE, Orlando, FL, USA. pp. 1130-1146.

Bastani A. (2008) Full-scale Experimental set-up for evaluating the performance of commercial air cleaners for building applications, thesis August 2008, Concordia University

Brunauer S., Deming L.S., Deming W.E., Teller E. (1940) On a theory of the van der Waals adsorption of gases. Journal of the American Chemical Society 62:1723-1732. DOI: 10.1021/ja01864a025.

Chiang Y.-C., Chiang P.-C., Huang C.-P. (2001) Effects of pore structure and temperature on VOC adsorption on activated carbon, Carbon 39:523-534. DOI: 10.1016/s0008-6223(00)00161-5.

Duong D.D. (1998) Adsorption analysis: equilibria and kinetics, Imperial College Press.

EPA. 2007. The Inside Story: A guide to indoor air quality, EPA Document #402-k-93-007, United State Environmental Protection Agency, Office of Radiation and Indoor Air (6609J) Cosponsored with the Consumer Product Safety Commission

EPA. 2008, September. A guide to indoor air quality, EPA document 402/F-08/008 US, United State Environmental Protection Agency, online available: http://www.epa.gov/iaq/pdfs/careforyourair.pdf (last access, August 22. 2011)

Guo B., Zhang J., Nair S., Chen W., Smith J. (2006) VOC removal performance of pellet/granular-type sorbent media - experimental results. ASHRAE Transactions 112, Part 2.

Gupta V.K., Verma N. (2002) Removal of volatile organic compounds by cryogenic condensation followed by adsorption. Chemical Engineering Science 57:2679-2696.

Haghighat F., Lee C.-S., Pant B., Bolourani G., Lakdawala N., Bastani A. (2008) Evaluation of various activated carbons for air cleaning - Towards design of immune and sustainable buildings. Atmospheric Environment 42:8176-8184. DOI: 10.1016/j.atmosenv.2008.07.061.

Henschel D.B. (1998) Cost analysis of activated carbon versus photocatalytic oxidation for removing organic compounds from indoor air. Journal of the Air and Waste Management Association 48:985-994.

Hines, A.L., Ghosh, T.K., Loyalka, S.K., and Warder, R.C. 1993. indoor air quality and control, PTR Prentice-Hall Inc., A Simon & Schuster Company, Englewood cliffs, New Jersey.

Holmberg R., Torkelsson S., Stringehag O. (1993) Suitability of activated carbon filters for air handling units, Proceeding of 6th International Conferece on IAQ and Climate, Indoor Air 93, Helsinki, Finland.

Hunter P., Oyama S.T. (2000) Control of volatile organic compound emissions: conventional and emerging technologies John Wiley.

Khazraei Vizhemehr A., Kholafaei H., Haghighat F., Lee C. (2011) The effect of relative humidity level, VOC type and multiple VOCs on the performance of full-scale GAC filters, Indoor Air, Texas, Austin.

Kwon K.C., Park Y., Simmons C.M., Tibere G.L., Ibrahim T.H. (2003) Molecular diffusion of volatile-liquid vapors into air. Chemical Engineering Communications 190:1449-1467. DOI: 10.1080/714909153.

Lide D.R. (2004) CRC handbook of chemistry and physics: a ready-reference book of chemical and physical data CRC Press.

Liu R.T., Huza M.A. (1995) Filtration and indoor air quality: a practical approach. ASHRAE Journal:February: 18-23.

Logan B.E. (1999) Environmental transport processes Wiley.

Mahajan B.M. (1987) Method for measuring the effectiveness of gaseous-contaminant-removal devices. Progress report, National Institute of Standard and Technology, US Department of Commerce, Gaithersburge, MD. pp. Medium: X; Size: Pages: 22.

Noll K.E., Gounaris V., Hou W. (1992) Adsorption technology for air and water pollution control Lewis Publishers.

Owen M.K., VanOsdell D.W., Jaffe L.B., and Sparks L.E. 1995. The effect of relative humidity on gaseous sir cleaner media performance: Toluene adsorption by activated carbon. In: engineering solution to indoor air quality problems, VIP-51, Air and Waste Management Association, Pittsburgh, PA: 551-562.

Pei J., Zhang J. (2010) Modeling of sorbent-based gas filters: development, verification and experimental validation. Building Simulation 3:75-86. DOI: 10.1007/s12273-010-0309-4.

Pei J., Zhang J., Nair S., Chen W., Guo B., Wong J. (2008) VOC removal performance of pellet/granular type sorbent media from testing to predictions. ASHRAE Transactions.

Perry R.H., Chilton C.H., Kirkpatrick S.D. (1963) Perry's chemical engineers' handbook McGraw-Hill.

Popa J., Haghighat F. (2003) The impact of VOC mixture, film thickness and substrate on adsorption/desorption characteristics of some building materials. Building and Environment 38:959-964. DOI: 10.1016/s0360-1323(03)00063-5.

Popescu R.S., Blondeau P., Jouandon E., I. C. (2007) Breakthrough time of activated carbon filters used in residential and office buildings: Modeling and comparisons with experimental data. Proceeding of Clima.

Popescu R.S., Blondeau P., Jouandon E., Colda I. (2008) Physically-based modelling of the influence of humidity on the efficiency of activated-carbon filters, Indoor Air 2008, Copenhagen, Denmark.

Popescu R. S. (2008) Modelisation du comportement des filtres en charbon actif utilises pour l'epuration de l'air interieur, These pour le grade de docteur, Universite de la rochelle (LEPTIAB)

Ruthven D. (1984) Principles of adsorption and adsorption processes University of New Brunswick, Fredericton.

Slejko F.L. (1985) Adsorption technology: a step-by-step approach to process evaluation and application M. Dekker.

Thibodeaux L.J., Mackay D. (2010) Handbook of Chemical Mass Transport in the Environment CRC Press.

Treybal R.E. (1990) Mass transfer operations. McGraw-Hill, 3rd edition.

Tsai M.C., Chen W.N., Cen P.L., Yang R.T., Kornosky R.M., Holcombe N.T., Strakey J.P. (1985) Adsorption of gas mixture on activated carbon. Carbon 23:167-173. DOI: 10.1016/0008-6223(85)90008-9.

VanOsdell D.W., Rodes C.E., Owen M.K. (2006) Laboratory testing of full-scale in-duct gas air cleaners. ASHRAE Transactions 112(2):418-429.

VanOsdell D.W. 1994. Evaluation of test methods for determining the effectiveness and capability of gas-phase air filtration equipment for indoor air applications-phase I: literature review and test recommendations, ASHRAE Trans. 100: 511-523.

Weber W.J. (1972) Physicochemical processes for water quality control Wiley-Interscience, New York.

Xu Q., Zhang Y., Mo J., Li X. (2011) A new method to evaluate the performance of adsorbents for indoor VOCs purification, Indoor Air, Austin, Texas.

Yang R.T. (1987) Gas separation by adsorption processes Stoneham (MA): Butterwoths Publishers.

Young D.M., Crowell A.D. (1962) Physical adsorption of gases Butterworths, Washington.

Yu J.W., Neretnieks I. (1993) The Effect of a Passive Adsorption Sheet on Reducing Organic Pollutants in Indoor Air, Indoor Air 3: 12-19.