

**MEASUREMENT AND SIMULATION OF ACTIVATED  
CARBON ADSORPTION AS A MEANS TO CONTROL  
INDOOR AIR QUALITY**

by

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## ABSTRACT

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The quality of indoor air has become an important issue in the creation and maintenance of a comfortable building environment. Sick Building Syndrome, SBS, is an Indoor Air Quality, IAQ, problem that encompasses the ill health effects resulting from indoor air contaminants. In an effort to address this problem the effect of adsorptive measures that employ activated carbon bonded filters on the concentration of volatile organic compounds, VOCs, in an indoor environment were measured and simulated. Gas chromatography was used to measure equilibrium and kinetic adsorption characteristics of propane on such filters. TRNSYS, a transient simulation program, was used to apply the experimentally derived adsorption data to a building simulation to determine pollutant concentrations in occupied zones.

A propane isotherm at 35° C was measured over a concentration range of 5 to 43.9 ppm. In addition to the collection of equilibrium data the kinetic adsorption data was recorded by monitoring the outlet concentration of the carbon filters as a function of time. The equilibrium and kinetic adsorption information were applied to two types of contaminant breakthrough models, longitudinal diffusion and mass transfer resistance. A filter model employing the longitudinal diffusion breakthrough model which was capable of solving the outlet concentration for a time varying inlet boundary condition was then developed and verified experimentally.

The carbon filter model was incorporated into a TRNSYS building simulation that calculated the transport of contaminant through the carbon filter and building zones. The effects of filter parameters and ventilation strategies on zone pollutant concentrations and energy uses were calculated. Three pollutant generation strategies were simulated: constant 24 hour generation, occupant generation, and short term large volume event generation. Additionally, two ventilation strategies were employed: 24 hour ventilation and 12 hour ventilation. The ventilation and generation schemes were simulated for a small filter, large filter, no filter, and a perfect filter.

The results of the study indicate that because of the filter's relatively low capacity and the high volumetric flow of air in indoor environments the bonded filters do not perform well for constant sources of pollutant generation. However, the filters do excel at alleviating the effects of short term large volume events by distributing the contaminant over a longer period at a lower concentration than would be experienced without a filter. Additionally, for occupant generated pollutants properly designed filters can reduce pollutant concentrations significantly if the ventilation system is able to desorb the contaminants from the filters during unoccupied periods such as overnight.



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## NOMENCLATURE

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### ROMAN SYMBOLS

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Symbol	Definition
A	area
b	conversion constant from ppms to contaminant mass per ml/min.
B	mass transfer coefficient
C	concentration of contaminant
COA	concentration of outdoor air
D	diffusion coefficient
F	volumetric flow rate
FID	flame ionization detector
Inf	infiltration
K	linear isotherm constant
L	filter length
m	mass
NWPE	non-woven polyester
p	fraction of outdoor air
PC	personal computer

ppm	parts per million
q	amount of contaminant adsorbed per unit mass of carbon
R	retentivity
ret	return
s	seconds
S	pollutant generation
sup	supply
t	time
u	interstitial gas stream velocity
U	uncertainty
v	volts
V	volume
Z	axis in the longitudinal direction

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### GREEK SYMBOLS

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Symbol	Definition
$\epsilon$	void fraction
$\rho$	density

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### SUBSCRIPTS

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Symbol	Definition
B	bias
c	activated carbon
d	diffusion



end	end of the experimental run
in	into the inlet of the carbon filter sample
L	longitudinal
max	maximum
o	initial value
IZF	inter-zone-flow
out	out of the outlet of the carbon filter sample
P	precision
T	total



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**CHAPTER  
ONE**

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**INTRODUCTION****1.1 Indoor Air Quality**

The quality of indoor air has been the focus of a great deal of attention because of a phenomena which has come to be known as Sick Building Syndrome, SBS. Health problems such as headaches, nausea, mucous membrane irritation, fatigue, and a number of other ailments which are attributed to the indoor environment constitute the symptoms of SBS. What seems to be a sudden emergence of this problem appears to stem from two causes. One cause is thought to be the advent of new synthetic building materials used in products like carpeting, wallpaper, and particle board that has created a large number of new pollutant generation sources. At the same time that pollutant generation has rapidly increased the infiltration of outdoor air to indoor spaces has been dramatically reduced in an effort to provide more energy efficient buildings. These two factors combine to produce indoor air concentrations of toxic organic chemicals that can be 70 times greater than those outdoors (Quellette and Doria, 1987).

### **1.1.1 Guidelines and Regulations**

Although it is generally accepted that exposure to a large number of low concentration volatile organic compounds, VOCs, can cause illness, it is far from clear what constitutes acceptable indoor air quality. Many government and professional agencies have provided standards that try to address the problem in a holistic manner by setting numerical requirements for some contaminants that have been judged to be indicative of indoor air quality. One of these contaminants is carbon dioxide, which alone is not harmful at the concentrations found indoors, but is thought to be an indicator of other pollutant levels. The American Society of Heating Refrigeration and Air Conditioning Engineers, ASHRAE, the National Institute for Occupational Safety and Health, NIOSH, the Occupational Safety and Health Administration, OSHA, and the American Industrial Hygiene Association AIHA have all established different and sometimes contradictory guidelines as to what constitutes acceptable indoor air quality.

ASHRAE set forth its indoor air quality guidelines in Standard 62-1989, "Ventilation for Acceptable Indoor Air Quality". Many different indicators of indoor air quality such as ventilation rates and fractions of limit values for VOCs proposed by other agencies are proposed in the standard. Ventilation rates recommended for some types of indoor spaces are typically on the order of 15-20 cfm per person. These rates were derived based on a carbon dioxide level which has been arbitrarily set at 1000 ppm reduced in 1989 from a value of 2500 ppm set in 1981. However, lower ventilation rates may be used if specified contaminants are kept below a certain value listed in the appendices of the standard. Unfortunately, only 20 or 30 contaminants are listed in the tables but several hundred commonly exist in indoor air. The limits provided are for exposure to individual contaminants and do not reflect the effects of mixtures. Thus, acceptable

indoor air quality ultimately defaults to its' definition by ASHRAE as air in which there are no known contaminants at harmful concentrations as determined by cognizant authorities and with which a substantial majority (80% or more) of the people exposed do not express dissatisfaction (ASHRAE, 1989).

AIHA has set a guideline of  $5 \text{ mg/m}^3$  for the total VOCs present in indoor air based on the work of Molhave et al. (1984) that found a majority of the people suffered from mucous membrane irritation at that level of  $5 \text{ mg/m}^3$ . As a reference, the generation rates of selected building materials (Molhave, 1982) and persons (Wang, 1975) are shown in Table 1.1.1 and 1.1.2.

OSHA set a 1/10 Threshold Limit Value, TLV, guideline based on the TLVs adopted by the American Conference of Government Industrial Hygienists, ACGIH. The TLV is a value placed on an airborne substance which represents the conditions under which almost all workers will not suffer ill health affects from repeated daily exposure (Brysse, 1992). However, Molhave found that a majority of the people suffer from membrane irritation at the 1/10 TLV level. After comparing the guidelines set by each of the organizations it becomes apparent that the creation and maintenance of acceptable indoor air quality is a difficult and complex issue because a generally agreed upon definition of what quantitatively constitutes acceptable indoor air quality has not yet been clearly defined.

**Table 1.1.1:** Emission Rates of Selected Building Materials (Molhave,1982).

<b>Material</b>	<b>Description</b>	<b>Concentration (mg/m<sup>3</sup>)</b>	<b>Specific Emission (mg/m<sup>2</sup>h)</b>
Particleboard	Urea formaldehyde glued	1.56	0.12
Particleboard	Urea formaldehyde glued	1.73	0.13
Plasterboard	12mm, paper board	0.66	0.026
Calcium- Silicate board	22.8 mm board	1.69	0.064
Sealing agent	Plastic compound	169.00	72.0
Sealing agent	Plastic silicone compound	77.90	26.0
Sealing agent	Putty, strips 5X7 mm	1.38	0.34
Insulation batch	Mineral wool	0.38	0.012
Particle board	Urea formaldehyde glued	3.56	0.14
Plywood lining	Teak	1.07	0.044
Wood fiber board	12 mm board	2.96	0.12
Tightening filet	Neoprene/polyethylene	0.81	0.16
Tightening filet	Plasticized PVC	1.05	0.056
Felt carpet	Synthetic fiber/plastic	3.15	0.11
Felt carpet	Synthetic fiber	1.95	0.08
Wall paper	Vinyl and paper	.95	0.04
Wall paper	Vinyl and glass fiber	7.18	0.30
Wall paper	Printed paper	0.74	0.031
Floor covering	Linoleum	5.19	0.22
Wall and floor glue	Water based EVA	1410.0	271.0
Texture glue	Water based EVA	9.81	2.1
Filler	PVA glue/cement	57.8	10.2
Filler	Sand, cement	3.95	0.73
Wall covering	Hessian	0.09	0.0054
Floor covering	Synthetic fiber/PVC	1.62	0.12
Floor covering	Rubber	28.40	1.4
Wall paper	PVC foam	5.50	0.23
Tightening fillet	Heat expanding neoprene	0.35	0.016
Fiber board	Glass fiber/polyester	0.40	0.017
Paint	Acrylic latex	2.00	0.43
Floor Varnish	Epoxy, clear	5.45	1.3
Floor Varnish	Isocyanate	28.90	4.7
Floor Varnish	Acid hardener	3.50	0.83
Wall covering	PVC	2.43	0.10
Laminated board	Plastic	0.01	0.0004
Floor covering	Soft plastic	3.84	0.59
Insulating foam	Polystyrene	40.50	1.4
Insulating foam	Polyurethane	3.59	0.12
Floor covering	Homogenous PVC	54.80	2.3
Floor/wall covering	Textile	39.60	1.6
Floor/wall covering	Textile	1.98	0.083
Cement flag	Concrete	1.45	0.073

A new federal office building located in Portland, OR was the subject of an indoor air quality study by Grot et al. (1991). The level of several VOCs were measured four separate times over a span of 15 months. The measurements were made as the ventilation rates were increased at each measurement, the values were 0.5, 1.36, 0.24, and 1.99 air changes per hour. The total VOC concentration ranged from  $1\text{mg/m}^3$  to  $5\text{mg/m}^3$  and were 1/1000 of recommended OSHA levels which is significantly lower than the 1/10 of the TLVs that OSHA recommended and that has been adopted as a preliminary guide in ASHRAE 62-89. As well, the ventilation rates were also above recommended ASHRAE 62-89 levels. Despite compliance with these standards, 20% of the building occupants rated the air quality as poor with an additional 30% complaining of stuffiness. Headaches, eye irritation, and sleepiness were also reported as complaints of some of the occupants.

**Table 1.1.2:** Emission rates of Organics produced by Humans (Wang, 1975).

Organic Compounds	Typical Concentration 389 people in Class (ppb)	Emission Rates (mg/day per person)	
		Lecture Class 225 People	During Examination
Acetone	20.65±2.8	50.7±27.3	86.6±42.1
Acetaldehyde	4.2±2.1	6.2±4.5	8.6±4.6
Acetic Acid	9.9±1.1	19.9±2.3	26.1±25.1
Allyl alcohol	1.7±1.7	3.6±3.6	6.1±4.4
Amyl alcohol	7.6±7.2	21.9±20.8	20.5±16.5
Butyric acid	15.1±7.3	44.6±21.5	59.4±52.5
Diethylketone	5.7±5.0	20.8±11.4	11.0±7.7
Ethyl acetate	8.6±2.6	25.4±4.8	12.7±15.4
Ethyl alcohol	22.8±10.0	44.7±21.5	109±31.5
Methyl alcohol	54.8±29.3	74.4±5.0	57.8±6.3
Phenol	4.6±1.9	9.5±1.5	8.7±5.3
Toluene	1.8±1.7	7.4±4.9	8.0
Carbon monoxide		48,400±1200	
Ammonia		32.2±5.0	
Hydrogen sulfide		2.73±1.32	2.96±0.68
Carbon Dioxide		642,000±34,000	930,000±52,000

### 1.1.2 Methods to Control Indoor Air Quality

The quality of indoor air can be improved by one of two methods, either elimination of the source of pollutant generation or removal of the pollutants from the air. While it is possible to remove some sources of pollutant generation it would be very difficult to remove all sources. Thus, it will most likely always be necessary to remove some pollutants from the air. This can be achieved by either exchanging the indoor air with outdoor air which is assumed to have a lower concentration of contaminants or to remove or destroy the contaminants by some filtering or conversion process.



Because air that is exchanged between indoors and outdoors must be conditioned, which depending on the ambient weather conditions may or may not be an expensive proposition, it is more desirable to remove the pollutants by some other means than increasing the ventilation rate. Removing pollutants by filtering is thus preferred to infiltration of outdoor air for two reasons, first there is the potential to save a great deal of energy by not conditioning outdoor air, and second it is that it is not necessary to limit the quality of the indoor air to that of the outdoor pollutant levels which depending on the location may not be acceptable.

## **1.2 Research Objective**

It is the objective of this research to measure and model the kinetic and equilibrium adsorption processes of VOCs onto activated carbon bonded filters. Once a model has been developed and verified, the effect of a filter on the indoor air concentrations of VOCs will be explored. The effect of different ventilation strategies and filter parameters will be investigated in an effort to assess both qualitatively and quantitatively the indoor air quality and energy ramifications of the integrated HVAC and carbon filter system design and operation.

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**CHAPTER  
TWO**

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**FUNDAMENTALS OF ACTIVATED CARBON  
FILTRATION****2.1 Adsorption**

The physical phenomena through which activated carbon filtration occurs is adsorption.

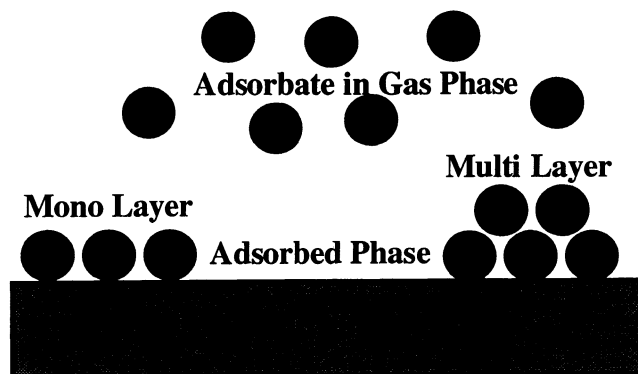
Adsorption is a phase change where molecules in a gas or liquid phase adhere to the surface of a solid, the reverse of which is known as desorption. The surface of an adsorbent with contaminant molecules adsorbed to it is shown schematically in Figure 2.1.1. The molecules that are adsorbed are referred to as the adsorbate, and the solid to which they adsorb is termed the adsorbent. In the case of activated carbon filtration, the contaminant is the adsorbate and the activated carbon is the adsorbent. The adsorption process has many applications, some typical ones include odor control, dehumidification, solvent recovery, and gas chromatography.

Adsorption is typically characterized as being one of two types, physical or chemical.

Chemical adsorption occurs when the bonds between the adsorbate and adsorbent are strong involving the sharing of electrons and it is generally not a reversible process.

Physical adsorption in contrast takes place when the bonds that hold the adsorbate to the

adsorbent are weak intermolecular forces and it typically is a reversible process. The type of adsorption explored in this investigation is physical and all further references to adsorption imply physical adsorption from the gas phase.



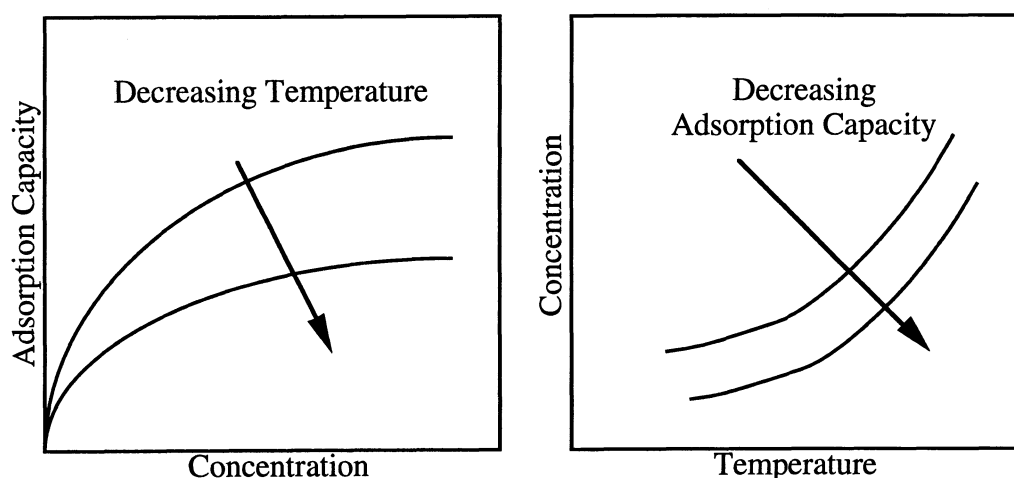
**Figure 2.1.1:** Mono and multi layer adsorption from the gas phase onto an adsorbent.

The weak intermolecular forces responsible for physical adsorption in non-polar adsorbates and adsorbents are dispersion forces. Dispersion forces result from temporary dipoles created by instantaneous shifts of electrons in the electron cloud. Because larger molecules have more electrons which are further away from the nucleus, they usually result in stronger bonds. Since molecule size increases with increasing molecular weight, so does the strength of the adsorptive bonds.

## 2.2 Isotherms and Isoteres

The amount of contaminant that can be adsorbed onto the surface of an adsorbent at equilibrium helps to determine the amount of carbon that might be needed for a particular adsorption application. Temperature and gas phase concentration are two factors that affect the equilibrium capacity of a particular adsorbent for a particular adsorbate. As temperature increases adsorptive capacity decreases and as concentration decreases

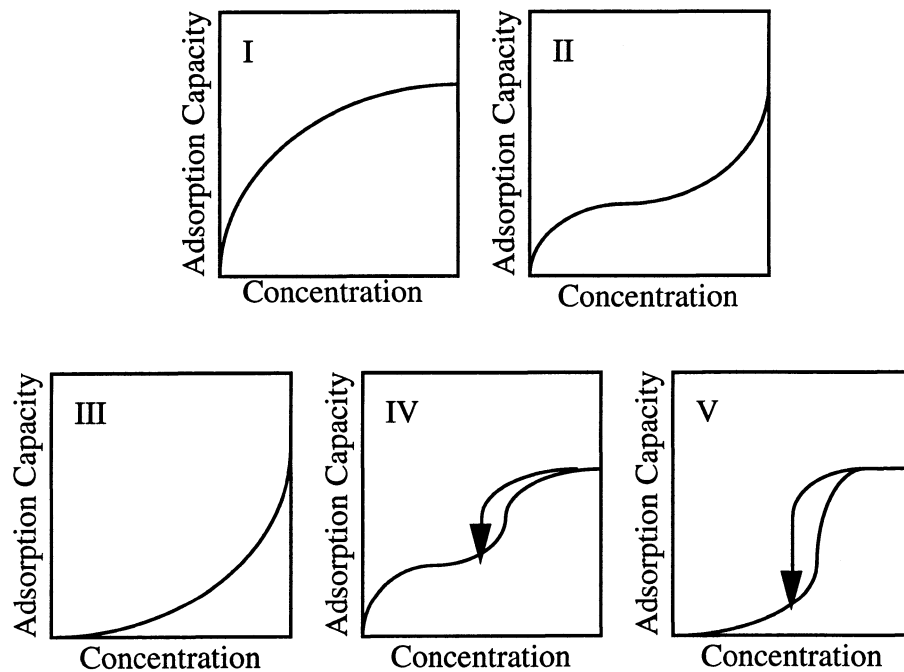
adsorptive capacity decreases. The representation of the equilibrium adsorptive capacity can be represented by either an isotherm or isotere as depicted schematically in Figure 2.2.1. The temperature is held constant in an isotherm with concentration as the independent variable, while in an isotere both the temperature and concentration are independent variables and lines of constant adsorption capacity are shown.



**Figure 2.2.1:** Schematics of an isotherm and an isotere respectively.

There exist many models to predict the isotherm of a contaminant based on a few experimentally derived parameters. Each of the models employs different physical assumptions. Brunauer (1940) has derived a classification system of the typical shapes of isotherms, shown in Figure 2.2.2, and the adsorption mechanisms that lead to them. The type I isotherm is termed the Langmuir isotherm where a single layer of contaminant is formed on the surface of the adsorbent which is limited by complete monolayer coverage. Type I isotherms are the most common for the adsorption of VOC's onto activated carbon. A special case of the type I isotherm is a linear isotherm where the coverage of the monolayer is very small compared to the available area, this is often referred to as the Henry isotherm. Type II is characterized by the formation of multiple

layers of contaminant adsorption. The occurrence of type III isotherms is uncommon and they result from multilayer adsorption also. Both types IV and V reflect capillary condensation and exhibit hysteresis upon desorption.

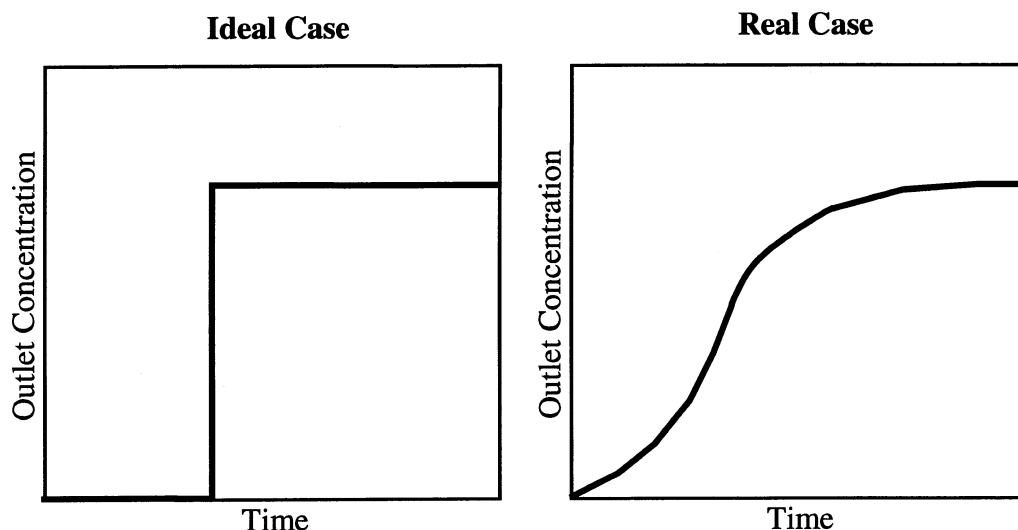


**Figure 2.2.2:** Brunauer isotherm classification system.

### 2.3 Breakthrough Curves

As contaminant passes through an adsorbing media there are resistances to mass transfer onto the media and driving forces that transport the contaminant longitudinally in the gas phase. If these phenomena did not occur, when contaminant entered the filter at a constant concentration there would be zero concentration at the outlet initially until the adsorbent reached its' equilibrium capacity. At that point the outlet concentration would instantaneously step to the inlet value. However, because these processes occur, the

outlet concentration slowly increases from zero to the inlet value as shown graphically in Figure 2.3.1 and is commonly referred to as a breakthrough curve.

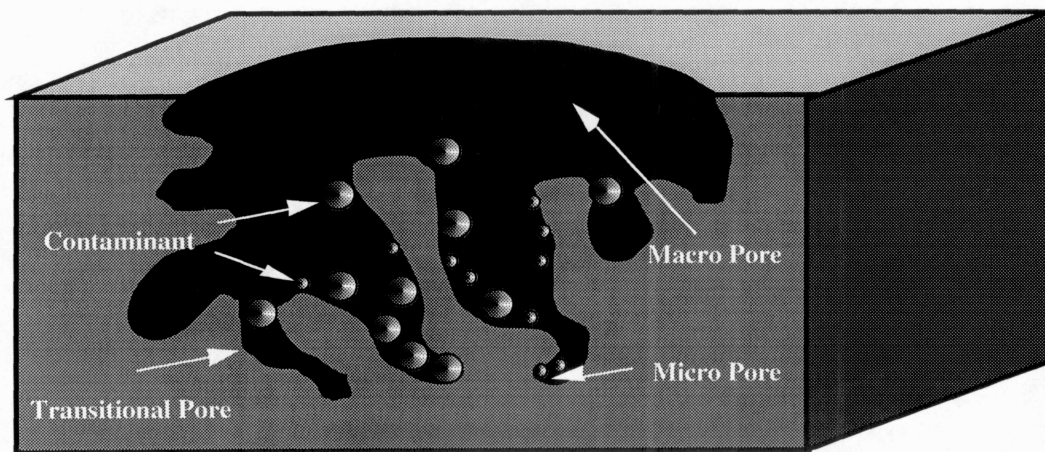


**Figure 2.3.1:** Schematic representation of ideal and real breakthrough curves.

## 2.4 Filters

### 2.4.1 Activated Carbon

Activated carbon is an excellent adsorbent and has been used for hundreds of years as such. Its high surface area, typically  $1000\text{--}1500\text{ m}^2/\text{g}$ , provides a large space for contaminants to adsorb. As well, it contains a wide distribution of pore sizes, schematically depicted in Figure 2.4.1, which makes it suitable for a wide variety of contaminants. The radii of the micropores range from approximately  $6\text{--}7\text{ \AA}$ , the transitional pores  $20\text{--}2000\text{ \AA}$ , and macropores are greater than  $2000\text{ \AA}$ . Approximately 95% of the total surface area is in pores with radii less than  $18\text{--}20\text{ \AA}$ . Additionally, the surface is non polar which tends to makes it hydrophobic and organophilic lending itself towards the filtration of organics.



**Figure 2.4.1:** Cross sectional schematic of activated carbon.

Activated carbon can be manufactured from any carbonaceous material, some typical materials are coconut shells, wood, and coal. The first step in the process is pyrolysis or thermal decomposition of the material at temperatures of approximately 400°C to 600°C. All of the non-carbon matter is removed in this process leaving a structure of micro crystallites of graphite arranged in a random order. In the spaces between the crystals there remains amorphous carbon which must be removed by "activation". The activation process is accomplished with steam or carbon dioxide at high temperature, (700°C-1100°C). The structure that is left behind creates the micropores whose size distribution and pore volume is a function of the base material and the exact process conditions. The final product can be manufactured into powdered, granular, or even fiber form depending on the industrial application.

### 2.4.2 Filter Configurations

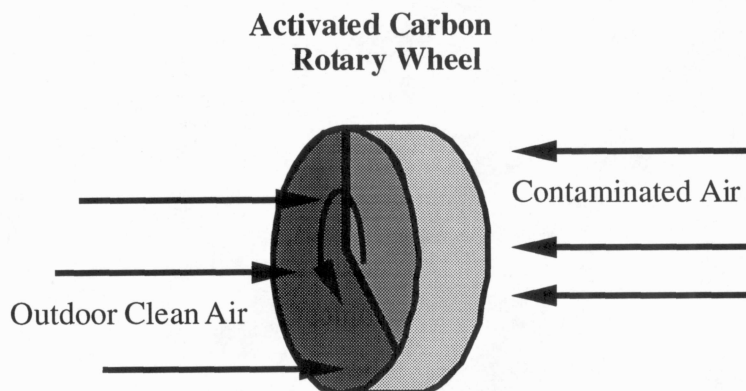
Once the activated carbon is manufactured it can be used in a filter. Filters are produced in many different forms and sizes. Of the more common filters are packed beds of granular carbon, powdered carbon bonded to polyester substrates, woven carbon fibers, and composites of all three.

Packed beds contain the greatest mass of carbon per unit volume and are used in situations that require a large adsorptive capacity like solvent recovery, water purification, and air purification. Unfortunately, packed beds produce large pressure drops which increases the cost of pumping a fluid through them. The cost of fan or pump power must then be weighed against other options.

To remedy the problem of large pressure drops and to make it easier to apply carbon filters to an existing system carbon powder has been bonded to rigid polyester substrates. The bonded filters significantly reduce pressure drop and permit direct installation into a plenum or duct. However, this has the effect of sharply decreasing the amount of carbon contained in a filter thus reducing its' lifetime significantly.

To both reduce the pressure drop and maintain lifetime activated carbon has been applied to rotary wheel technology. The activated carbon is contained in a wheel across which a relatively low pressure drop is experienced. On one part of the wheel an incoming air stream is filtered while on the other part of the wheel another air stream cleanses the filter. The wheel rotates so that the filter is continuously adsorbing and desorbing as shown in Figure 2.4.2. If designed properly, the wheel can operate for an indefinite amount of time without requiring the replacement of the adsorbent material.





**Figure 2.4.2:** Rotary wheel technology application to activated carbon filtration.

### 2.4.3 Application in Larger Systems

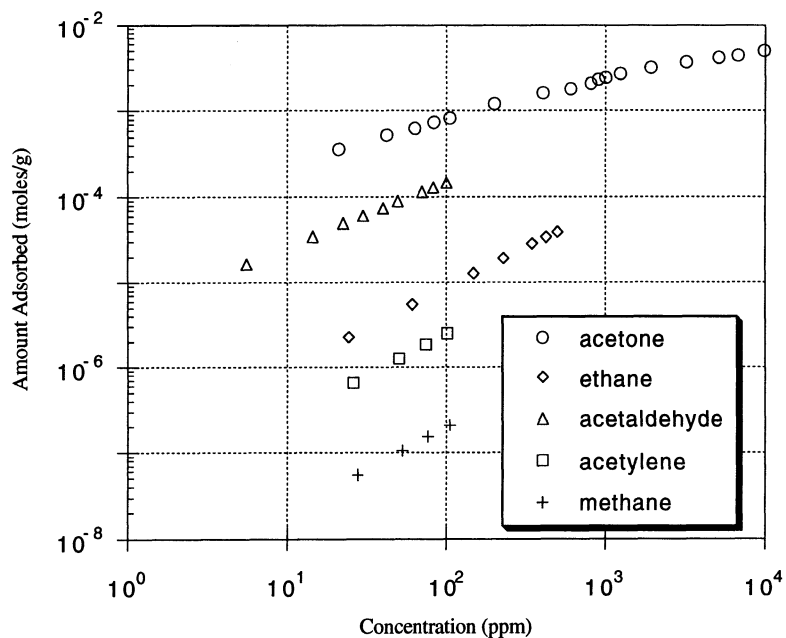
To solve an air quality problem activated carbon adsorption need not be the only method employed. Combinations of several technologies have been used to more effectively take advantage of the virtues of each process. NASA used a catalytic oxidizer in conjunction with an activated carbon bed to maintain the air quality in space craft (Olcott, 1972). As well, there are certain common contaminants that are not compatible with activated carbon adsorption such as ammonia and formaldehyde which must be eliminated by other means. Additionally, desiccant systems can be used to control the humidity of the air streams passing through the filter to control the rates of adsorption and desorption. Thus, when approaching an air quality problem activated carbon may be used in conjunction with other means to most effectively realize its potential.

## 2.5 Literature Survey

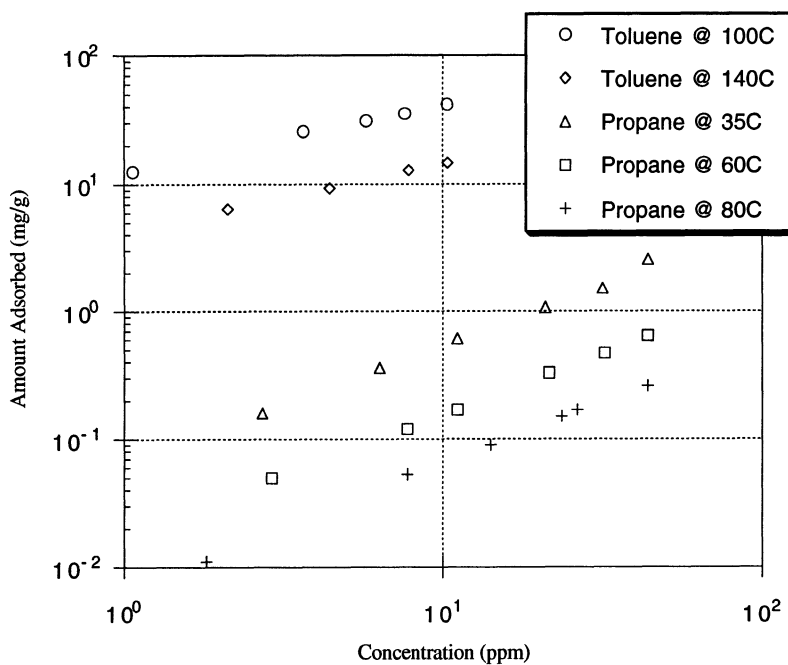
Several authors have investigated the adsorption of VOC's onto activated carbon at concentrations in the low ppm. While these studies have produced some data, there does

not exist a large number of contaminant isotherms in the concentration range typically found in indoor air applications. In an effort to collect the available data Hines et al. (1990) have compiled a literature data base of articles that contain information about the co-sorption of organic and inorganic pollutants from air. Knight (1992) performed a literature search that produced six sources of low concentration isotherm data. In addition to the equilibrium data, the kinetic behavior of adsorbents is an important issue in the design of adsorption equipment not only for adsorption but desorption as well. Studies have been conducted by NASA (Olcott, 1972) , the United States Air Force (Coutant, 1987), and industry that have provided some kinetic and equilibrium data obtained for spacecraft, waste clean up, and indoor air quality applications. A discussion of the findings and a reproduction of some of the data of the aforementioned investigators follows.

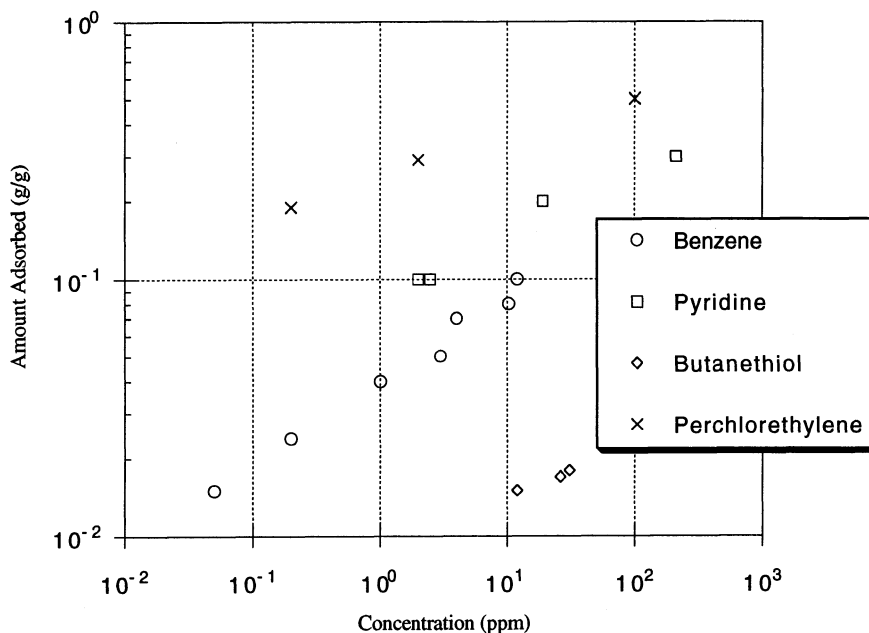
Isotherm data from some of the representative sources identified by Forsythe (1988) Boor (1992) and Clapham (1970) are replotted in Figures 2.5.1 through 2.5.3.



**Figure 2.5.1:** Isotherms at 25°C and 1 atmosphere on Columbia 4LXC 12/28 activated carbon replotted from Forsythe (1988).



**Figure 2.5.2:** Isotherms for G65 50X150 on activated carbon at 1 atmosphere replotted from Boor (1992).



**Figure 2.5.3:** Isotherm data at 70 to 75°F and 1 atmosphere on Pittsburgh PBL activated carbon from Clapham (1970).

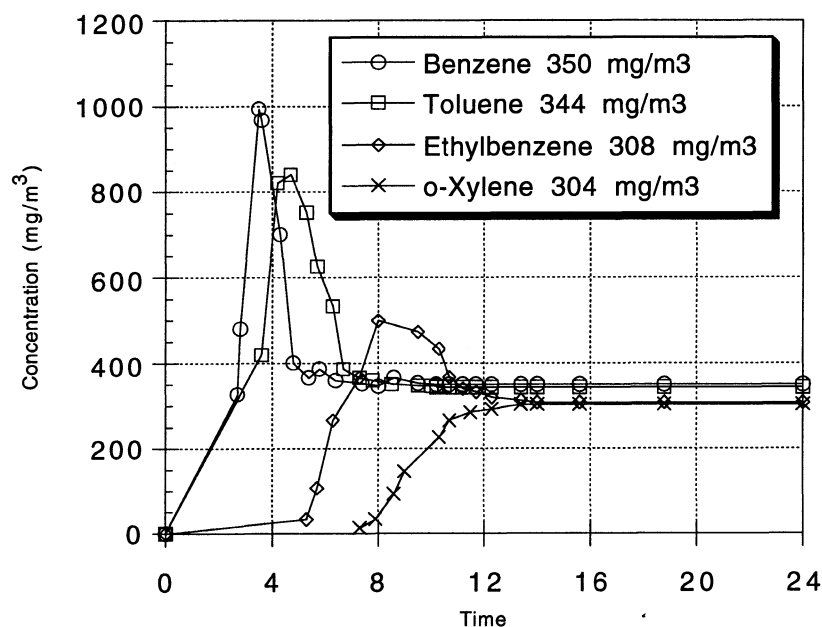
In an effort to remove VOC's from a humidified air stream that had been contaminate during a process used to clean ground water Coutant et al. (1987) examined the effects of temperature, species competition, concentration, and humidity on VOC adsorption. These parameters are also of concern for indoor air quality applications because of the large number of species found in indoor air and the temperature and humidity changes involved in HVAC equipment. The effect of humidity on adsorption processes can be seen from its' affect on equilibrium capacities listed in Table 2.5.1.

**Table 2.5.1:** The effect of relative humidity and temperature on the adsorption of VOC's reprinted from Coutant (1987).

VOC	Concentration (ppm)	Temperature (F)	Relative Humidity (%)	Adsorption Capacity (mg/g)
Benzene	1.65	55	90	0.1
Toluene	1.65	55	90	0.5
Ethyl benzene	1.65	55	90	2.0
o-Xylene	1.65	55	90	3.0
Benzene	1.65	93	25	0.2
Toluene	1.65	93	25	1.2
Ethyl benzene	1.65	93	25	5.7
o-Xylene	1.65	93	25	8.7
Benzene	16.5	55	90	0.9
Toluene	16.5	55	90	4.4
Ethyl benzene	16.5	55	90	14.6
o-Xylene	16.5	55	90	18.1
Benzene	16.5	93	25	48.9
Toluene	16.5	93	25	113.3
Ethyl benzene	16.5	93	25	152.9
o-Xylene	16.5	93	25	112.0

The effect of multiple contaminant mixtures can be seen in the breakthrough curve of an experimental run of four contaminants through an activated carbon bed in shown in Figure 2.5.4. From the figure is apparent that the contaminant mixture separated into its' constituents in the carbon bed and formed zones of high concentration with the more volatile components being pushed towards the outlet. Olcott (1972) expressed that this result gives way to two limiting case scenarios when designing carbon filters. At one extreme the contaminants are assumed to be at such a low concentration that they are adsorbed as if the others were not present. The filter would then be designed for the single contaminant that required the largest filter. The other extreme occurs when the contaminants are at a sufficiently great enough concentration that they cannot coexist in

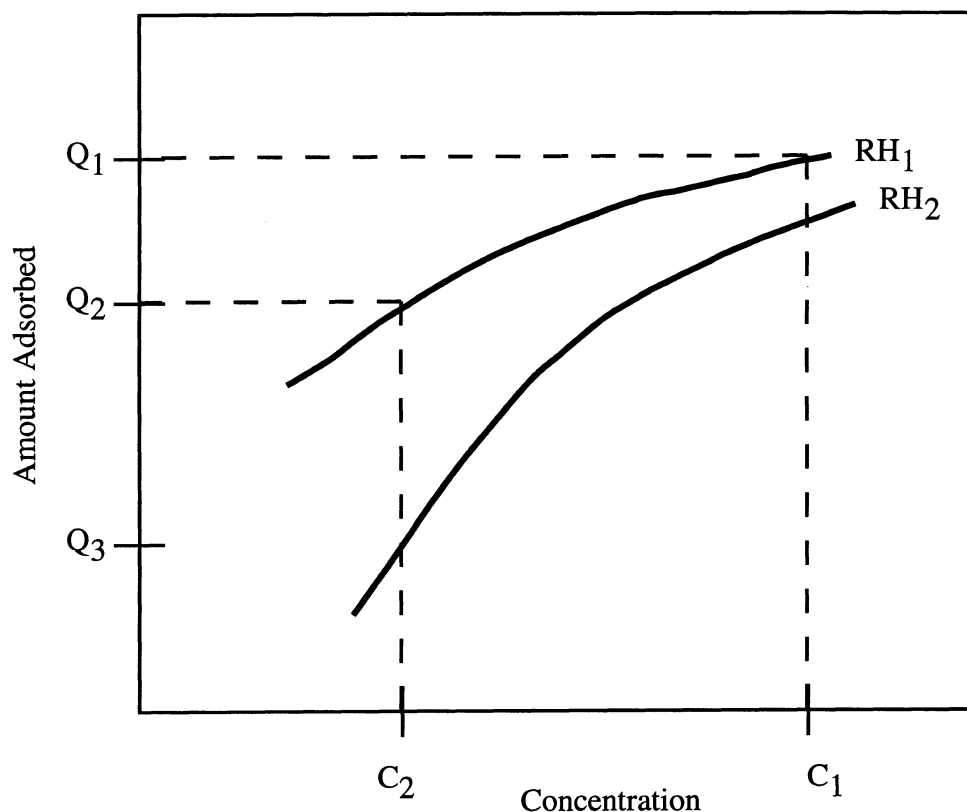
the adsorbed state and a filter large enough to contain each contaminant separately is required. Most situations should lie somewhere between the two extremes.



**Figure 2.5.4:** Multiple contaminant breakthrough curve replotted from Coutant (1987)

While increased humidity most often inhibits the adsorption of VOC's, it can be controlled through the air temperature and the use of desiccants so that humidity is used to ones advantage. In principle it is advantageous to decrease relative humidity for adsorption, which increases the filters capacity for contaminants, and to increase relative humidity for desorption, which decreases the filter's capacity thus aiding in the removal of contaminants from the filter. This basic principle is illustrated by Liu (1992) in Figure 2.5.5 where adsorption occurs indoors, at low humidity and high concentration, RH1 and C1, and desorption is achieved with outdoor air, at high humidity and low concentration, RH2 and C2. Thus, the driving force to desorb the filter for reuse is the

difference between  $Q_1$  and  $Q_3$  rather than  $Q_1$  and  $Q_2$ , thereby accelerating the desorption process.

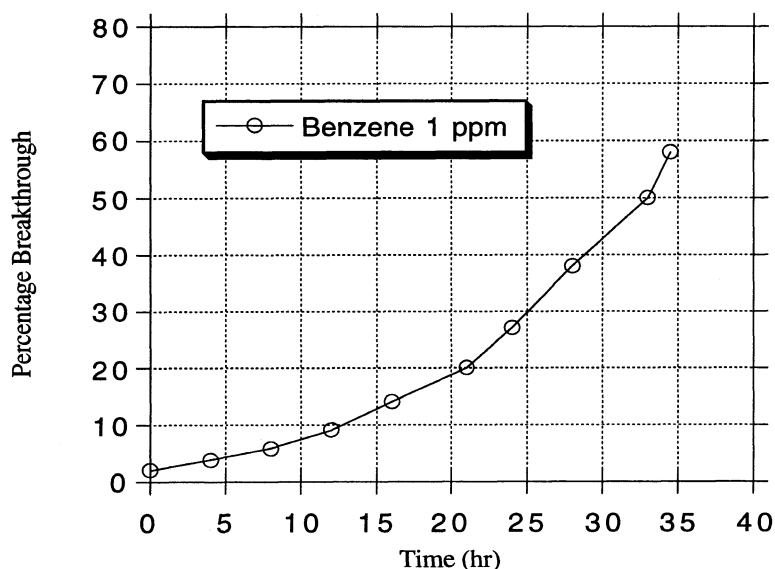


**Figure 2.5.5:** Schematic isotherm shift because of humidity adapted from Liu (1992).

Filter service lifetime was part of the focus of an investigation by Clapham et al. (1970) that explored the application of bonded activated carbon filters because of their adaptability for small installations. A breakthrough curve for Benzene at 1 ppm for a 2.5 inch filter is shown in Figure 2.5.6. The lifetime of the filter is measured in hours rather than weeks or months which is not very useful in an HVAC application. However, Clapham made the observation that,

...when clean air is passed through the carbon filter the contaminant is slowly desorbed at a very low level. This means that in an average residential or commercial air

conditioning system where odors are encountered intermittently the carbon is regaining capacity during those periods when no fresh odor is being generated. Life of a carbon filter in such circumstances could be measured in months or even years.



**Figure 2.5.6:** Breakthrough curve for Benzene at 1 ppm and 100 FPM with a one and one half inch 12X30 BPL bonded filter.

A more conventional approach to filter lifetime and service is provided by Munkelt (1948) in the ASHRAE Refrigerating Engineering Application Data. Where the lifetime of a filter is calculated based on the retentivity of it for a particular vapor under consideration. The retentivity is the percentage of the adsorbent weight of the adsorbate which is retained in the adsorbent after it has been exposed to a saturated concentration of the adsorbate and then placed in a sorbate free atmosphere. The lifetime can then be calculated by Equation 2.5.1 where  $W$  is the weight of the carbon in pounds,  $t$  is time in minutes,  $R$  is retentivity by percentage,  $P$  is the fraction of air which is new and odor free, and  $S$  is the rate of generation of contaminant in pounds per min. This practice disregards the changing capacity for contaminant at different concentrations and the



kinetic behavior of the filters thus assuming that the contaminant passes through as a sharply defined boundary.

$$t = \frac{W \cdot R \cdot (1 - p)}{S \cdot 100} \quad (2.5.1)$$

## 2.6 Summary

There exists experimental data that provides kinetic as well as equilibrium information for the adsorption of VOCs onto activated carbon. As well, the effects of multiple contaminant mixtures, temperature, and humidity on adsorption behavior have been explored by several investigators and their qualitative effects have been documented. All of the results indicate that these factors deviate significantly from the ideal case where the contaminant concentration and kinetic effects are ignored. Thus, to properly engineer an adsorption process the influence of each of these factors must be considered and an appropriate model developed.

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CHAPTER  
**THREE**

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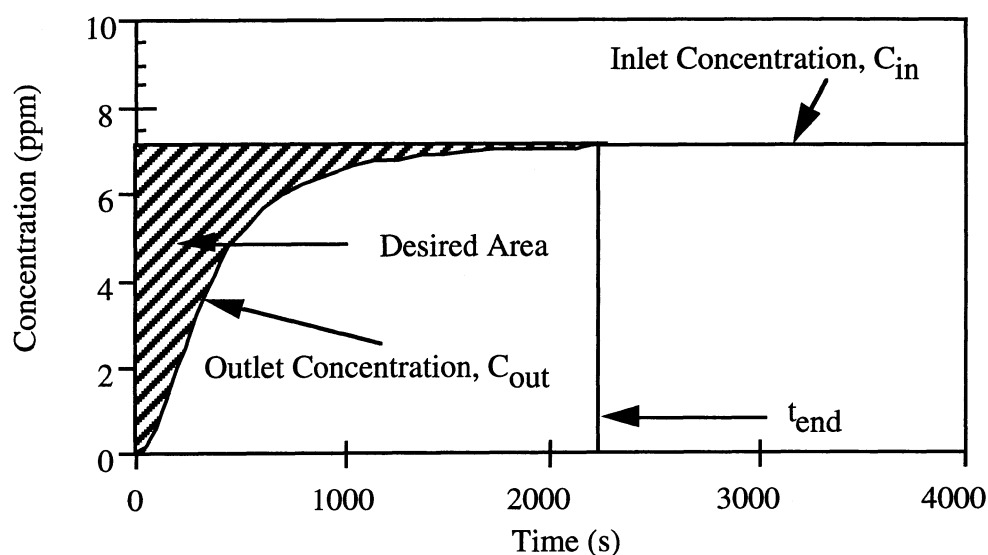
## ADSORPTION ISOTHERM MEASUREMENT

The methods and equipment employed to measure the contaminant isotherm and other adsorption data for the activated carbon bonded filters used in this study are described in the following chapter. The chromatography method termed frontal analysis, which is used to measure the equilibrium capacity of a filter for a given gas phase concentration of a contaminant and ultimately to determine the contaminant isotherm, is discussed. A detailed description of the experimental system and procedures that are used to execute the frontal analysis technique follows. Finally, an examination of the uncertainty associated with the isotherm measurement is presented along with the results.

### **3.1 Frontal Analysis**

The frontal analysis technique is essentially a mass balance on a contaminant stream passing through a gas chromatograph. To perform the mass balance, a known concentration of contaminant is introduced into the inlet of the carbon filter sample in the oven of the chromatograph over a period of time. The contaminant concentration at the inlet of the filter is constant and known, while the outlet concentration of the filter is monitored. The outlet concentration is initially zero and slowly increases as the carbon filter sample becomes saturated with contaminant and eventually equals the inlet

concentration. Once the contaminant concentration in the effluent at the outlet of the filter sample equals the concentration at the inlet the experiment is terminated. To determine the amount of contaminant adsorbed by the filter, the mass of the contaminant that exited at the outlet of filter is subtracted from the mass of contaminant that was introduced into the inlet.



**Figure 3.1.1:** Frontal analysis chromatogram.

The mass of the contaminant that exits the filter at the outlet is calculated from the chromatogram of the experiment, which is a graphical representation of the concentration of contaminant at the filter outlet,  $C_{out}$ , as a function of time as shown in Figure 3.1.1. This particular chromatogram is also commonly referred to as a "breakthrough curve". With the flow rate through the filter known, the mass can be calculated by integrating the area under the breakthrough curve from time zero to  $t_{end}$ . The integrated quantity can then be multiplied by the flow rate,  $F$ , and some constant,  $b$ , which is dependent upon the units of each term, as given by

$$m_{\text{out}} = F \cdot b \cdot \int_0^{t_{\text{end}}} C_{\text{out}} \cdot dt \quad (3.1.1)$$

Once the mass of the contaminant that exited the filter is determined it must be subtracted from the mass of the contaminant that entered the filter at the inlet. With a constant inlet concentration the entering mass is calculated by the product of the flow rate, the constant  $b$ , and the area in Figure 3.1.1 represented by the rectangle with sides  $C_{\text{in}}$  and  $t_{\text{end}}$ .

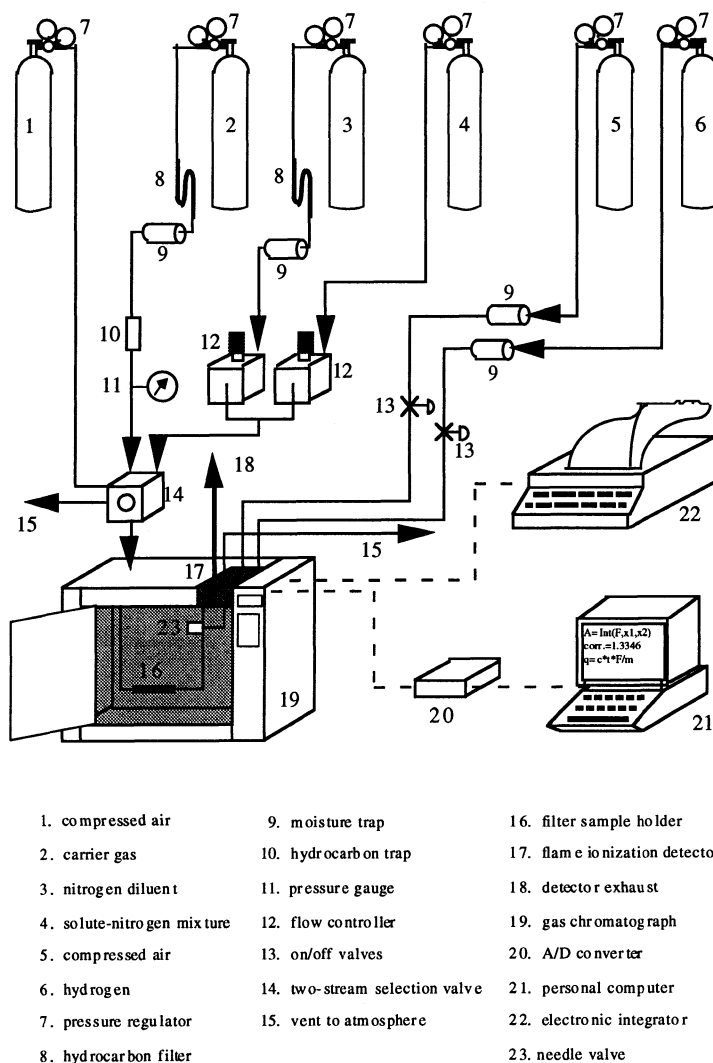
$$m_{\text{in}} = F \cdot b \cdot C_{\text{in}} \cdot t_{\text{end}} \quad (3.1.2)$$

Thus, the amount of contaminant adsorbed per unit mass of carbon for a filter is the difference between Equations 3.1.2 and 3.1.1, divided by the mass of the carbon contained in the filter.

$$q = \frac{m_{\text{in}} - m_{\text{out}}}{m_{\text{carbon}}} \quad (3.1.3)$$

## 3.2 System Components

A schematic representation of the main components in the experimental system is shown in Figure 3.2.1. A brief description of the function that each of the components in the system performs follows.

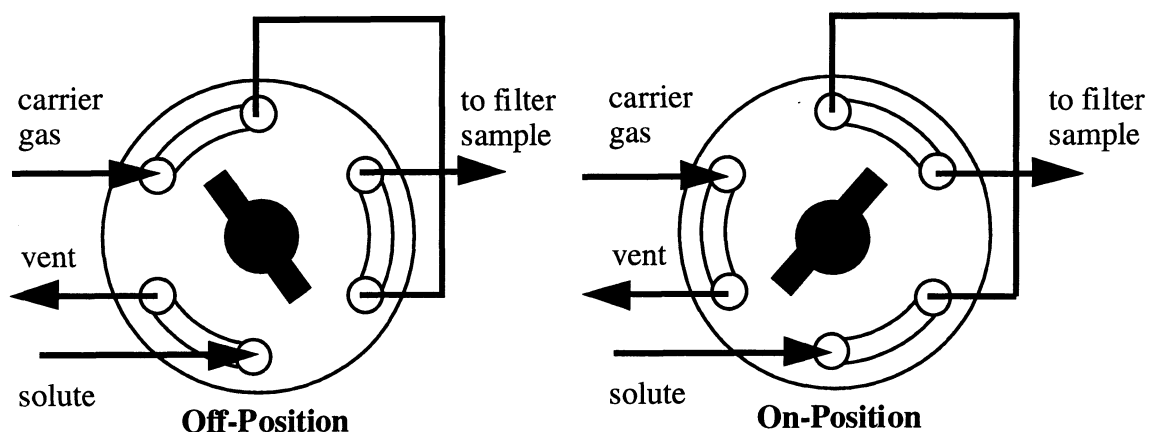


**Figure 3.2.1:** Experimental system components adapted from Schaefer (1991).

### 3.2.1 Gas Chromatograph

The Hewlett-Packard 5890 Series II gas chromatograph is the central piece of equipment in the experimental system. One function of the HP 5890 is to maintain the filter sample at a constant temperature in its oven. The oven is capable of maintaining a constant temperature from slightly above room temperature to 175°C. It cannot maintain

temperatures at or below that of the room because it is not fitted with an optional cryogenic attachment.



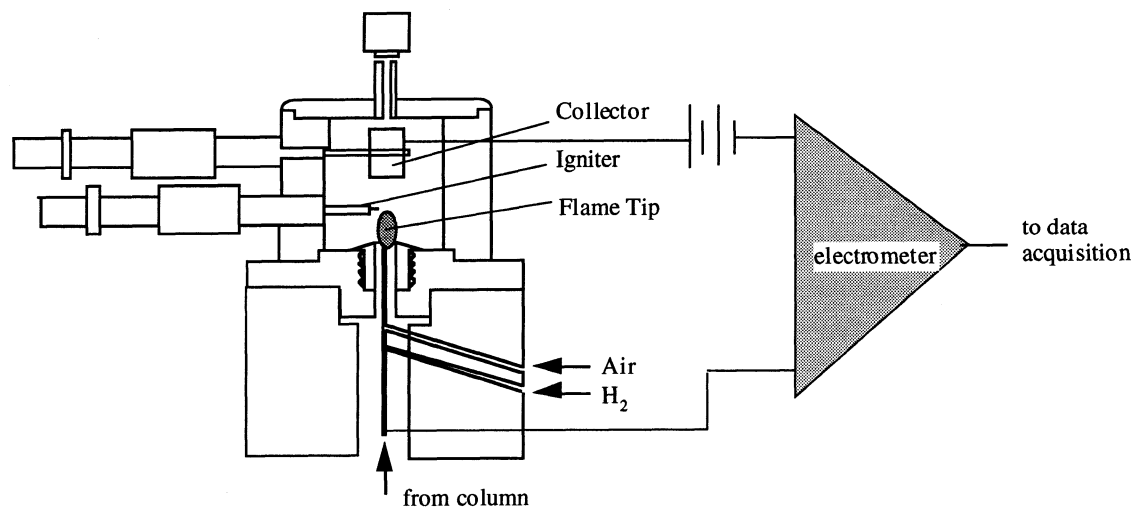
**Figure 3.2.2:** Pneumatic gas stream selection valve adapted from Schaefer (1991).

Control of the gas stream passing through the filter by means of a pneumatic valve, shown in Figure 3.2.2, is also performed by the HP 5890 chromatograph. The valve has been configured to have two positions; in the on position a gas stream of a known contaminant concentration is passed through the filter sample, in the off position pure nitrogen is passed through the filter sample. This task is accomplished through either a manual command from the keypad or as a timed event programmed through the keypad. It is possible to program the control of the pneumatic valve for a time period of up to 650 minutes.

### 3.2.2 Flame Ionization Detector (FID)

The FID measures the concentration of contaminant in the effluent stream of the filter sample. The FID is suitable for use with most organic compounds except those that do not burn or ionize. All organic compounds used in this experiment are appropriate for

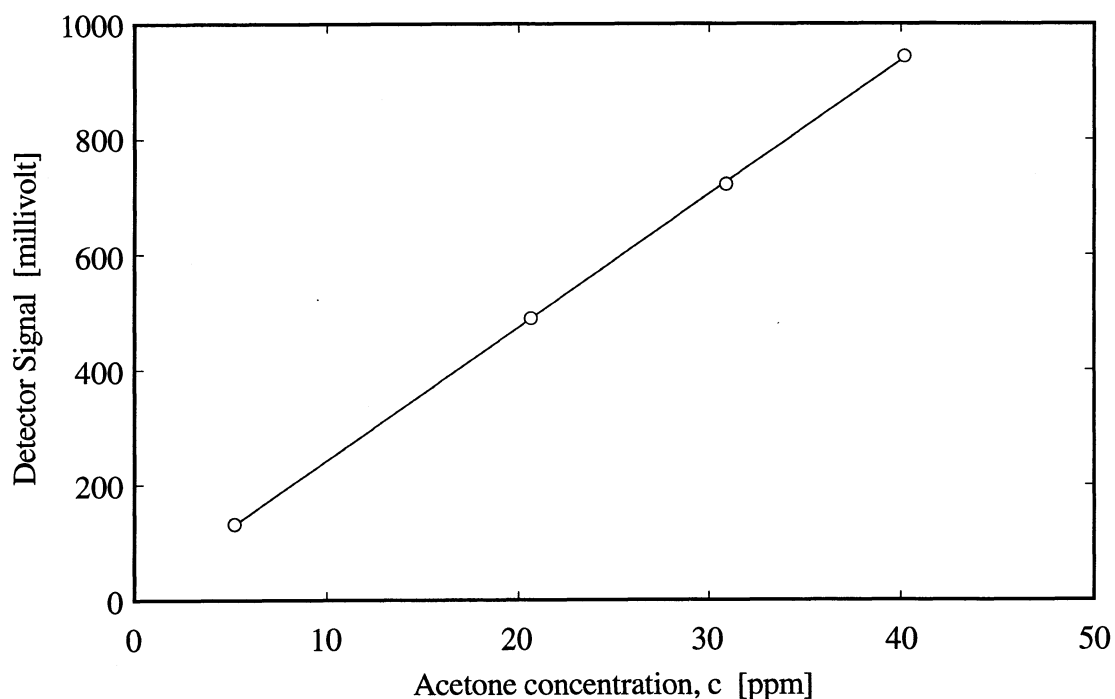
use with the FID. A schematic of the detector is shown in Figure 3.2.3. The operating principle of the detector is the measurement of a current generated by ions that are produced when organic compounds are burned by the detector's flame. The current is passed through a resistor across which a voltage is measured. The current and thus the voltage are proportional to the amount of organic being burned. The voltage is then amplified and recorded. Once the signal is calibrated the concentration of the effluent stream can be determined directly from the FID voltage. Control of the sensitivity of the flame ionization detector (FID) is achieved from the keypad of the chromatograph as well.



**Figure 3.2.3:** Flame Ionization Detector adapted from Schaefer (1991).

An FID rather than a different type of detector was selected because it exhibits linearity over a large range of concentrations. It is typically linear over a range of six orders of magnitude from the minimum detectable concentration. A plot of the response of the detector to effluent concentrations representative of the ones measured in this experiment

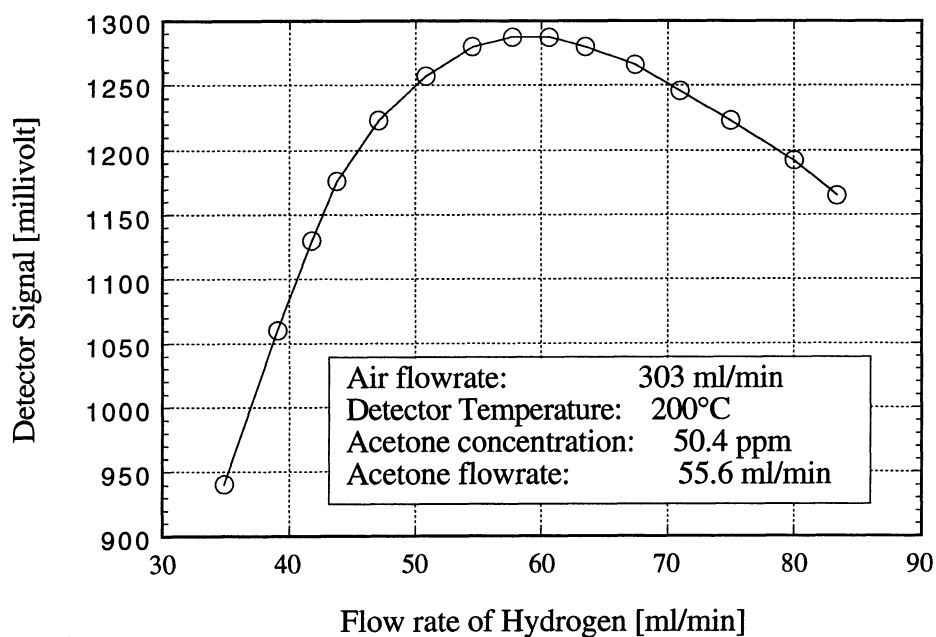
is shown in Figure 3.2.4. The linear response shown in the plot demonstrates the appropriateness of the detector selection to this application.



**Figure 3.2.4:** FID response as a function of acetone concentration from Schaefer (1991).

The sensitivity of the detector is related to the shape and size of its' flame which is in turn a function of the flow rates of the air and hydrogen and jet size. For a given jet diameter the air and hydrogen flow rate can be optimized for greatest sensitivity. The hydrogen flow rate has a greater effect on the sensitivity of the FID than the air flow rate. A plot of the FID voltage for a fixed contaminant concentration and air flow rate versus the flow rate of hydrogen is shown in Figure 3.2.5. The sensitivity of the FID in this system was maximized by adjusting the hydrogen flow rate to approximately 57 ml/min.





**Figure 3.2.5:** FID sensitivity as function of hydrogen flow rate from Schaefer (1991).

Once the flame shape has been optimized for greatest sensitivity it is important to ensure that the maximum signal from the detector does not exceed 1 volt. The output of the FID is an analog signal that ranges from 0 to 1 volt and all information exceeding 1 volt is truncated. The maximum signal is set by the Range 2 command on the chromatograph keypad. The effect of the setting is to enter the value of Range in Equation 3.2.1 where each increase by integer values of the Range parameter lowers the voltage to the PC by one half.

$$\text{Voltage to PC} = \frac{\text{Detector Signal}}{2^{\text{Range}}} \quad (3.2.1)$$

### 3.2.3 Data Acquisition

The components that perform the data acquisition functions of the system are the junction box, Apple IIe personal computer, and Hewlett-Packard 3396A Integrator. The signal from the output of FID goes to the junction box which sends it to the Apple IIe. The personal computer converts the analog signal to a digital signal and records it on floppy disk using data acquisition software. The integrator is used only as a plotter so that real time output of the FID can be monitored to make a determination of when the test should be terminated and to provide a hard copy of the test.

### 3.2.4 Gas Supply

The equipment used to supply the chromatograph with gas is comprised of gas cylinders, flow controllers, moisture traps, hydrocarbon traps, and pressure regulators. Six gas cylinders, two nitrogen, two air, one hydrogen, one contaminant, six pressure regulators, six moisture traps, two hydrocarbon traps, two flow controllers, and one chemical trap were used.

One air cylinder is used to operate the pneumatic valve that selects which gas stream flows through the filter sample. The other air cylinder is connected to the FID and is used to supply the flame. The hydrogen cylinder is also connected to the FID and provides fuel to the flame. One nitrogen cylinder is used to purge the contaminant from the filter during desorption. The other nitrogen cylinder is used to dilute the contaminant gas to obtain different concentrations of contaminant gas. All the nitrogen cylinders have a grade of Ultra High Purity which implies a purity of 99.999% and the contaminant gas cylinder is certified to a  $\pm 5\%$  bias error.

There are moisture traps between all cylinders and their end uses. There is also a hydrocarbon trap between the nitrogen cylinders and their end uses. Additionally, a chemical trap is located between the nitrogen used for desorption and the pneumatic valve.

Every cylinder is fitted with a pressure regulator that brings the tank pressure down to a much lower working pressure. The regulators are designed to maintain a constant working pressure and mass flow rate regardless of changes in the tank pressure. Therefore, once the flow rates are set at the beginning of an experiment they remain constant throughout the entire experiment.

The flow controller is used to mix the diluent nitrogen cylinder and the contaminant gas to achieve the desired concentration at the filter sample inlet. The concentration is adjusted by setting the contaminant flow rate to an estimated required value and measuring it precisely while the nitrogen stream is off. The flow rate of the nitrogen is measured while the contaminant is flowing by subtracting the contaminant flow from the total flow and is adjusted until the desired concentration results. The inlet concentration is calculated by multiplying the concentration of the contaminant cylinder by the fraction of the total flow provided by the contaminant gas cylinder.

### **3.2.5 Flowmeter**

A Hewlett-Packard soap film flowmeter was used to measure the flow rates of all the gases that were passed through the filter sample. The flowmeter was connected to the exhaust of the FID by means of a special adapter that used an o-ring to seal itself. The

flow was measure by initiating a film of soap to form over the inlet to the flowmeter and measuring the time elapsed from the 0.0 ml mark to the 10 ml mark. The flow rate was then equal to the inverse of the elapsed time multiplied by 10 to yield units of ml/min.

### **3.3 Filter Sample and Holder**

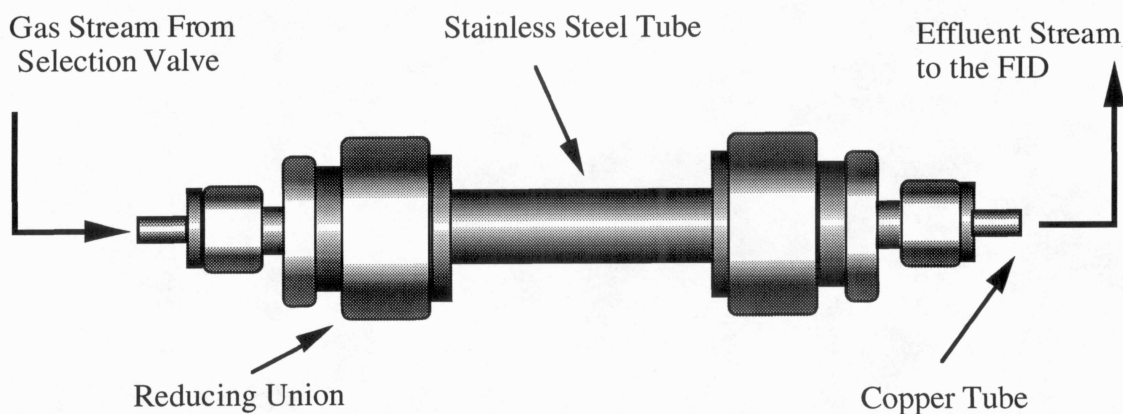
#### **3.3.1 Carbon Filter**

The carbon bonded filter used in this experimental investigation was manufactured by the Lewcote Corporation. The particular filter employed contained 150% add on carbon, meaning that 60% of the weight of the filter was that of the carbon and the remaining 40% was polyester. On a square foot piece of filter there are approximately 49 grams of carbon. Lewcote's designation for this filter is NWPE-12-150. The carbon that was bonded to the filter was manufactured by the Calgon Corporation and is Calgon® Type PCB activated carbon. The specifications for the activated carbon are provided in Appendix A.

The activated carbon bonded filters were investigated rather than the more conventional granular packed bed because they offer some potential advantages. Very little special equipment is needed to implement this type in an existing system. The filters are rigid and free from carbon dust which allows them to be placed directly in a duct or plenum. Another potential benefit is the low pressure drop across the filter as compared to a packed bed thereby reducing fan power costs. However, a drawback of this type of filter is that it contains much less carbon than a conventional packed bed of the same size which minimizes its' overall capacity to adsorb volatile organic compounds.

### 3.3.2 Filter Sample Holder

A piece of equipment was designed to contain a sample of the filter so that the frontal analysis technique could be performed. A schematic of the holder is shown in Figure 3.3.1. The sample holder is essentially a polished stainless steel tube with an outside diameter of a half of an inch and a wall thickness of approximately a thirty-second of an inch. There were many holders manufactured and the length varied from two to 6 inches. The ends of the holder were fitted with stainless steel reducing unions manufactured by Swagelok® to reduce the diameter to a quarter inch. A stainless steel screen was placed inside the unions to prevent any particles of carbon from entering the FID. The sample holder is located inside the oven of the gas chromatograph with the inlet connected to the pneumatic valve which selects the proper gas stream, and the outlet is connected to the FID.



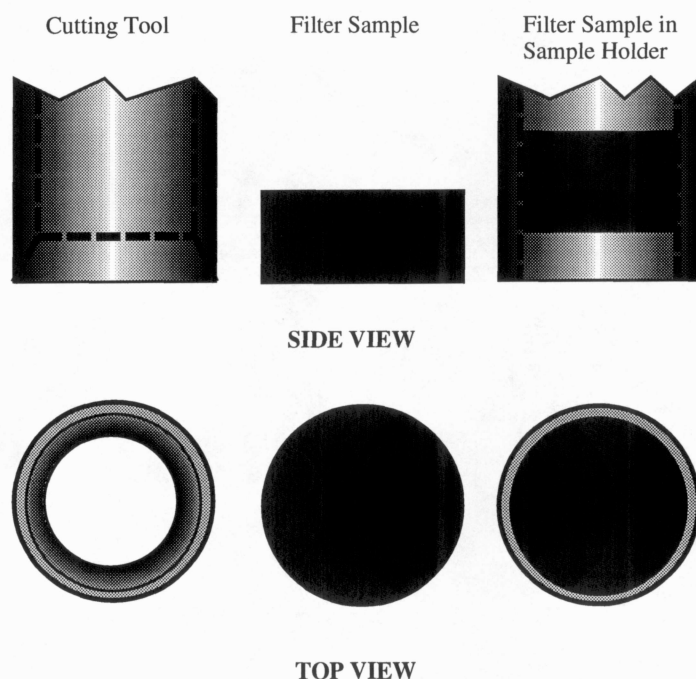
**Figure 3.3.1:** Activated carbon filter sample holder.

### 3.3.3 Filter Sample Preparation

The inside of the filter holder is slightly smaller than one half inch in diameter, and therefore a sample must be cut from the larger filter to be placed inside of it. To perform

this task a piece of the same stock used to manufacture the sample holder was sharpened from the inside diameter to the outside to make a cutting tool for the filter sample. Thus, the pieces of filter that were cut with it were larger in diameter than the inside of the sample holder by twice the wall thickness. The side view and end view of the sample holder, the sample, and the cutting tool are depicted in Figure 3.3.2. The result of this difference in diameter is a snug fit that prevents any part of the contaminant stream from bypassing the filter at its edges.

Preparation of a sample to be tested was performed by first covering the hands with vinyl examination gloves to prevent contaminating the filter with oils through excessive handling. The filter was then placed on a wooden block and the cutting tool pushed into it and twisted. It was then removed from the inside of the cutting tool with a plastic rod and weighed with a digital micro balance. The sample was finally placed inside of the sample holder and lodged about one half of an inch into it with the plastic rod. The reducing unions were then placed on the ends of the holder and secured to the proper fittings inside of the gas chromatograph oven.



**Figure 3.3.2:** Top and side views of the filter sample cutting tool, filter sample, and the filter sample placed in its holder.

## 3.4 Experimental Procedure

### 3.4.1 Pre-Run Execution

Once the sample was installed inside of the gas chromatograph oven a series of operations were performed to prepare for a run to be executed. These operations included oven temperature selection, range selection, flow rate setting, filter desorption, data acquisition initialization, and FID ignition. A description of each operation and the rationale behind each parameter selection follows.

The temperature of the oven was set to 35°C for the measurement of the propane isotherm. It was necessary to ensure that the oven temperature set point was always above the room temperature because the oven temperature control system employs a

heating element only and a fan. 35°C was chosen as a temperature that was high enough above room temperature and low enough to provide data applicable to normal room conditions.

The range parameter set for gas chromatograph was set to a value of one for the concentrations of propane used in this investigation, which ranged from 43.9 ppm to 5.2 ppm.

Adjustment of the flow rate of the contaminant gas stream and the diluent nitrogen stream was usually performed at the end of the previous run because measurement of the flow rate is performed with the soap film flowmeter at the outlet of the filter causing the filter to be contaminated during flow rate measurement. These flow rates were adjusted with the flow controllers to achieve the desired inlet concentration. Thus, the filter sample must be desorbed after flow rate adjustment, prior to the next run. Once the proper flows were attained the On/Off valves at the regulators of the contaminant and diluent nitrogen gas cylinders were turned off until just a few minutes prior to the next run.

After flow adjustment a stream of pure nitrogen was passed through the filter sample to desorb it of any contaminants. The stream of pure nitrogen was initiated by switching the On/Off valve on the pressure regulator of the carrier gas cylinder to on and setting the pneumatic valve to the off position. The desorption was usually performed at the same temperature as adsorption and for a period of approximately 12 hours. This time period was well in excess of the time that should have been sufficient to completely purge the filter of the contaminant, propane, being used in this investigation. Higher temperatures



were not used to increase the rate of desorption because it was observed that temperatures above 50°C had a degrading affect on the carbon filter sample.

The time increment at which the FID output was recorded by the data acquisition software was then selected. The length of the time increment parameter was dependent on the length of the run. The runs for propane as the contaminant typically took approximately 5 or 6 hours and the logging time increment was set at one minute.

The On/Off valves on each of the regulators for each of the gas cylinders were turned to the on position several minutes prior to run execution so that steady state conditions were achieved. Even though the contaminant gas was flowing, the pneumatic valve was in the off position, directing only pure nitrogen to the filter sample and the contaminant gas to the fume hood.

The hydrogen and air On/Off valves at the FID were then switched to the On position and the FID was ignited. Once the FID was ignited, all the gas streams were flowing at steady state, and the ready indicator light on the chromatograph indicated that the set oven temperature was established, the system was ready to begin an experimental run.

### **3.4.2 Run Execution**

To execute the run all that was necessary was to start the data acquisition program, switch the pneumatic stream selection valve on the gas chromatograph to the on position, and enter the plot command to the integrator keypad. The sequence and timing of those events was determined by two factors; the length of time it takes for the contaminant gas

stream to travel from the stream selection valve to the FID, and the logging time interval of the data acquisition software.

Using an empty filter sample holder and the response of the FID, it was determined that the contaminant travel time from the pneumatic stream selection valve to the FID for a volumetric flow rate of 55 ml/min. at an oven temperature of 35°C was approximately 15 seconds. The oven temperature is important because the volumetric flow rate is measured at room temperature and the travel path is at the oven temperature. Therefore, to maintain continuity the velocity in the travel path is dependent on temperature.

The data acquisition software takes approximately 25 seconds to initialize and then pauses for the length of the period between data loggings before the first measurement is logged. For example, if the program is set to record the FID output every 60 seconds then there would be a 85 second delay from the moment the command was entered to the recording of the first point.

The time period between entering the command into the personal computer to begin logging, and switching the pneumatic stream selection valve to the on position, is equal to the data acquisition time delay less the contaminant travel time. There is no delay between the time that the integrator is instructed to begin plotting and the time that plotting begins. That instruction is entered after the stream selection valve is switched on by a time delay equal to the contaminant travel time. The exact timing and sequence of events in the previous example would be as follows; the command to begin logging would be given to the PC, 70 seconds later the pneumatic stream selection valve would be switched

to the on position, and 15 seconds later the integrator would be instructed to begin plotting.

After the outlet concentration reached 99% of the inlet concentration the experiment was allowed to collect approximately 200 more data points before it was terminated. It was determined by Boor (1992) that this was the number of data points after which the calculated adsorbed quantity of contaminant would not change. These points were required to eliminate the effect of noise on the calibration of the FID voltage to the inlet concentration.

### **3.4.3 Post-Run Analysis**

A sample analysis of a raw data file collected during one of the experimental runs used to calculate the propane isotherm follows. The abbreviated raw data file is shown in Table 3.4.1. The start time must be zeroed because the data acquisition program uses the computer clock card and does not start at zero and the FID does not begin at zero voltage. The resulting manipulated data file is also shown in Table 3.4.1. A chromatogram or breakthrough curve can then be constructed from this data as shown in Figure 3.4.1. Based on the frontal analysis method, Boor et. al. (1992) developed a consistent analytical procedure to calculate the quantity of contaminant adsorbed by the carbon filter from the chromatogram obtained with this experimental system. That procedure is used here to calculate that quantity with the data file in Table 3.4.1.

**Table 3.4.1:** Raw and Manipulated data file from an experimental run.

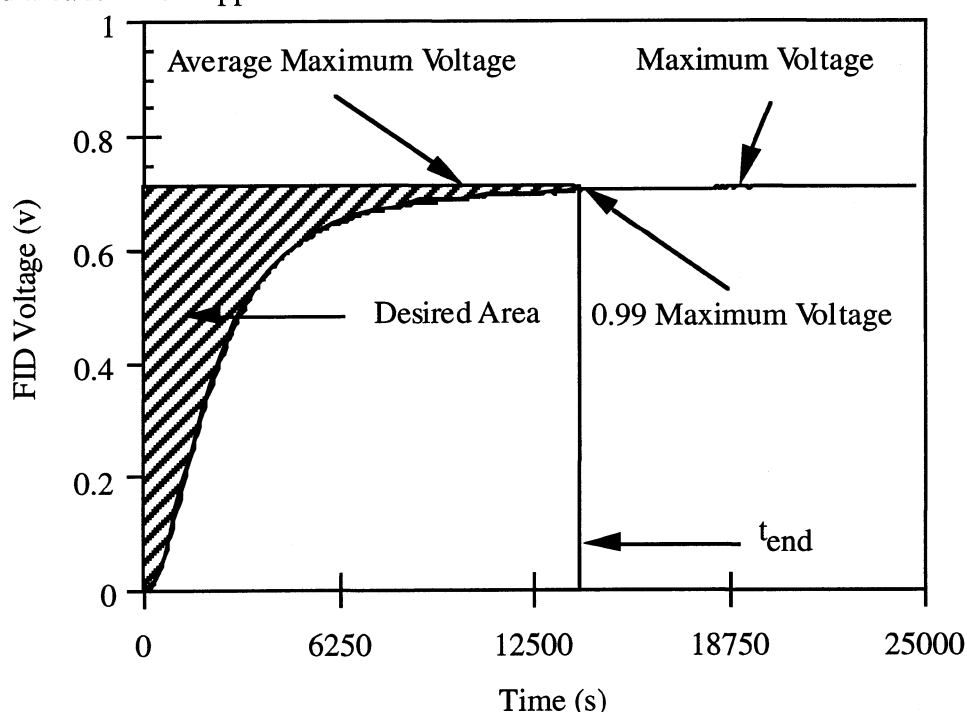
Raw Data		Manipulated Data		
Time(s)	Signal(v)	Time(s)	Signal(v)	Signal(ppm)
39789	0.00834	0.0000	0.00000	0.00000
39847	0.00834	58.000	0.00000	0.00000
39910	0.01126	121.00	0.00291	0.18093
39965	0.01418	176.00	0.00583	0.36186
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
53589	0.71286	13800	0.70451	43.656
53645	0.71286	13856	0.70451	43.656
53710	0.71286	13921	0.70451	43.656
53766	0.70994	13977	0.70159	43.475
.	.	.	.	.
.	.	.	.	.
64268	0.72120	24479	0.71286	44.173
64326	0.72120	24537	0.71286	44.173
64391	0.72120	24602	0.71286	44.173
64447	0.72120	24658	0.71286	44.173

The first step in the analysis procedure was to find the maximum voltage, including any noise. The maximum voltage for the data file in Table 3.4.1 was 0.7129 v. The first time at which 99% of this voltage occurs is considered the point at which the outlet concentration reaches equilibrium with the inlet concentration, this is  $t_{end}$ . The first time that this occurs in the example is at 13800 seconds. The average of every point after that time is then considered to be the value for the average maximum voltage which corresponds to the inlet concentration, which in this case is 0.7085 v. The area under the curve was then integrated numerically from 0 to 13800 seconds and is equal to 7793

vs. That area was then converted to units of ppms by calibrating the average maximum voltage to the inlet concentration.

$$C(\text{ppm}) = \frac{C_{\text{max}}(\text{ppm})}{V_{\text{max}}(\text{v})} \cdot \text{FID signal}(\text{v}) \quad (3.4.1)$$

An area of 605820 ppms is calculated in this example, which represents the contaminant that exited the outlet of the filter. To determine the amount of propane that was adsorbed by the filter this area must be subtracted from the total area of contaminant that entered the inlet of the filter represented by a rectangle with the from time zero to  $t_{\text{end}}$ . The resulting desired area is 122929 ppms.



**Figure 3.4.1:** Chromatogram constructed from the data collected during an experimental run.

The desired area can then be used to determine the amount of propane adsorbed per gram of carbon bonded to the filter sample using the relation.

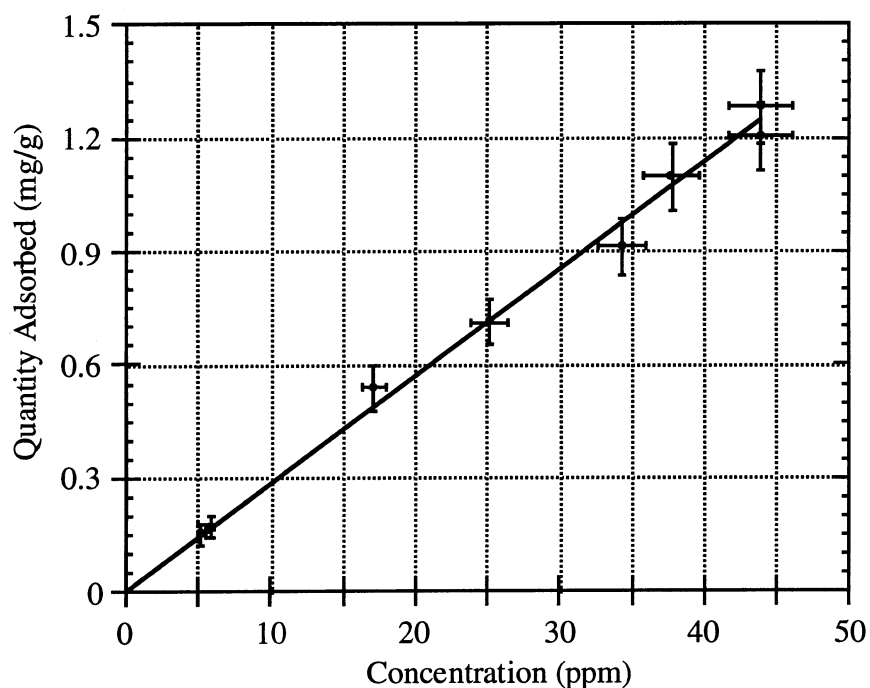
$$q = b \frac{F \cdot A \cdot \rho_{N_2}}{m_c} \quad (3.4.2)$$

Where  $b$  is a function of the atmospheric pressure and temperature,  $A$  is the desired area calculated previously from the chromatogram, and  $m_c$  is the mass of the carbon bonded to the filter sample. All of the adsorption calculations are included in an EES® worksheet located in Appendix B. The quantity adsorbed in the example was 1.206 mgpropane/gc.

### 3.5 Results

An isotherm for propane on activated carbon bonded filters at 35°C was measured employing the experimental methods and system described previously. The filter was manufactured by the Lewcott Corporation with the designation Activfilter™ ACF-NWPE-12-150. The designation denotes that the filter is comprised of a non-woven polyester substrate weighing 284 g/m<sup>2</sup> having a nominal thickness of 1.27 cm with activated carbon bonded to it in the amount of 150% of the weight of the substrate. The isotherm was measured for a range in concentration from approximately 5 to 44 ppm and is shown in Figure 3.5.1 fit to a straight line using a least squares fitting routine.

### Propane Isotherm @35C for Activfilter™ 12-150



**Figure 3.5.1:** Measured propane isotherm.

As was expected from the literature the isotherm is linear. However, the capacity of the activated carbon contained in the filter is much less than for similar carbons in granular form as reported by Boor (1992). This difference may result from the process of bonding the carbon to the substrate which renders a large amount of the surface area of the carbon inaccessible for adsorption.

### 3.6 Uncertainty Analysis

A very rigorous examination of the uncertainty error contained in measurements made using this experimental system was conducted by Boor (1992). The experimental system used by Boor was identical to the one used here with the exception of the filter sample

and sample holder. The additional uncertainty error associated with these pieces of equipment will be considered after a brief summary of the major topics analyzed by Boor.

The uncertainty associated with a measurement is formed from two components, bias error and precision error. The bias error is the amount the average measurement made differs from the true value. The precision error is an indication of how close each individual measurement is to the average measurement. The precision error thus indicates the repeatability of a measurement while the bias indicates its trueness. The error can then be combined as a root sum square error with a confidence of 99% if the errors are of the same magnitude.

The measurement of the capacity of the filter sample is a function of four variables as indicated by Equation 3.4.2. Because all of the variables are independent the bias and precision error can be expressed as Equation 3.6.2 and 3.6.3.  $U_B$  and  $U_P$  represent the bias and precision error respectively. The total error can then determined from Equation 3.6.4. The error for each measurement made in the calculation of the isotherm are represented by error bars in Figure 3.5.1.

$$U_B^2 = \left(\frac{\partial q}{\partial F}U_{BF}\right)^2 + \left(\frac{\partial q}{\partial A}U_{BA}\right)^2 + \left(\frac{\partial q}{\partial \rho_{N_2}}U_{B\rho_{N_2}}\right)^2 + \left(\frac{\partial q}{\partial m}U_{Bm}\right)^2 \quad (3.6.2)$$

$$U_P^2 = \left(\frac{\partial q}{\partial F}U_{PF}\right)^2 + \left(\frac{\partial q}{\partial A}U_{PA}\right)^2 + \left(\frac{\partial q}{\partial \rho_{N_2}}U_{P\rho_{N_2}}\right)^2 + \left(\frac{\partial q}{\partial m}U_{Pm}\right)^2 \quad (3.6.3)$$

$$U_T = \sqrt{U_B^2 + U_P^2} \quad (3.6.4)$$

The bias and precision errors as determined by Boor (1992) for the terms in Equations 3.6.2 and 3.6.3 are as follows:



## Bias errors and sources

UB<sub>m</sub>: bias uncertainty caused by mass balance,  $\pm 0.00007$  gram

UB<sub>F</sub>: bias uncertainty for flow rate, (ml/min.)

flowmeter :  $\pm 2.5\%$  (ml/min) for both 1.0 and 10.0 ml volumes

time : one-half least significant digit of clock,  $\pm 0.05$  seconds

UB<sub>A</sub>: bias uncertainty for area, (ppms)

A/D converter :  $\pm 0.0012$  volt

FID :  $\pm 0.001$  volt (assumed)

contaminant

concentration :  $\pm 5.0\%$  for all contaminants

time :  $\pm 1.0$  second (applied to area determination)

UB<sub>pN2</sub>: bias uncertainty for density, (gmole/m<sup>3</sup>)

temperature : one-half least significant digit of thermometer,  $\pm 0.5$ K

gas constant : property value assumed to have an error of  $\pm 2\%$

pressure :  $\pm 1.7$ pa, negligible relative to the average total pressure of 98,508 pa.

## Precision errors and sources

UP<sub>m</sub> : precision uncertainty caused by mass balance,  $\pm 0.00005$  gram

UP<sub>F</sub> : bias uncertainty for flow rate, (ml/min.)

High flow rate :  $\pm 0.8$  ml/min

Low flow rate :  $\pm 0.5$  ml/min

UP<sub>A</sub>: precision uncertainty for area, (ppms)

t<sub>end</sub> : error for time at end of test; 0.5 seconds

Avg. V<sub>max</sub> : error caused by noise in signal; 0.005 volts

UP<sub>pN2</sub>: precision uncertainty for density, (gmole/m<sup>3</sup>)

pressure :  $\pm 2.7\%$

The additional error caused by the filter sample and holder are difficult to determine. The difficulty results from the inability to measure the mass of carbon bonded to the filter independently. Only the entire filter sample could be weighed and then multiplied by the fraction of the weight the manufacturer states is carbon. Error arises from variations in the true percentage of weight of the activated carbon contained in a filter sample.

However, measurements at 43.9 ppm were repeated using eight individual filter samples from different locations on a 0.5 ft<sup>2</sup> piece of filter material in four experiments and the measurements agreed within 5.1%.

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**CHAPTER  
FOUR**

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**MASS TRANSFER PROCESSES IN CARBON  
BONDED FILTERS**

Mathematical model of varying complexity have been proposed to describe the transport of mass through an adsorbing media. Two such models that employ a simplified approach are presented: the single parameter diffusion model and the mass transfer resistance model. Both models employ three basic assumptions to simplify the analysis; flow through the filter is uniform and in one dimension, the boundary conditions experience only step changes in concentration, and that there is a single contaminant and its' isotherm is linear. A development of the differential mass balance for the processes and the solution to each model follows.

**4.1 Governing Differential Equations**

A differential element of the carbon filter is shown in Figure 4.1.1. It is assumed that mass is transported through the filter as the sum of two components. The first component being convective and equal to the velocity of the gas contaminant stream,  $u$ , multiplied by the gas phase contaminant concentration,  $C$ . The second is the mass flow resulting from longitudinal diffusion,  $m_d$ , which is proportional to the gas phase concentration gradient as expressed by,

$$m_d(z,t) = D_L \cdot \frac{\partial C}{\partial z} \quad (4.1.1)$$

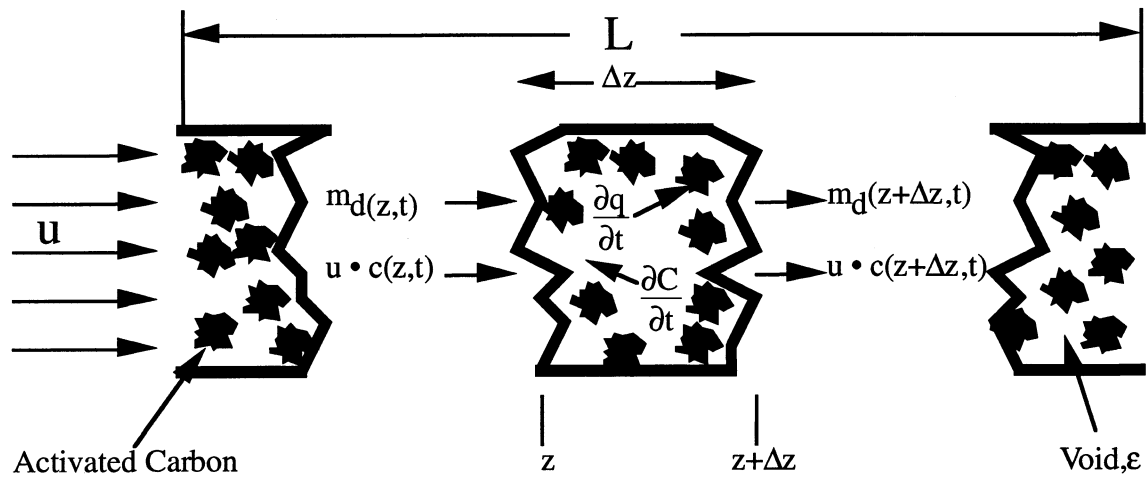
A mass balance on the differential element then yields Equation 4.1.2, where  $\frac{\partial q}{\partial t}$  is the storage term in the adsorbed phase as expressed in Equation 4.1.3 and  $\frac{\partial C}{\partial t}$  is the storage term in the gas phase. If the limit of Equation 4.1.2 is taken as  $\Delta z$  goes to 0 the resulting differential equation takes the form of Equation 4.1.4.

$$\begin{array}{ll} \text{Diffusion term} & \text{Convection term} \\ -D_L \cdot \left( \left[ \frac{\partial C}{\partial z} \right]_{z+\Delta z} - \left[ \frac{\partial C}{\partial z} \right]_z \right) + u \cdot ([C]_{z+\Delta z} - [C]_z) & \end{array} \quad (4.1.2)$$

$$\begin{array}{l} \text{Storage term} \\ = \left( \frac{\partial C}{\partial t} - \left( \frac{1-\epsilon}{\epsilon} \right) \frac{\partial q}{\partial t} \right) \cdot \Delta z \end{array}$$

$$\frac{\partial q}{\partial t} = B \cdot (q(z,t) - q_*) \quad (4.1.3)$$

$$-D_L \cdot \frac{\partial^2 C}{\partial z^2} + u \cdot \frac{\partial C}{\partial z} + \frac{\partial C}{\partial t} + \left( \frac{1-\epsilon}{\epsilon} \right) \cdot \frac{\partial q}{\partial t} = 0 \quad (4.1.4)$$



**Figure 4.1.1:** Differential element of a carbon filter.

To solve this differential equation, each of the two models makes one of two additional simplifying assumptions. Those assumptions are either that there is no mass transfer due to longitudinal diffusion or that there is no resistance to mass transfer.

## 4.2 Single Parameter Diffusion Model

### 4.2.1 Assumptions

The single parameter diffusion model employs the additional assumption that there is no resistance to mass transfer from the gas state to the adsorbed state. Thus, the coefficient  $B$  in Equation 4.1.3 becomes infinite and the mass of contaminant in the adsorbed phase is assumed to be in equilibrium with the gas phase concentration at all times. Thus, if the gas phase concentration at a point is known the adsorbed phase concentration can be determined from the contaminant isotherm. Equation 4.1.3 can now be restated as,

$$\frac{\partial q}{\partial t} = K \cdot \frac{\partial C}{\partial t} \quad (4.2.1)$$

#### 4.2.2 Solution

The solution to a step input in concentration at the inlet of the filter to this equation has been reported by many investigators including Forsythe (1988) and Famularo, et al. (1980). Aside from a few differences in notation, the solution that follows will be that of Madey (1981) et.al. The boundary conditions can be stated as

$$C(z,0) = 0 \quad (4.2.2)$$

$$C(0,t) = C_0 \quad (4.2.3)$$

The solution for the concentration at the outlet can then be stated as a fraction of the step input given by,

$$F = \frac{1}{2} \cdot \exp\left(\frac{1}{\Delta}\right) \cdot \operatorname{erfc}(S_+) + \frac{1}{2} \cdot \operatorname{erfc}(S_-) \quad (4.2.4)$$

where

$$\Delta \equiv \frac{D_L}{u \cdot L} \quad (4.2.5)$$

$$t_p \equiv \left[ \frac{(1-\epsilon) \cdot K}{\epsilon} + 1 \right] \cdot \frac{L}{u} \quad (4.2.6)$$

$$S_{\pm}(t) \equiv \frac{1}{2 \cdot \sqrt{\Delta}} \left[ \sqrt{\frac{t_p}{t}} \pm \sqrt{\frac{t}{t_p}} \right] \quad (4.2.7)$$

Thus, for a filter at equilibrium with constant gas and solid phase concentrations of contaminant throughout, this solution will calculate the outlet concentration for a step change in inlet concentration. The solution is valid for both positive and negative steps in

inlet conditions and because the differential equations are linear they can theoretically be superimposed to solve for more complex boundary conditions.

#### 4.2.3 Diffusion Coefficient Fitting and Model Verification

Verification of the single parameter diffusion model was conducted by comparing the solution to the differential equation with the real data obtained from the experimental setup used to measure the propane isotherm. All of the parameters used in the solution were measured or calculated with the exception of the diffusion coefficient. The coefficient could not be derived analytically because it is a lumped parameter that accounts for the effects of a large number of resistances and driving forces. Therefore, the diffusion coefficient was fitted with a least squares regression analysis in comparison to the real data.

The void fraction,  $\epsilon$ , represents the volume of the filter that is not occupied by carbon and was calculated by

$$\epsilon = 1 - \frac{m_c \cdot \frac{1}{\rho_c}}{V_{\text{filter}}} \quad (4.2.8)$$

where  $\rho_c$  is the bulk density of the carbon and  $V_{\text{filter}}$  is the volume of the filter. The void fraction of the filters used in this investigation was 0.906. The isotherm constant,  $K$ , was derived from the slope of the isotherm measured for propane.  $K$  can be calculated as,

$$K = \frac{q [\text{moles/m}^3]}{C [\text{moles/m}^3]} \quad (4.2.9)$$

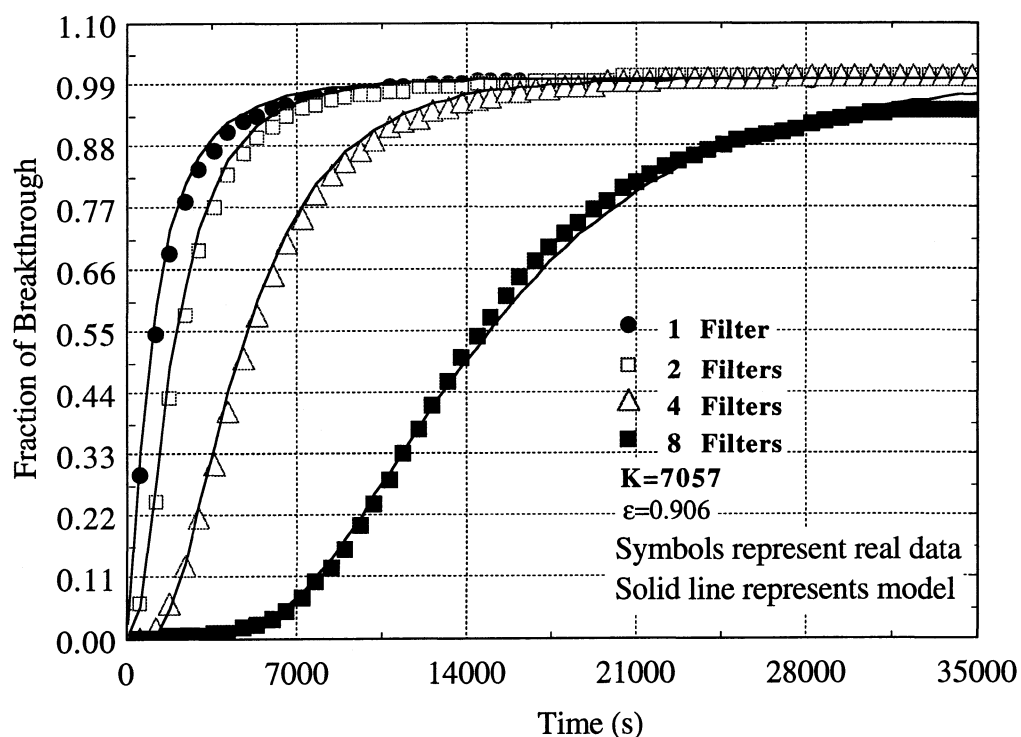
where  $q$  is equal to the amount of contaminant in units of moles that was adsorbed per  $\text{m}^3$  of carbon, and  $C$  is in units of moles of contaminant per  $\text{m}^3$  of gas phase. The dimensionless value for  $K$  obtained from the isotherm in Figure 3.5.1 was 7057. Because the filter sample was small and the length may not necessarily reflect the amount of carbon contained in it, the filter length used in the model was based on the weight of the sample. A conversion factor of weight to length was calculated using the nominal filter length of one half of an inch and an average filter sample weight based on the manufacturers specifications. The value of the length to weight conversion factor was calculated as 0.190 meters per gram of carbon.

Four breakthrough curves with four filters of length 1.70, 2.61, 5.61, and 11.0 cm were measured. The filter lengths greater than 1.70 cm were obtained by placing multiple filter samples in series. The data was then used to fit the diffusion coefficient using a least squares regression analysis for each of the filters. The parameters and results of each of the experimental runs are shown in Table 4.2.1 and Figure 4.2.1.

**Table 4.2.1:** Diffusion coefficients and model parameters.

Length (cm)	Diffusion Coefficient ( $\text{cm}^2/\text{s}$ )	Sum of Squares	Interstitial Velocity ( $\text{cm}/\text{s}$ )
1.70	1.02	0.014	0.8
2.61	0.708	0.016	0.8
5.61	0.869	0.017	0.8
11.0	0.714	0.037	0.5

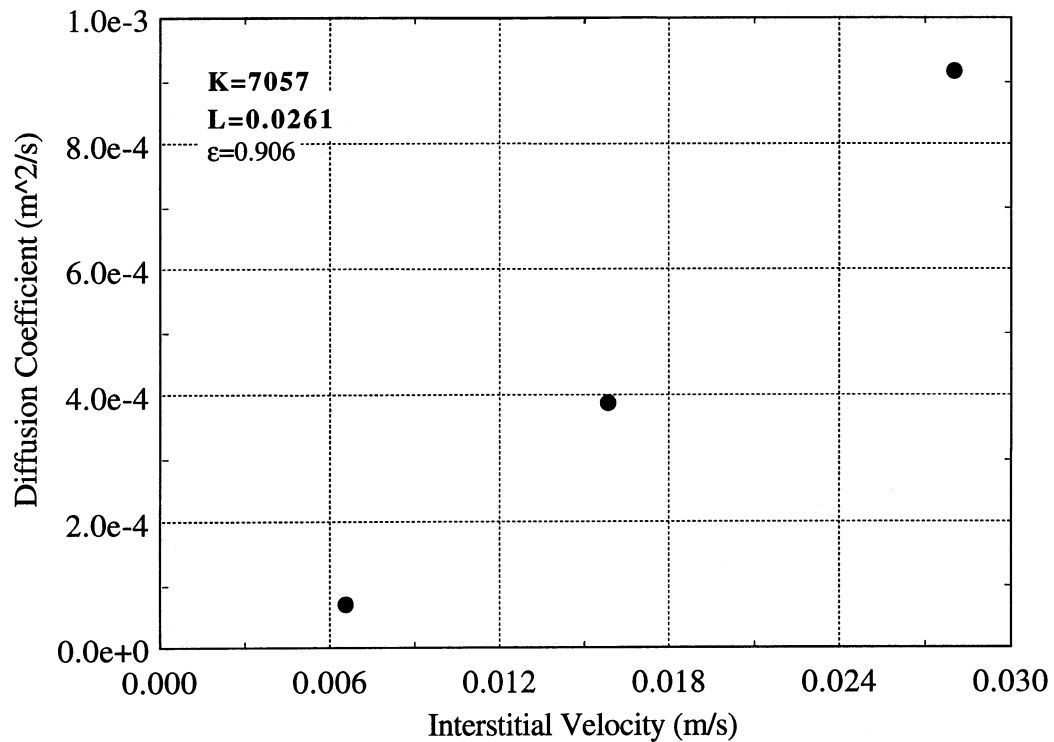




**Figure 4.2.1:** Single parameter breakthrough model comparison to real data.

#### 4.2.4 Velocity Dependence of the Diffusion Coefficient

The diffusion coefficient was found to be dependent upon the interstitial velocity of the gas stream passing through the filter. The results of three experiments executed with increasing velocities are shown in Figure 4.2.2. The dependence of the diffusion coefficient appears to be parabolically related to the velocity. This result seems reasonable because the diffusion coefficient is an indication of how quickly contaminant moves from an area of high concentration to low concentration. Thus, the greater the velocity the more turbulence and mixing that occurs.



**Figure 4.2.2:** Single parameter diffusion coefficient as a function of velocity.

### 4.3 Single Parameter Mass Transfer Resistance Model

#### 4.3.1 Assumptions

The additional assumption applied by the single parameter mass transfer model is that there is no significant transport of contaminant through longitudinal diffusion. Thus, the  $-D_L \frac{\partial^2 C}{\partial z^2}$  term can be dropped from Equation 4.1.4. As well, the assumption is also made that the rate of mass transfer from the gas phase to the adsorbed state is linearly proportional to the difference between the amount of contaminant adsorbed at any instant and the equilibrium value. The proportionality constant is represented by B in Equation 4.1.3.

### 4.3.2 Solution

The solution as reported by Ruthven[1984] can be calculated by,

$$F = \frac{1}{2} \cdot \operatorname{erfc}\left(\sqrt{\xi} - \sqrt{\tau} - \frac{1}{8} \sqrt{\xi} - \frac{1}{8} \sqrt{\tau}\right) \quad (4.3.1)$$

where,

$$\xi = \frac{B \cdot K \cdot L}{u} \left( \frac{1-\epsilon}{\epsilon} \right) \quad (4.3.2)$$

$$\tau = K \left( t - \frac{Z}{u} \right) \quad (4.3.3)$$

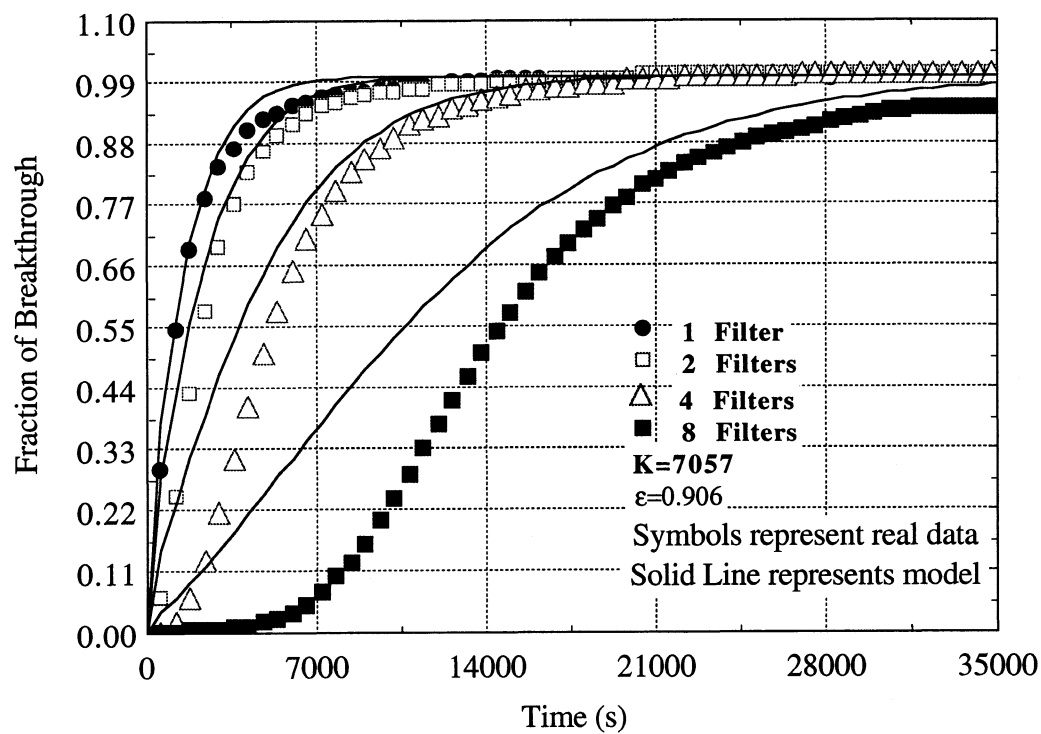
The solution is approximate with an error of less than 0.6% for  $\xi > 2.0$ . The boundary conditions for the solution are the same as those for the single parameter diffusion model.

### 4.3.3 Mass Transfer Coefficient Fitting and Model Verification

All of the parameters for the solution to the mass transfer model were calculated in the same manner that they were calculated for the diffusion model with the mass transfer coefficient fit by a least squares regression analysis in comparison to real data. The results of the regression analysis are presented in Table 4.3.1 and Figure 4.3.1. From the graphical difference between the model and the real data, as well as the magnitude of the sum of the squares it is apparent that for the conditions of the experiment that the mass transfer model does not match the real data very well.

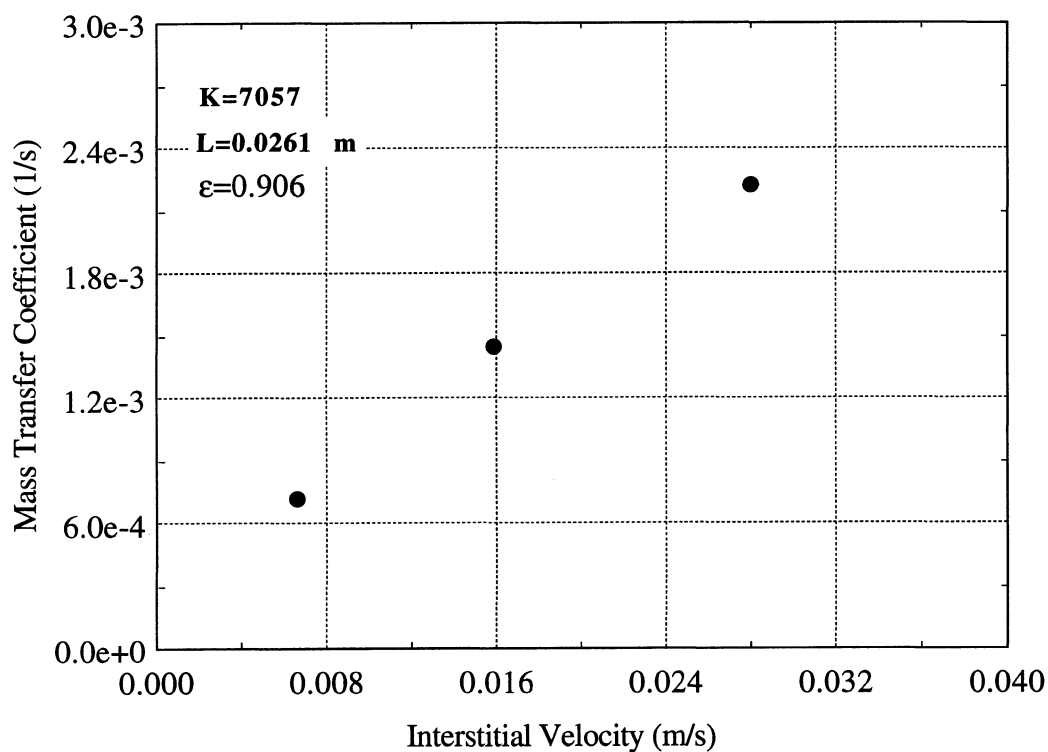
**Table 4.3.1:** Results of the mass transfer model fitting.

Length (cm)	Mass Transfer Coefficient (1/s)	Sum of Squares	$\xi$	Interstitial Velocity (cm/s)
0.0170	0.00088	0.050	1.4	0.8
0.0261	0.00067	0.234	1.7	0.8
0.0569	0.00040	0.939	2.2	0.8
0.1100	0.00023	3.357	3.6	0.5

**Figure 4.3.1:** Comparison of the mass transfer model and real data.

#### 4.3.4 Velocity Dependence of the Mass Transfer Coefficient

The value of the mass transfer coefficient is also related to the velocity of the gas stream passing through it however as the velocity increases it tends to level out. This result again seems reasonable because the mass transfer coefficient is an indication of how quickly mass changes from the gas phase to the adsorbed phase. It is possible that as the velocity increases the film resistance decreases to a level where other resistances not related to the velocity dominate the rate of mass transfer.



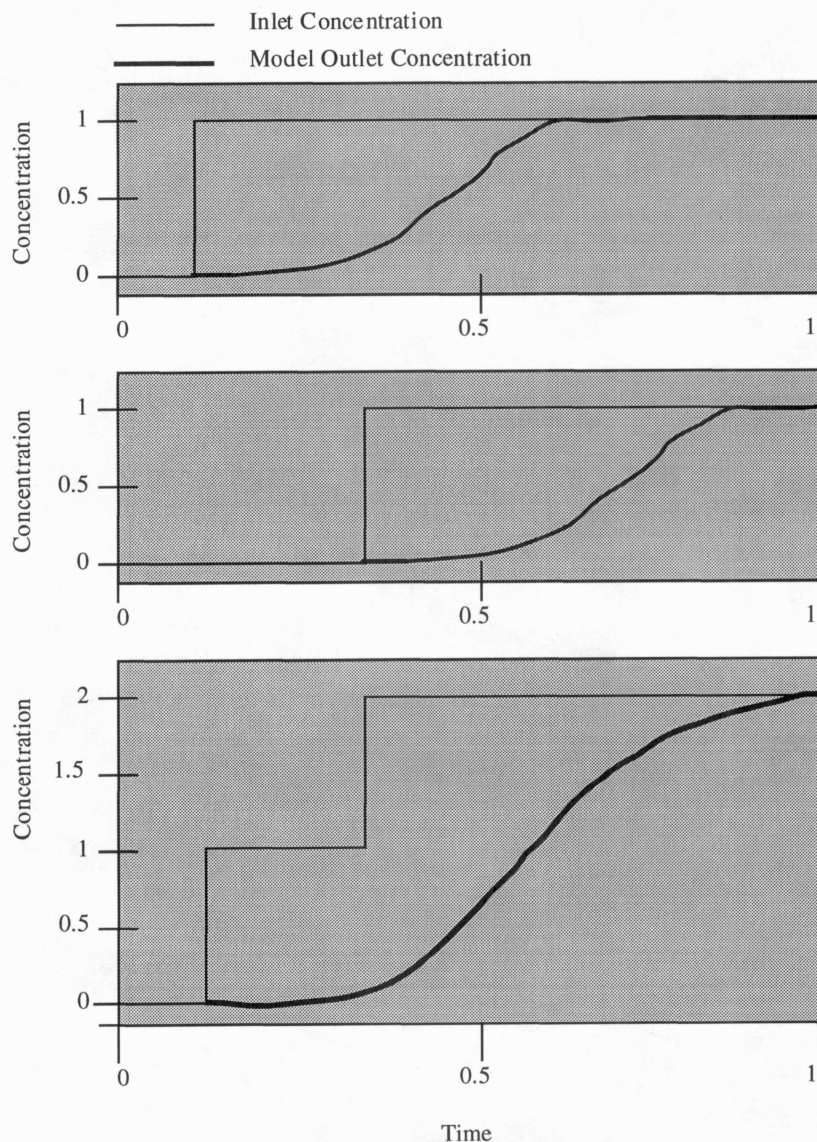
**Figure 4.3.2:** Mass transfer coefficient as a function of velocity.

#### 4.4 Superposition of Single Parameter Diffusion Model

Because the breakthrough models are solutions to linear differential equations they can theoretically be superimposed to determine the solution to a superimposed set of

boundary conditions. Thus, many inlet concentration steps both positive and negative can be superimposed in a differential approach to approximate a time varying inlet condition. To determine the outlet concentration for an increasing ramp function of the inlet concentration two inlet steps starting at successive time steps can be added as shown in Figure 4.4.1. In this manner the outlet concentration for any inlet concentration function can be solved for by simply adding the solutions to incremental steps to approximate the inlet condition.



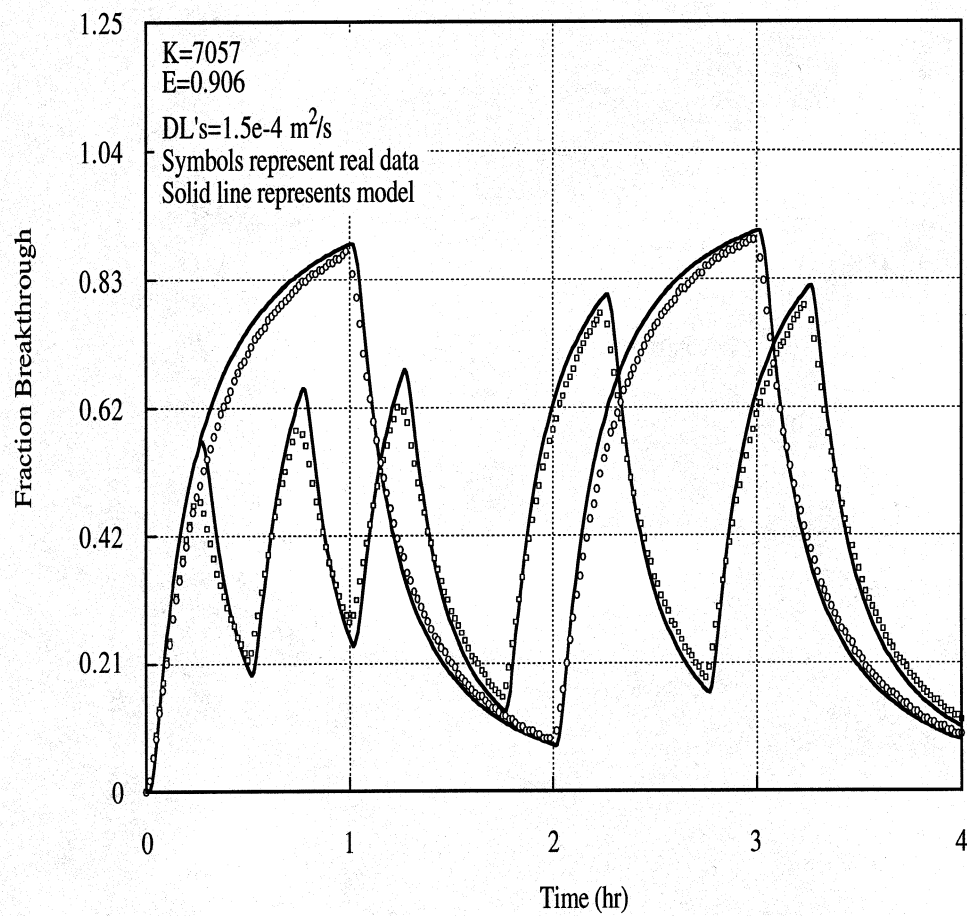


**Figure 4.4.1:** Superposition of breakthrough curves to determine outlet concentration for an increasing ramp of the inlet concentration.

To verify the validity of the superposition technique, a filter sample was subjected to a series of step increases and decreases of inlet contaminant concentration at different intervals. The measured outlet concentration data, indicated by the symbols, is compared to the predicted outlet concentration depicted by the solid line in Figure 4.4.2 as a fraction



of the inlet concentration for two different sets of boundary conditions. The diffusion model was selected because it more closely fit the observed filter behavior at these conditions and a diffusion coefficient fit to a single step change in concentration in previous experiments was selected.



**Figure 4.4.2:** Superposition of diffusion model in comparison to real data.

## 4.5 Conclusions

From the results of the regression analysis for the conditions under which the filters were tested the single parameter diffusion model more accurately represents the adsorption process in the carbon bonded filters. However, the velocities employed in these experiments were in the range of 1 fpm which is slower than would be expected in an actual application and results may vary as the velocity is increased.

The technique of superimposing solutions of the diffusion model appears valid from the results shown in Figure 4.4.2. However, the conditions for which the experimental data were obtained were conducive to meeting the assumptions of the model. The assumptions being a linear contaminant isotherm and uniform flow in one direction. This result will allow a filter model to be developed for use in a simulation where the boundary condition is a complex time varying input.

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**CHAPTER  
FIVE**

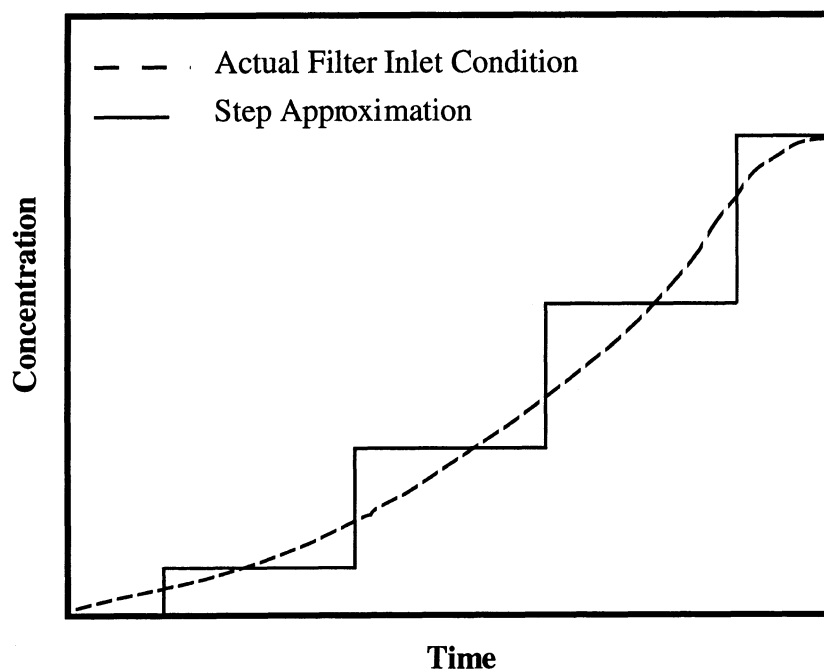
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**BUILDING ZONE POLLUTANT REMOVAL  
MODELING**

The objective of modeling adsorption processes in activated carbon air filters is to design a filter and ventilation system that reduces pollutant concentration levels in an indoor environment to an acceptable level. To realize this end, a model that calculates the transport of pollutants through an activated carbon filter and building ventilation system is essential. The method of breakthrough curve superposition developed previously will be used to create a filter model for use with the TRNSYS (Klein et al., 1990) a transient simulation program that will calculate the filter outlet concentration for a time varying inlet concentration. The filter model will be used in conjunction with a pollutant transport model created by Knoespele (1990) and later modified by Emmerich (1993) to create a tool that will allow one to assess the impact of filter parameters and ventilation controls on the pollutant concentrations and associated energy costs in a building zone. Development of the governing equations and methodology used to create the filter and pollutant transportation models for TRNSYS follows.

## 5.1 Activated Carbon Filter Model

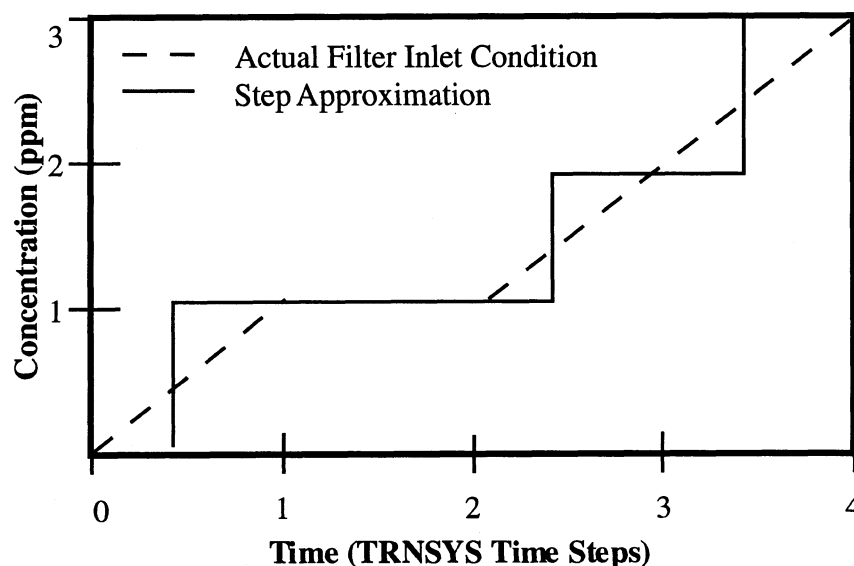
It has been demonstrated that the solution to the breakthrough model for single step inputs in concentration can be superimposed to obtain the solution to more complex inlet boundary conditions. Based on this premise any varying inlet condition can be approximated by dividing it into small step changes in a differential approach as shown in Figure 5.1.1. This technique is the principle on which the filter model is based.



**Figure 5.1.1:** Approximation technique used to model the filter inlet concentration.

The method used to approximate the inlet condition into a series of step increments begins with choosing a threshold step size entered as a model parameter. The step size determines how closely the model approximates the actual inlet concentration. The threshold step size is compared to the absolute value of the difference between the last

inlet concentration value of the model and the current inlet value, and a new step change in the models' inlet concentration is initiated when the threshold step size is exceeded. An illustration of the application of this concept is shown in Figure 5.1.2. Because TRNSYS solves for each time step in the simulation, the concentrations between time steps are represented by a straight line connecting the concentrations at adjacent time steps. In the example, the threshold step size was set at 0.5 ppm and the actual inlet concentration began at zero and increased to 1 ppm, in the first time step of the simulation. Therefore, because the inlet condition started at 0 ppm and increased to 1 ppm the absolute difference between the value of the previous model inlet concentration, 0, and the actual inlet concentration, 1, was greater than the threshold step size and the model was triggered to initiate a step change equal to the difference of 1 ppm. The time the model recorded the step as occurring was equal to the simulation time less one half of a time step to conserve mass.



**Figure 5.1.2:** Illustration of the concentration threshold step size used to construct the filter inlet concentration.

The size of each inlet concentration step and the time that it was initiated are stored in an array. All of the other variables used to calculate the solution to the breakthrough model are constant throughout the entire simulation. Once a breakthrough curve has completely passed through the filter, the value that the breakthrough model calculates for that particular step's outlet concentration is constant at the value of the inlet step concentration and therefore, need not be calculated by the filter model at the end of each TRNSYS time step. Instead, the value of the completely broken through curves can be summed and stored in a single variable that is added to the outlet concentration by the filter model at the end of each time step. This procedure prevents the array that stores the breakthrough information from exceeding the available storage space. However, if the step size is too small the model may create more concentration steps than can be stored simultaneously in the array. If this condition occurs TRNSYS will warn the user with an error message, and the threshold step size or the storage array size can be increased to remedy this problem by either reducing the number of concentration steps or increasing the storage space respectively.

Of the two models investigated in chapter 2 the single parameter diffusion breakthrough model more closely represented the kinetic adsorption phenomena observed in the experimental portion of this investigation. However, it is possible that in other situations the mass transfer model may better represent the processes taking place in a filter. Therefore, both models were incorporated in the TRNSYS carbon filter type. The user may select which breakthrough model they wish to use through the model selection parameter in the TRNSYS deck.

Most ventilation systems shut down during some portion of the day. Because the filter model records only the start time of a concentration step and assumes the flowrate to be constant the model would calculate the outlet concentration as if air were always passing through the filter even if the ventilation system was not operating. Thus, an adjustment was made to account for the time that there is no flow of air through the filter. It is assumed that when the ventilation system is not operating no mass transfer takes place in the filter. This effect is achieved by adding the amount of time the ventilation system is not operating to the start time of each of the breakthrough curves in the storage array. The filter then calculates the transport of mass through the filter only for the time that air is passing through the filter.

The parameters of the filter model are values that remain constant throughout the entire simulation. The parameters are entered in what is called a deck. The TRNSYS deck is a description of the simulation that includes a declaration of the components used in the simulation, the value of constants used by the components, and the relationship of the components to each other. An example of one of the decks used in this investigation is located in Appendix C.

There are twelve parameters used by the carbon filter model and a description of each follows:

**Adsorption Coefficient:** Depending upon the selection of breakthrough model it represents either the single parameter diffusion coefficient or the mass transfer coefficient. The units are square meters divided by seconds or the inverse of seconds respectively.

**Desorption Coefficient:** In the case of a linear isotherm the desorption coefficient would generally be the same as the adsorption coefficient but if there is some other factor which affects the rate of desorption this parameter allows the user to specify a different value.

**Void Fraction:** The void fraction parameter is the fraction of the filter cross-section that contains no carbon and is dimensionless.

**Filter Length:** The length of the filter in units of meters.

**Filter Area:** The cross-sectional area of the filter in units of meters squared.

**Isotherm Constant:** The value of the isotherm constant of the contaminant being used in the model. There are hundreds of contaminants present in indoor air, therefore the isotherm constant for an average contaminant will be used in this study. The constant is dimensionless and is calculated by dividing the equilibrium capacity of the filter in units of moles of contaminant per unit volume of carbon by the concentration in units of moles of contaminant per unit volume.

**Threshold Concentration Step:** The magnitude of the difference between the last inlet concentration recorded by the model and the actual inlet concentration calculated by TRNSYS. When this value is exceeded the filter model initiates a new inlet step with a magnitude equal to the aforementioned difference. Concentrations are dimensionless consisting of units of cubic meters of contaminant per cubic meter of air.



**Volumetric Flow Rate:** The flowrate of air moving through the filter in units of meters cubed per second. This value is a parameter must be a constant (when the ventilation system is operating) and therefore the HVAC systems simulated with this filter model are limited to constant air volume systems.

**Initial Concentration:** The equilibrium gas phase concentration at which the filter begins the simulation. The filter model need not begin at zero concentration but it must begin at equilibrium with a constant concentration throughout the entire filter. Concentrations are dimensionless consisting of units of meters cubed of contaminant per meter cubed of air.

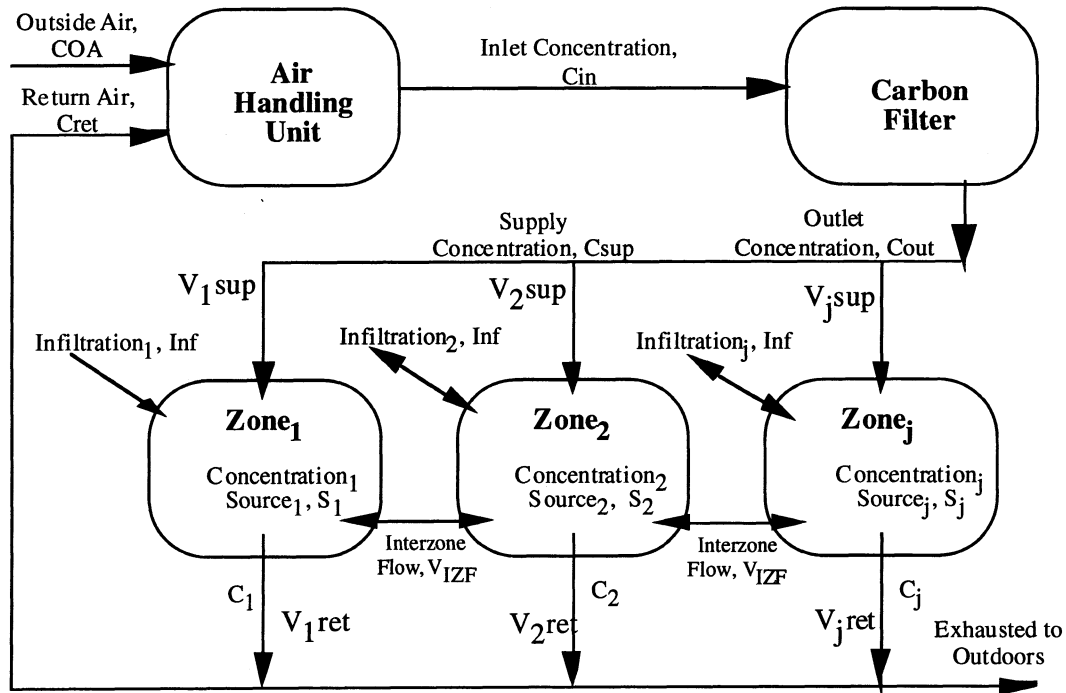
**Model Selection:** The user can either select the single parameter diffusion model by entering a 1 or the mass transfer resistance model by entering a 2.

**Time Step:** The time step of the TRNSYS simulation in units of hours.

**Array Size:** The size of the storage array that contains the time and magnitude of the step changes in inlet concentration. The array must be large enough to accommodate the number of inlet step changes in concentration that occur before additional space is made available by the complete breakthrough of previous step changes. The simulation calculation time increases as the array size is increased because the filter model calculates the fraction breakthrough of each inlet step in the array for each TRNSYS time step. Therefore, it is best to use the smallest array size possible that can satisfy the storage space requirements.

## **5.2 Pollutant Transport Model**

The pollutant transport model was developed by Knoespel and later modified by Emmerich. A brief explanation of model will follow and a more rigorous development of the theory and mathematics can be found in Knoespel (1990) and Emmerich (1993). The model consists of a Kirchoff network where each building zone and the ambient are modeled as nodes at uniform pressure, temperature, and pollutant concentration. The nodes are connected by infiltration and ventilation mass transportation pathways as shown in Figure 5.2.1. A mass balance is performed on each node and the system of equations is then solved simultaneously. To simplify the model, all of the infiltration flows are calculated by the air change method used by the TRNSYS Type 56 building heating and cooling load module. The simplification arises from the decoupling of the nodal balance equations from the element flow equation since all flow terms are known. This simplification, which allows transient calculations of pollutant concentrations as contaminant generation or ventilation rates change, is also employed by the Environmental Protection Agency's program INDOOR (Owen et al., 1989).



**Figure 5.2.1:** Multiple zone contaminant transport model schematic diagram.

To develop a system of equations that can be solved simultaneously to determine the concentration in each zone, a mass balance is performed on each node. Assuming that the density of the air remains constant, volumetric terms can be used to perform the mass balance. The concentration terms are the volumetric fraction of air occupied by contaminant. Summing all of the mass transfer pathways on Zone<sub>j</sub> yields,

$$\frac{dm_j}{dt} = \text{Inf}_j \cdot (\text{COA} - C_j) + S_j - \sum V_{\text{IZF}} \cdot (C_j - C_i) - (C_j V_{j\text{ret}} - C_{\text{sup}} V_{j\text{sup}}) \quad (5.2.1)$$

The first term on the right hand side of the equation represents the user specified volumetric infiltration of outdoor air into a zone. The volumetric pollutant generation term,  $S_j$ , is user specified and can remain constant or vary with time of day. The third

term is the volume of pollutant transfer into the zone through infiltration from other zones. The magnitude of the flow is set by the user but the sign of the term depends upon the zone concentrations. The last term results from the ventilation system transport of pollutant into or out of the zone depending on the supply concentration and the zone concentration.

The return flowrate is calculated by performing a mass balance on total flow of mass through a zone. The supply, infiltration, and inter-zone flow rates are set by the user therefore the return flow rate can simply be calculated by,

$$V_{jret} = V_{jsup} + Inf_j - V_{IZFj,i} + V_{IZFj,i} \quad (5.2.2)$$

Because the filter model requires that the flowrate remain constant the model operates as a constant air volume, CAV, system that can be turned on or off.

## 5.3 Office Simulation Model

### 5.3.1 Building Description

The building model used in the simulation is a two zone modern office building located in Madison, Wisconsin that was previously developed by Ruud (1990). The first zone is 3370 m<sup>3</sup> (119000 ft<sup>3</sup>) in volume covering 1300 m<sup>2</sup> (14000 ft<sup>2</sup>) of floor area with a maximum occupancy of 100 people. The second zone is an interior space 81 m<sup>3</sup> (2850 ft<sup>3</sup>) in volume covering 31m<sup>2</sup> (340 ft<sup>2</sup>) of floor area with a maximum occupancy of 10 people. The ventilation system maintains a constant total air flowrate of 6 air changes per hour, 345 cmm (12,186 cfm), which includes 1 air change per hour of outdoor air, 58 cmm (2031 cfm). The outdoor air flowrate in Zone 1 complies with ASHRAE 62-1986

by delivering 19.8 cfm/person. However, based on maximum occupancy the outdoor air flowrate in Zone 2 only provides 4.8 cfm/person. Data files that contain the building zone dimensions are included in Appendix C.

### 5.3.2 Pollutant Generation

The generation of pollutants in the office space was modeled for three different situations: 24 hour constant generation, occupant generated, and a short term large volume event.

The first situation, 24 hour constant generation, was based on the emission rates measured by Molhave (1982) listed in Table 1.1.1. It was assumed that the entire floor air of Zone 1 ( $1300 \text{ m}^2$ ) was covered by synthetic carpet that emitted  $0.1 \text{ mg/m}^2\text{hr}$ .

Because no specific contaminant was listed in the table a molecular weight of  $60 \text{ g/gmole}$  was assumed in order to calculate a volumetric flowrate of  $1.34\text{E-}08 \text{ m}^3/\text{s}$ . In addition, a generation rate of  $0.4 \text{ mg/m}^2\text{hr}$  for the wall paper produced  $6.13\text{E-}08 \text{ m}^3/\text{s}$  for a wall area of  $1440 \text{ m}^2$  with the same  $60 \text{ g/gmole}$  molecular weight assumption. There was no generation of contaminant in Zone 2.

The occupant generated case was derived from values supplied by Wang (1975) in Table 1.1.2. The mass generation values were converted to volumetric rates by assuming they behaved as ideal gases produced during an eight hour period. A value of  $4.74\text{E-}09 \text{ m}^3/\text{s}$  per person was calculated for the first twelve volatile organics listed in the table. The generation in Zone 1 was determined by the maximum occupancy of 100 people from 9 am to 5 pm. No generation was produced in Zone 2.

The short term large volume event is an attempt to assess the activated carbon filter's ability to distribute a high concentration release of contaminant into a indoor environment

over a longer time period at a lower concentration than would normally occur thereby protecting the occupants from high concentrations at which they would experience discomfort. A generation rate of  $1.0\text{E-}05 \text{ m}^3/\text{s}$  for a period of one hour was chosen for this case.

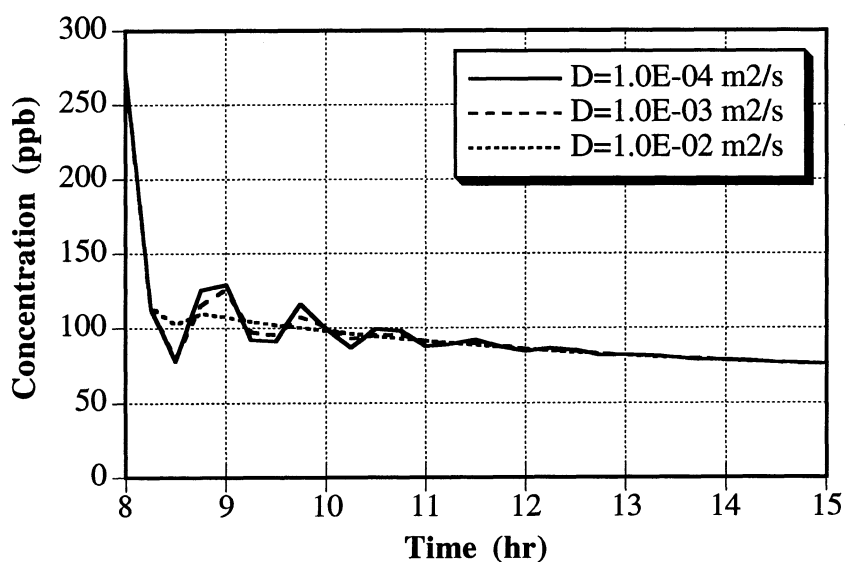
### 5.3.3 Activated Carbon Filter Description

Two filter sizes were employed in the simulations. One filter was  $10 \text{ m}^2$  by  $0.1 \text{ m}$  containing  $41.4 \text{ kg}$  of activated carbon and the other filter was  $10 \text{ m}^2$  by  $0.0127 \text{ m}$  containing  $5.3 \text{ kg}$  of activated carbon. Large surface areas were employed because it was envisioned that the activated carbon bonded filters would be placed in the supply air plenums of the building zone. The first filter's thickness would result from multiple layering of individual filters, the second filter's thickness is that of a single filter similar to the one used in the experimental portion of this investigation. Also, to provide a reference point for the performance of the filters two additional cases were simulated. One case was that of no filter and the other case was that of a perfect filter. The perfect filter was simulated by setting the supply concentration to zero.

The void fraction was calculated as  $0.906$  and the flowrate through the filter,  $5.75 \text{ m}^3/\text{s}$ , is equal to the total circulation flowrate through the zones.

The threshold step size concentration of the simulation was set to zero to ensure that, for each time step, which the ventilation system is operational, a concentration step change in the filter inlet will result. This parameter selection has the effect of increasing the computational time, but minimizes the difference between the actual inlet concentration to the filter and the filter model's inlet concentration.

The adsorption and desorption coefficients were chosen to be the same maintaining the assumption that the isotherm constant is linear. The value of the sorption coefficients in the experimental phase of this investigation were on the order of  $0.001 \text{ m}^2/\text{s}$  at a velocity of approximately  $0.028 \text{ m/s}$ . The velocity in the simulation,  $0.575 \text{ m/s}$ , was much greater than that of the experiments. Because the sorption coefficients increase as velocity increases the coefficients used in the simulation ought to be greater than those of the experiment. The effect of increasing sorption coefficients can be seen in Figure 5.2.1 where all conditions are identical for the three simulations except for the sorption coefficients. The coefficients for the simulations were arbitrarily chosen to be  $0.01 \text{ m}^2/\text{s}$  to reflect the increased velocity and expected smoothness of the zone concentration levels.



**Figure 5.2.1:** Effect of sorption coefficient on the smoothness of zone concentration levels.

The isotherm constant was chosen as 150,000 to represent an average value for the type of VOCs commonly found in indoor air. The linear isotherm constant is calculated by dividing the amount of contaminant adsorbed by the gas phase concentration of the contaminant. At concentration of 43.9 ppm, 1.26 mg of propane is adsorbed per gram of carbon. The isotherm constant can be calculated by converting the quantities to units of moles per cubic meter and dividing the propane adsorbed by the concentration as shown in Equation 5.2.1. The value of the isotherm constant for propane, which is not a strongly adsorbed contaminant, was calculated as 7057. Forsythe measured isotherms ranging from 40 to 671000 for several other contaminants on granular carbon which is similar to the carbon bonded to the filters used in this investigation. Thus, 150,000 should represent the isotherm constant of an average contaminant relevant to indoor air quality.

$$K = \frac{\frac{1.25 \text{ mg}_{\text{propane}}}{1.0 \text{ g}_{\text{carbon}}} \cdot 440000 \frac{\text{g}_{\text{carbon}}}{\text{m}^3}}{44090 \frac{\text{mg}_{\text{propane}}}{\text{mole}} \cdot 4.39\text{E-}05 \frac{\text{part}}{\text{part}} \cdot 40.2 \frac{\text{moles}_{\text{nitrogen}}}{\text{m}^3}} = 7057 \quad (5.2.1)$$

### 5.3.4 Ventilation Strategies

Two ventilation strategies are employed in the building simulations. The first ventilation control scheme switches the system on at 8 am and off at 8 pm. The second system operates the ventilation system 24 hours a day. The benefits of operating the system 24 hours a day is that the filter is able to desorb itself of contaminants that were adsorbed during the day provided those contaminants are absent at night. However, the benefit comes with the cost of operating the fans for an additional 12 hours a day and the cost of conditioning the outside air that is circulated through the building for those additional hours.



## 5.4 Simulation Description

The variations that have been outlined for each variable in the simulation are summarized in Table 5.3.1 with a number associated to each value that will be used in a subsequent table.

**Table 5.3.1:** Description of simulation variables.

Variable Type	Variable Label	Description
Filter Size	1	10m <sup>2</sup> x0.1m (41.4 kg)
	2	10m <sup>2</sup> x0.0127m (5.3 kg)
	3	No Filter
	4	Perfect Filter*
Ventilation Schedule	1	8 am to 8 pm
	2	24 Hour Operation
Pollutant Generation	1	24 Hour Generation 7.47E-08 m <sup>3</sup> /s
	2	Occupant Generated 4.74E-09 m <sup>3</sup> /s person 8 am to 7 pm
	3	Short Large Volume 1.0E-06 m <sup>3</sup> /s 15 minutes

\* Perfect filter case simulated by setting supply concentration,  $C_{sup}$ , to zero.

Sixteen of the possible combinations for the simulation variables which will be computed are summarized in Table 5.3.2. Also provided in the table is the section number where the results of the simulation are discussed and a simulation number that corresponds to the simulation numbers that appear on each of the graphs of the results.

**Table 5.3.2:** Summary of the simulation variable values.

Section Number	Simulation Number	Filter Number	Ventilation Number	Generation Number
5.5.1	1	1	1	1
	2	2	1	1
	3	3	1	1
	4	4	1	1
5.5.2	5	1	1	2
	6	2	1	2
	7	3	1	2
	8	4	1	2
5.5.3	9	1	2	2
	10	2	2	2
	11	3	2	2
	12	4	2	2
5.5.4	13	1	1	3
	14	2	1	3
	15	3	1	3
	16	4	1	3

## 5.5 Results

A plot of the concentration of pollutants in each of the zones for each simulation follows. The plot displays the concentration over the course of a typical day. Also, provided on the page following each concentration plot is a histogram displaying the number of hours per 5 day week that the zone concentration was within a particular concentration range from 8am to 8pm. The histogram is useful in comparing the length of time that the occupants are subjected to particular levels of concentrations for each filter case. The

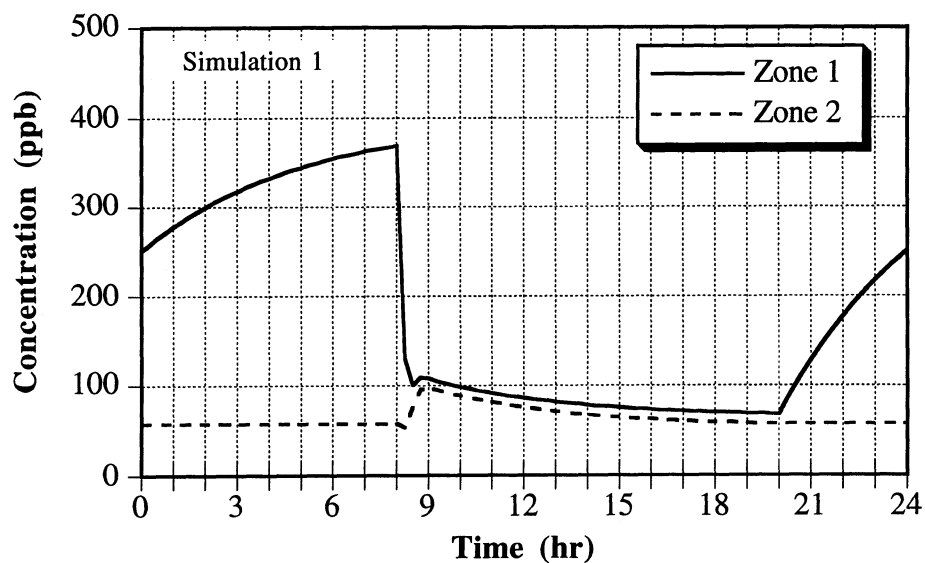
concentration of total VOCs in a lecture hall occupied by 225 students from Table 1.1.2 is approximately 150 ppb. The concentrations experienced in the zones for the occupant generated pollutant cases are less than 150 ppb for the perfect filter case and greater than 150 ppb for the no filter case. This result is a positive indication of the appropriateness of the pollutant generation rates for the occupants and of the accuracy of the filter transport model.

#### **5.5.1 Constant 24 Hour Pollutant Generation with 12 Hour Ventilation**

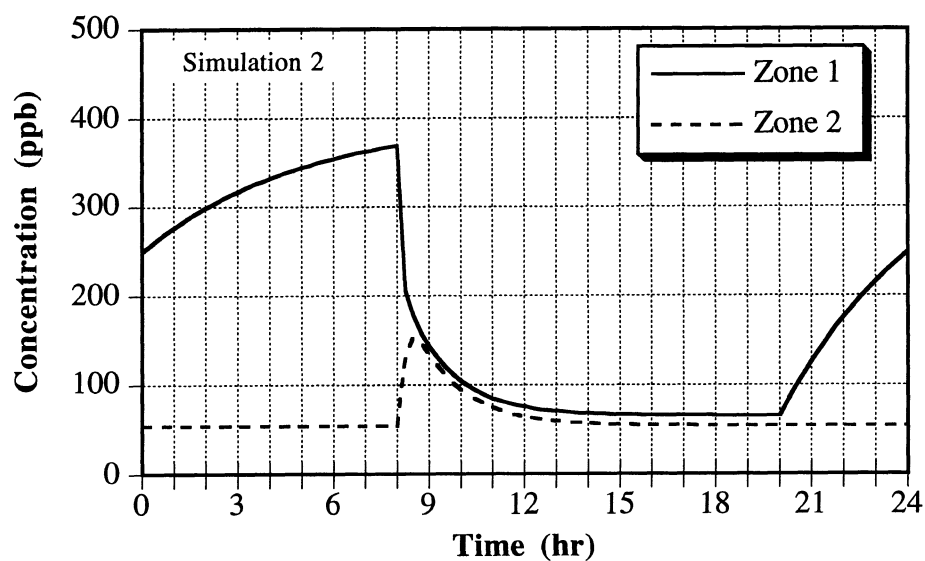
The general trend for the concentration in each zone over a typical day was similar for each of the four filter cases as was expected. During the time that the ventilation system was not operating the trend was for the concentration in Zone 1 to rise asymptotically towards the concentration at which the rate of contaminant removal through infiltration of outdoor air was equal to the rate of generation from 8pm to 8am. While the ventilation system was not operational the concentration of contaminants in Zone 2 remained constant because it was an interior zone into which no outdoor air infiltrated. When the ventilation system was switched on at 8am a dramatic decrease in the contaminant level of Zone 1 occurred. A corresponding increase in the concentration of Zone 2 ensued because of the introduction of contaminant through the supply air which was now contaminated by the return air from Zone 1. It was the decrease of the zone concentrations during the occupied hours from 8am to 8pm that differed significantly for each of the filter cases.

The large filter, shown in Figure 5.5.1, quickly decreased the concentration in Zone 1 at the start of the day until the contaminant began to break through after a half of an hour and the filter slowly desorbed the contaminant back into the zone over the course of the

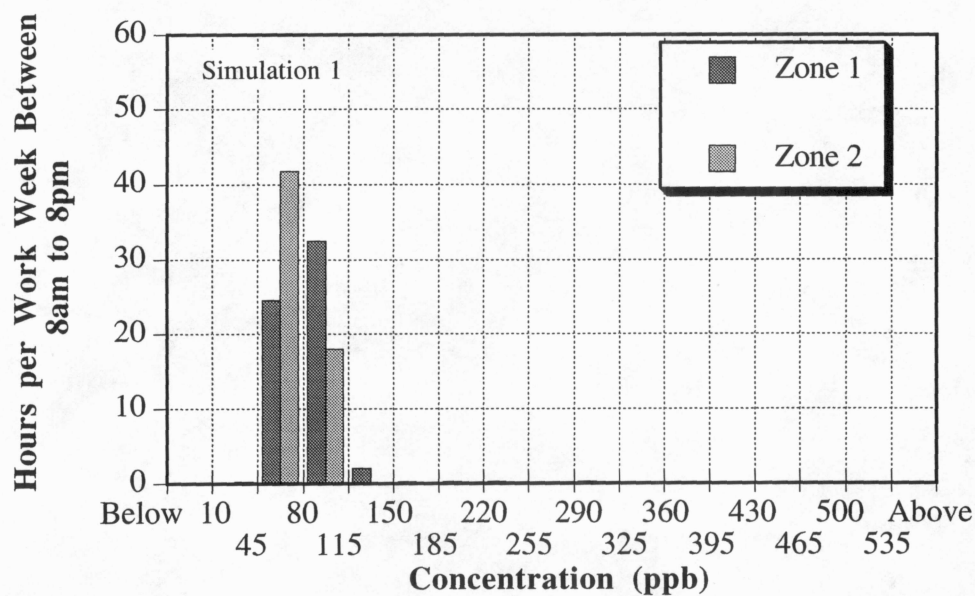
day. The concentrations in the small filter case, shown in Figures 5.5.2, broke through more quickly than the large filter allowing the room concentration to initially remain higher. But because the small filter had a lower capacity for pollutants it desorbed less contaminant back into the zone and allowed the zone to reach a lower concentration than with the larger filter more quickly. The result of this effect on the hours of exposure to particular concentration levels can be seen in the histograms in Figures 5.5.3 and 5.5.4 where the small filter case experienced a greater range of concentrations than the large filter case. The limiting case as the filter size decreased to zero can be seen in Figure 5.5.5. In the no filter case the concentration initially decreased more slowly than the filter cases but decreased to a lower level where the contaminant was removed as quickly as it was generated because no contaminant was desorbed back into the zone. The perfect filter case, shown in Figure 5.5.6 almost immediately decreased the Zone 1 concentration to the point where the contaminant removal was equal to generation. The histograms for the no filter case and the perfect filter case in Figures 5.5.7 and 5.5.8 demonstrate the high and low limits of contaminant level exposure times. The perfect filter case underwent very low concentrations for all of the occupied hours while the no filter case experienced a broad range of concentrations. The only way the concentration could have been lowered any further in the perfect filter case would have been to increase the ventilation rate. The concentration in Zone 2 was so low for the perfect filter case that it is not visible on the graph.



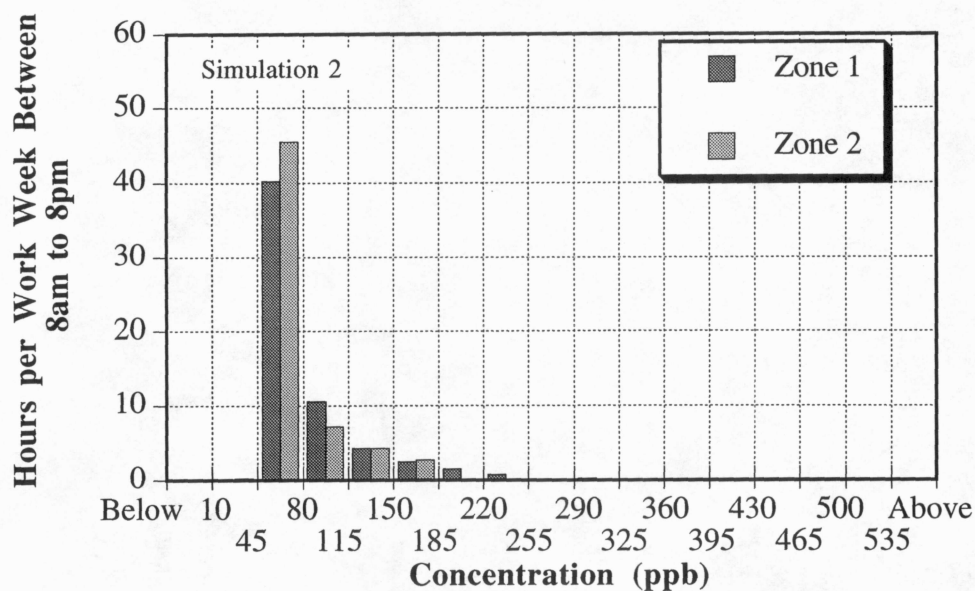
**Figure 5.5.1:** Zone concentrations for the large filter, 12 hour ventilation, and 24 hour pollutant generation.



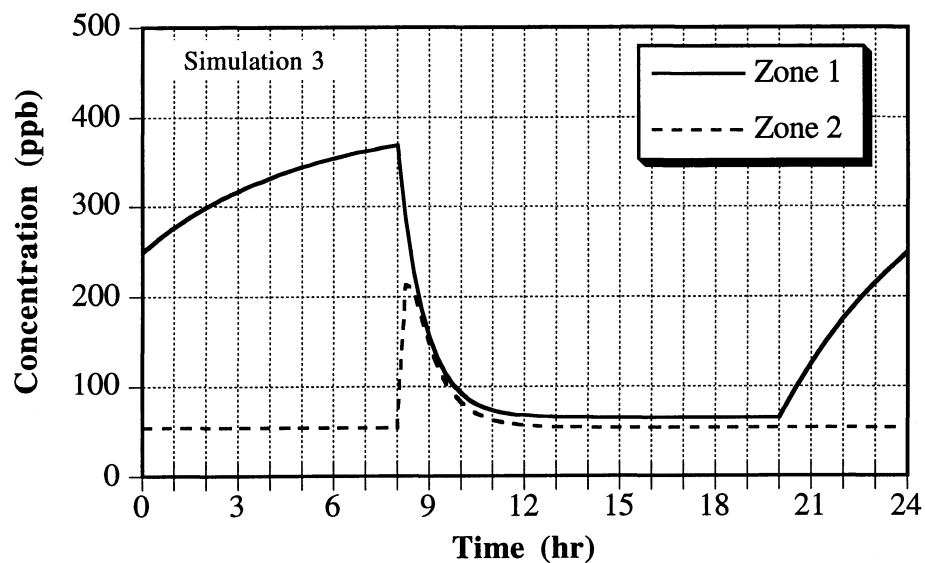
**Figure 5.5.2:** Zone concentrations for the small filter, 12 hour ventilation, and 24 hour pollutant generation.



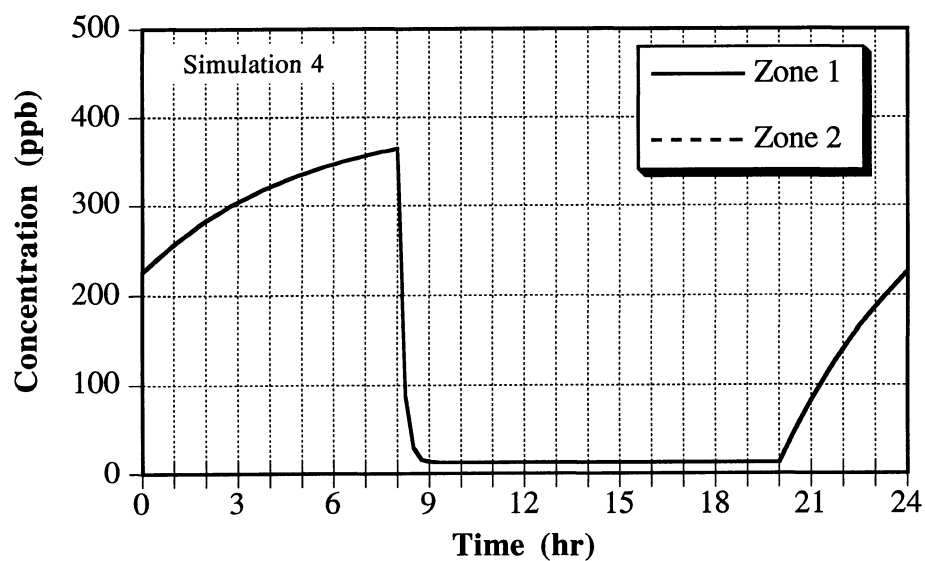
**Figure 5.5.3:** Zone concentration histogram for the large filter, 12 hour ventilation, and 24 hour pollutant generation.



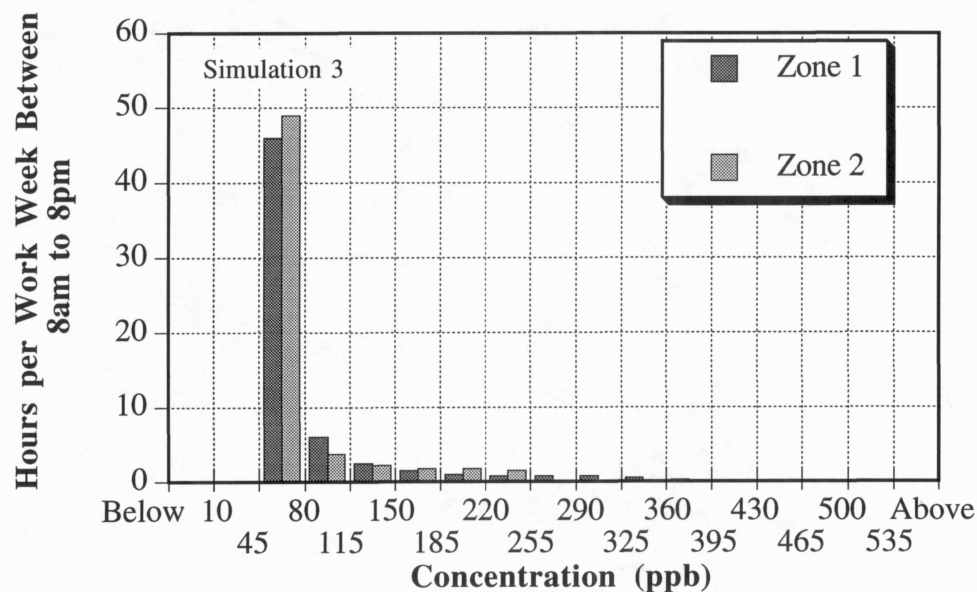
**Figure 5.5.4:** Zone concentration histogram for the small filter, 12 hour ventilation, and 24 hour pollutant generation.



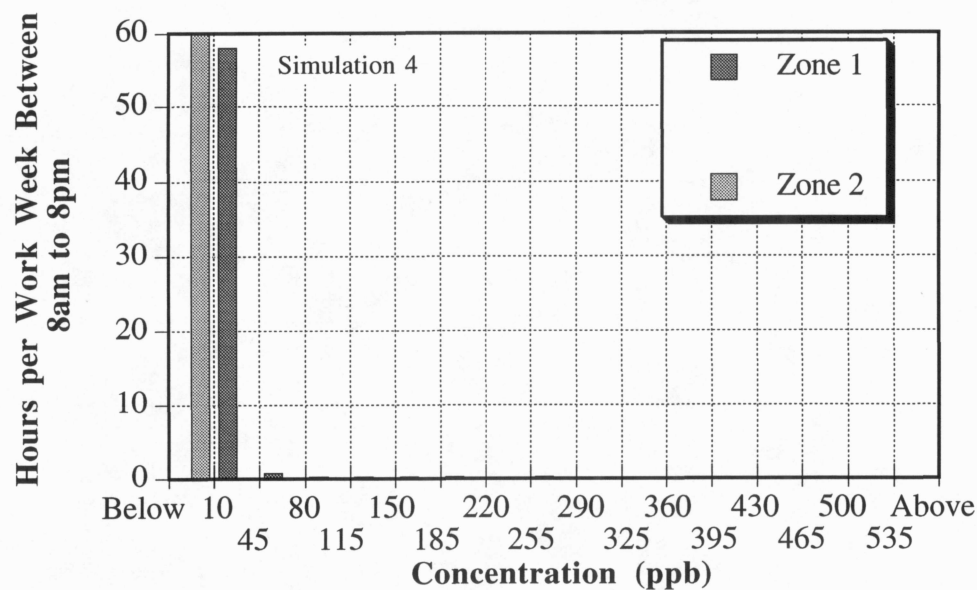
**Figure 5.5.5:** Zone concentrations for no filter, 12 hour ventilation, and 24 hour pollutant generation.



**Figure 5.5.6:** Zone concentrations for the perfect filter, 12 hour ventilation, and 24 hour pollutant generation.



**Figure 5.5.7** Zone concentration histogram for no filter, 12 hour ventilation, and 24 hour pollutant generation.



**Figure 5.5.8:** Zone concentration histogram for the perfect filter, 12 hour ventilation, and 24 hour pollutant generation.

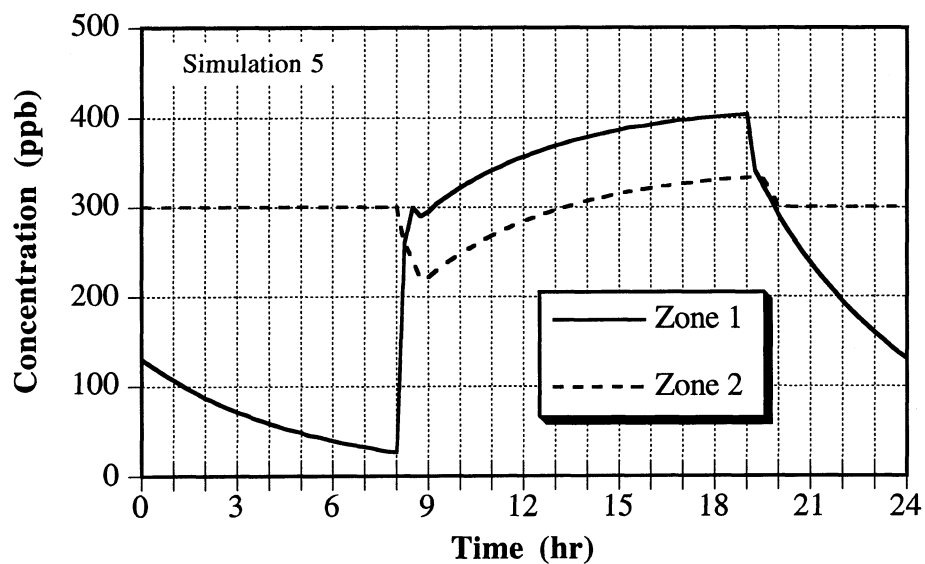


### 5.5.2 Occupant Generated Pollutants with 12 Hour Ventilation

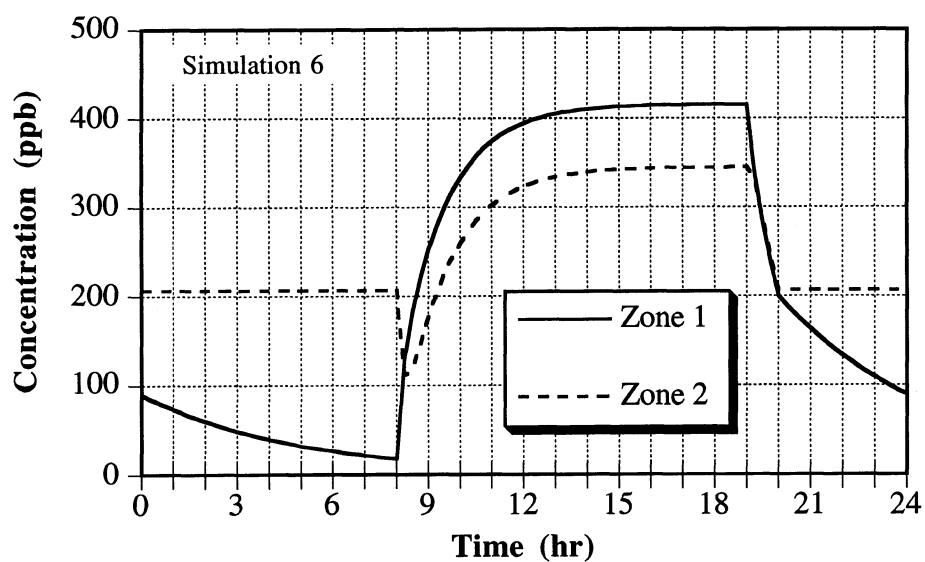
The concentration trends for the occupant generated case with 12 hour ventilation consisted of three phases, an asymptotic increase in concentration to the level at which generation equaled removal, constant concentration in Zone 2 while no pollutant was generated, and a decreasing portion in Zone 1 and 2. The increase started at 8am with the initiation of pollutant generation and continued until pollutant generation terminated at 7pm. From 7pm to 8pm the ventilation system was able to desorb the filters and lower both zone concentrations because of the absence of pollutant generation. At 8pm the ventilation system shut down and the concentration in Zone 1 decreased because of outdoor air infiltration while the Zone 2 concentration remained constant due to a lack of outdoor air infiltration. Although the Zone 1 concentration decreased, the ventilation system was not operating, and thus the filter still contained contaminant that was released back into the zone when the ventilation system was switched on again at 8am.

The large filter case, shown in Figure 5.5.9, initially exhibited a quick increase in the Zone 1 concentration at 8am from contaminant that remained in the filter after the ventilation system was shut down at 8pm. However, the Zone 1 concentration increased very slowly thereafter because of the remaining capacity in the filter created by the hour of desorption from the previous night from 7pm to 8pm. The concentration levels in Zone 2 followed those in Zone 1 at a lower level during the occupied hours. The concentration in Zone 1 and Zone 2 for the smaller filter, shown in Figure 5.5.10, started at a lower concentration than the larger filter because it had a smaller capacity and was able to more completely desorb the previous evening. However, the lower capacity also caused the Zone 1 and Zone 2 concentrations to increase more quickly and achieve a higher concentration than the large filter case. The effect of the filter capacity on

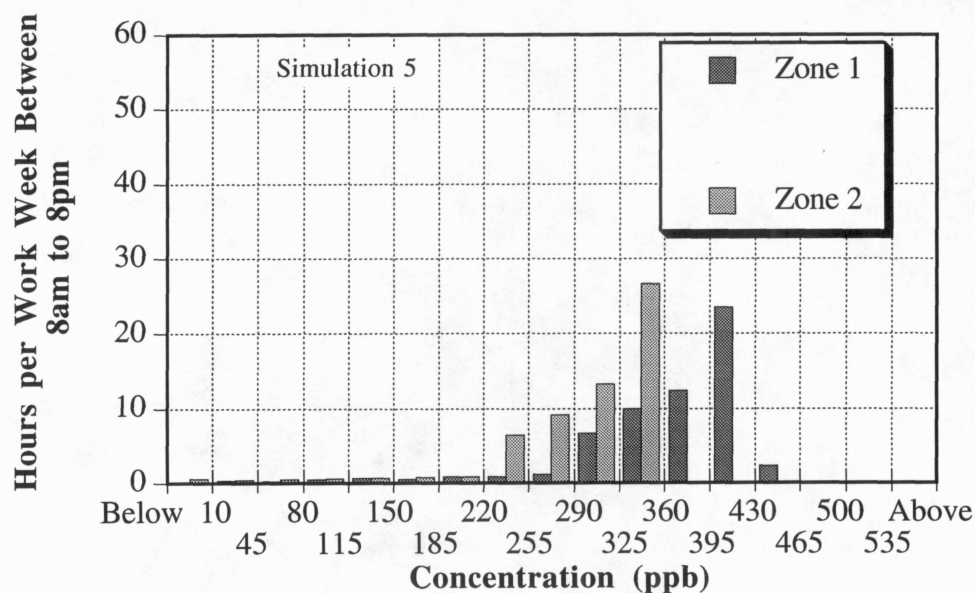
contaminant level exposure times is shown in the histograms in Figures 5.5.11 and 5.5.12. From the histograms it is apparent that the large filter case experienced lower concentrations for a longer period than the small filter case. The limiting case as the filter size decreased to zero can be seen in Figure 5.5.13 where the zone concentration increased even more rapidly than in the small filter case and reached the pollutant removal and generation equilibrium. The perfect filter case, shown in Figure 5.5.14, almost immediately brought the Zone 1 concentration to the level where the contaminant removal was equal to the generation at a lower concentration than the other cases because no contaminant ever broke through the filter and back into the zone. The concentration in Zone 2 was so low for the perfect filter case that it is not visible on the graph. The histograms in Figures 5.5.15 and 5.5.16 dramatically illustrate the extremes in contaminant exposure times where the perfect filter case experienced all of the occupied hours below 115 ppb and the no filter case encountered concentrations above 360 ppb for most of the occupied hours.



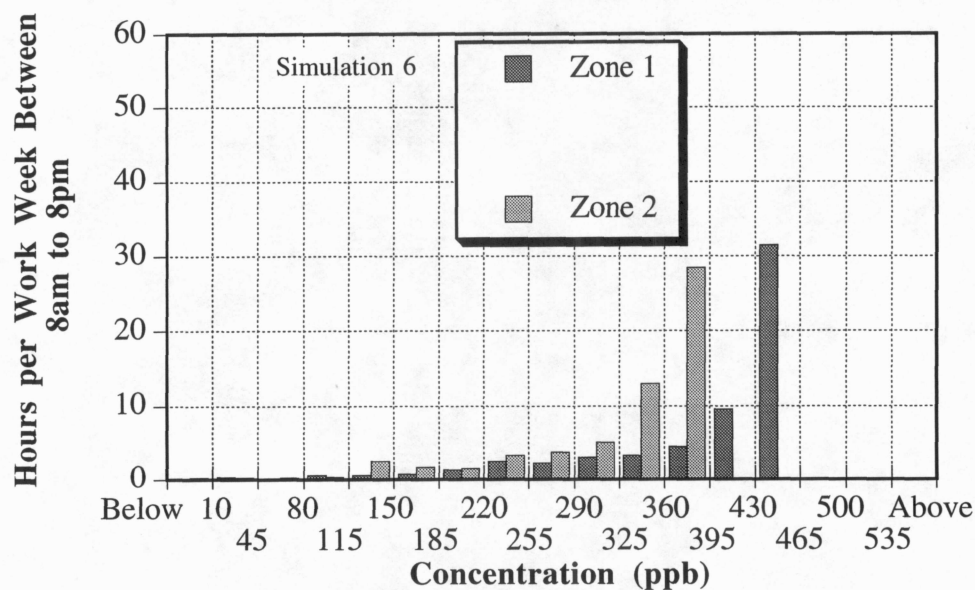
**Figure 5.5.9:** Zone concentrations for the large filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.



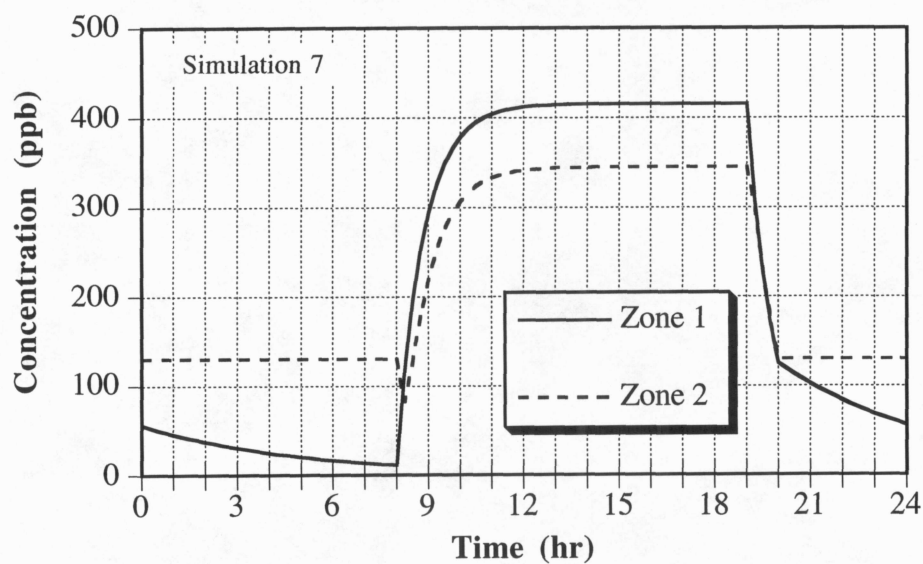
**Figure 5.5.10:** Zone concentrations for the small filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.



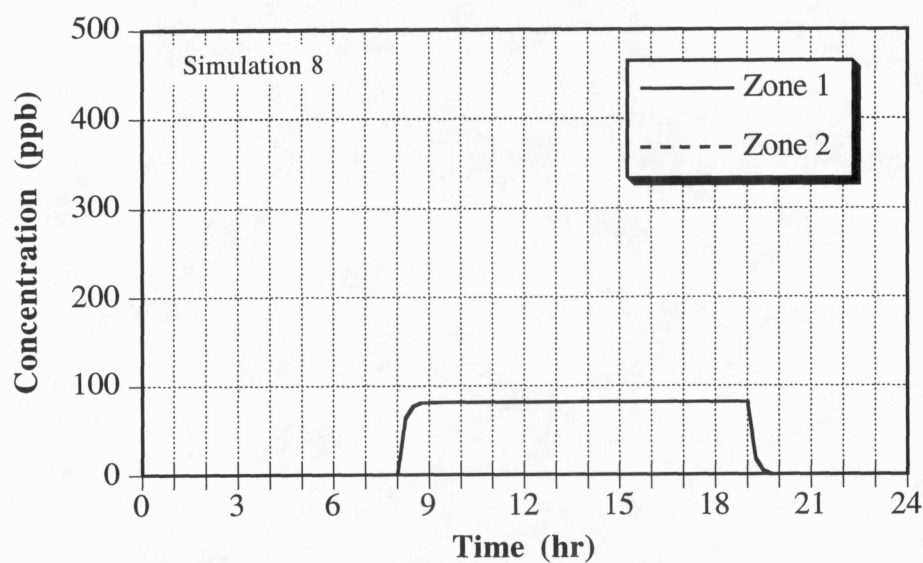
**Figure 5.5.11:** Zone concentration histogram for the large filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.



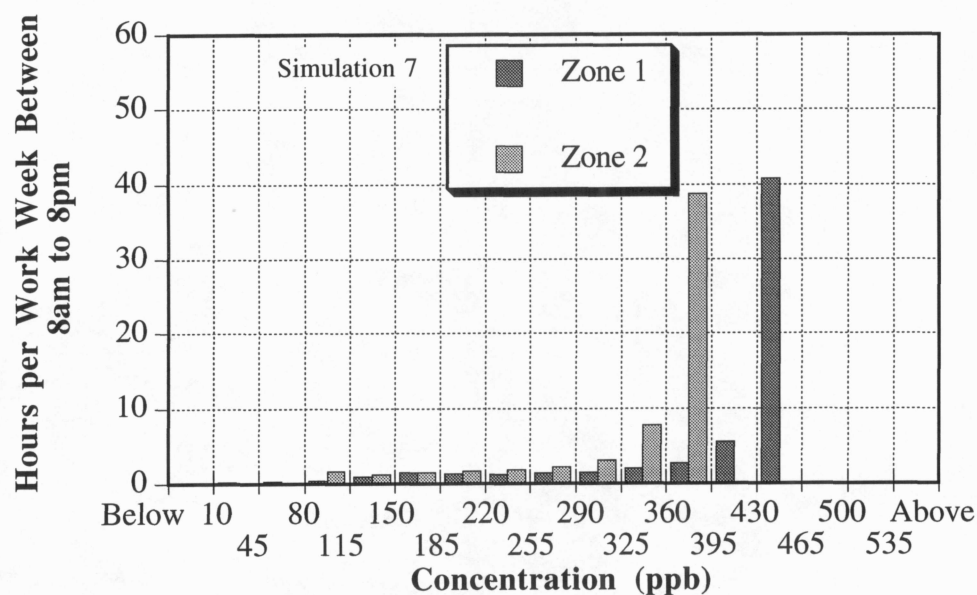
**Figure 5.5.12:** Zone concentration histogram for the small filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.



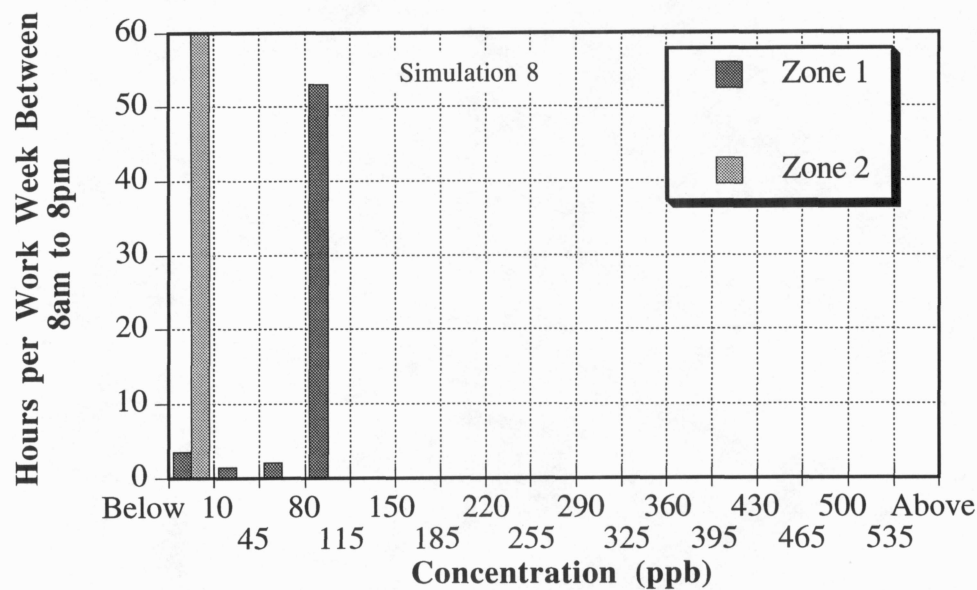
**Figure 5.5.13:** Zone concentrations for no filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.



**Figure 5.5.14:** Zone concentrations for a perfect filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.



**Figure 5.5.15:** Zone concentration histogram for no filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.

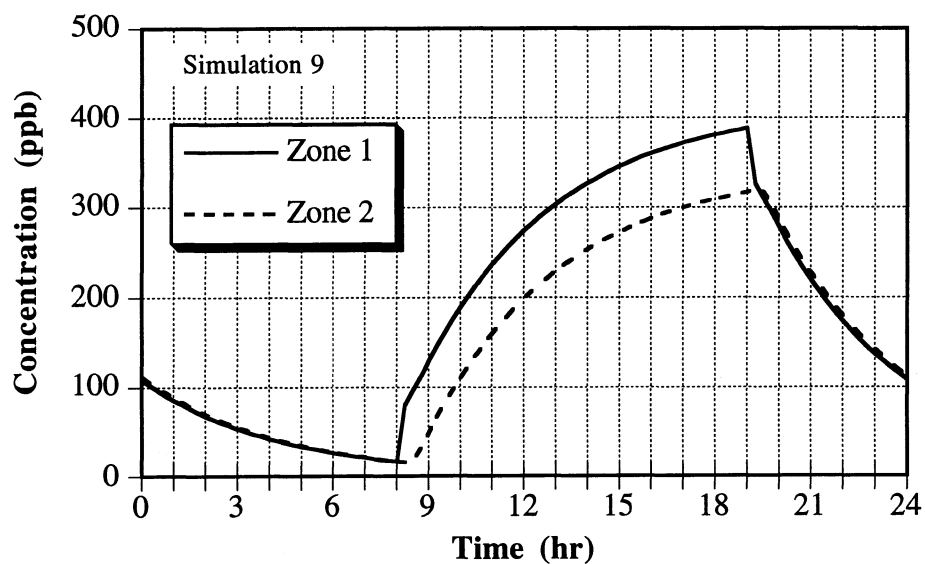


**Figure 5.5.16:** Zone concentration histogram for a perfect filter, 12 hour ventilation, and occupant pollutant generation from 8am to 7pm.

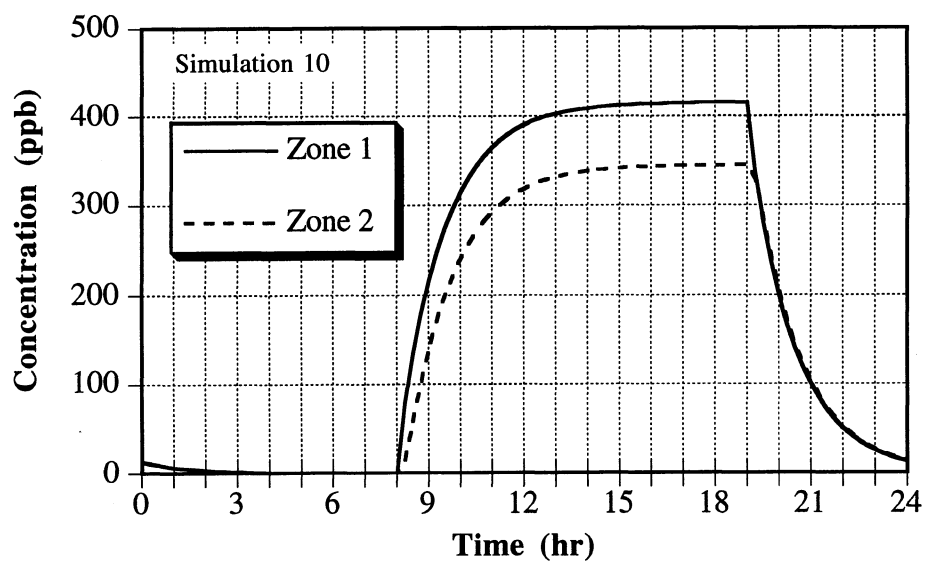
### 5.5.3 Occupant Generated Pollutants with 24 Hour Ventilation

The concentration trends for the occupant generated case with 24 hour ventilation differed from 12 hour ventilation case because the filter was able to desorb itself overnight since the occupants were not present. Thus, each morning the filter started the day with a much larger fraction of its original capacity than in the 12 hour case.

The large filter case, shown in Figure 5.5.17 began each day at 8am with very little contaminant present in the filter which caused the concentration to increase much more gradually than in the 12 hour ventilation case. The concentration in Zone 1 for the smaller filter, shown in Figure 5.5.18, started at the same concentration as in the large filter case but because of its smaller capacity the concentration rose much quicker than in the large filter. Because the ventilation system operated continuously the Zone 2 concentration followed the Zone 1 concentration more closely than in the 12 hour ventilation case where the Zone 2 concentration remained constant once the ventilation system shut down. The histograms in Figures 5.5.18 and 5.5.19 demonstrate the effect 24 hour ventilation has on desorbing the filters overnight to recover their capacity. The histograms show a significant decrease in exposure times at the higher concentration levels over 12 hour ventilation in both cases, but more so in the large filter case because of its greater capacity. The no filter case, shown in Figure 5.5.21, is very similar to the small filter case. The no filter and perfect filter case, shown in Figure 5.5.21 and 5.5.22, were identical to the 12 hour ventilation cases. The histograms for the no filter and perfect filter cases are shown in Figures 5.5.23 and 5.5.24 and were also identical to the 12 hour cases.

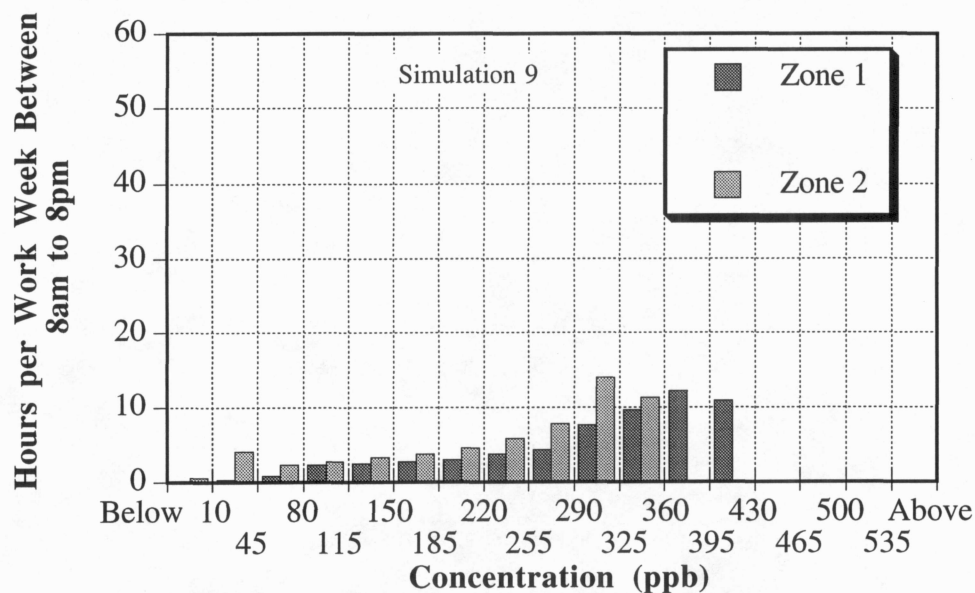


**Figure 5.5.17:** Zone concentrations for the large filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.

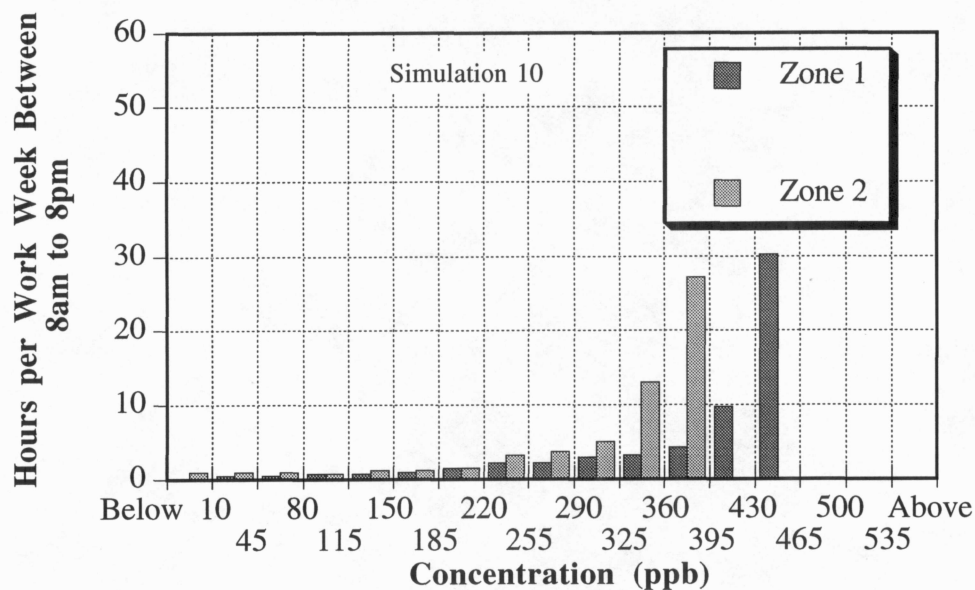


**Figure 5.5.18:** Zone concentrations for the small filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.

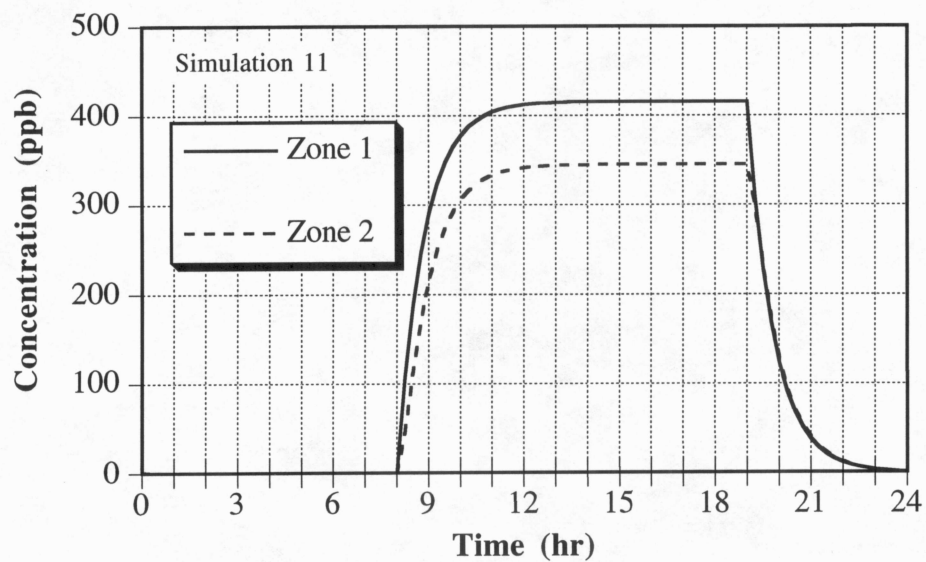




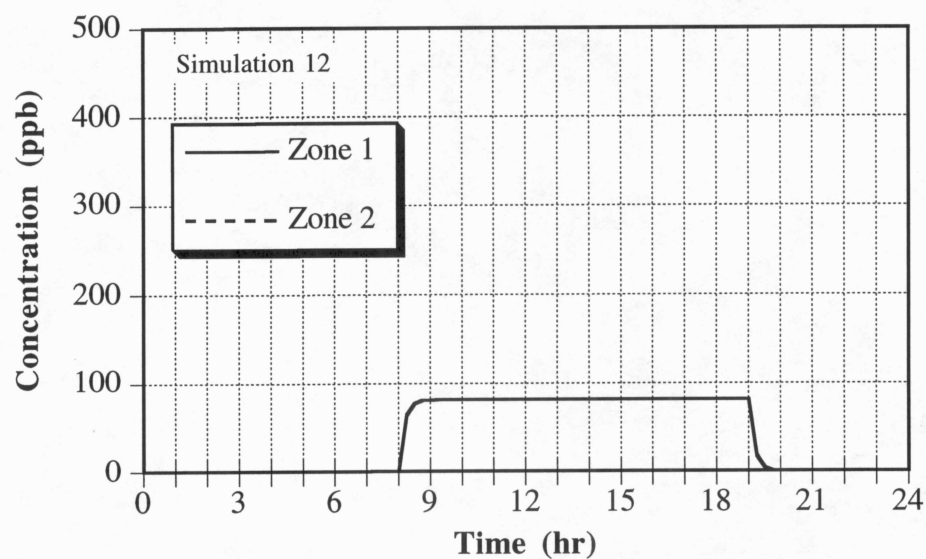
**Figure 5.5.19:** Zone concentration histogram for the large filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.



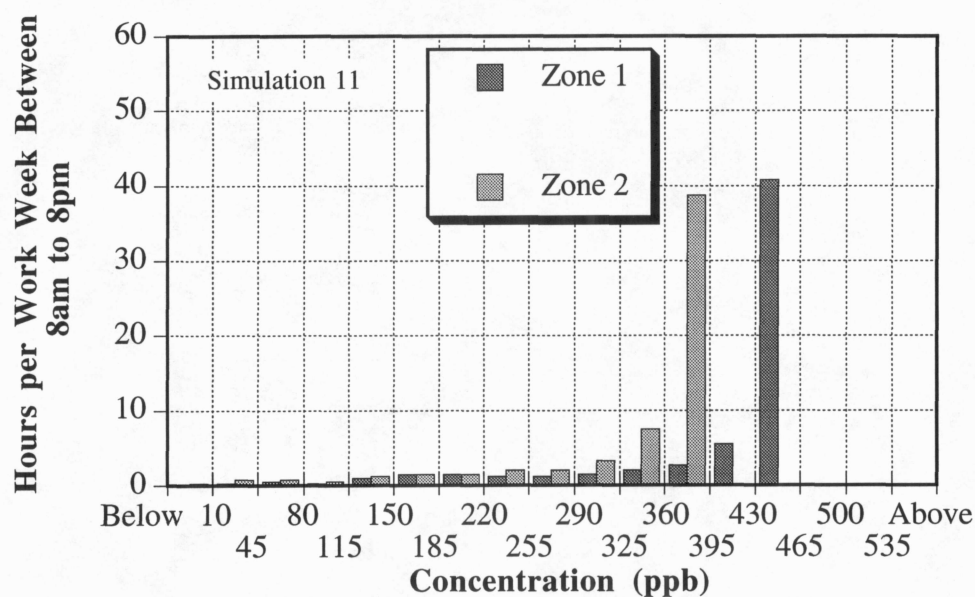
**Figure 5.5.20:** Zone concentration histogram for the small filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.



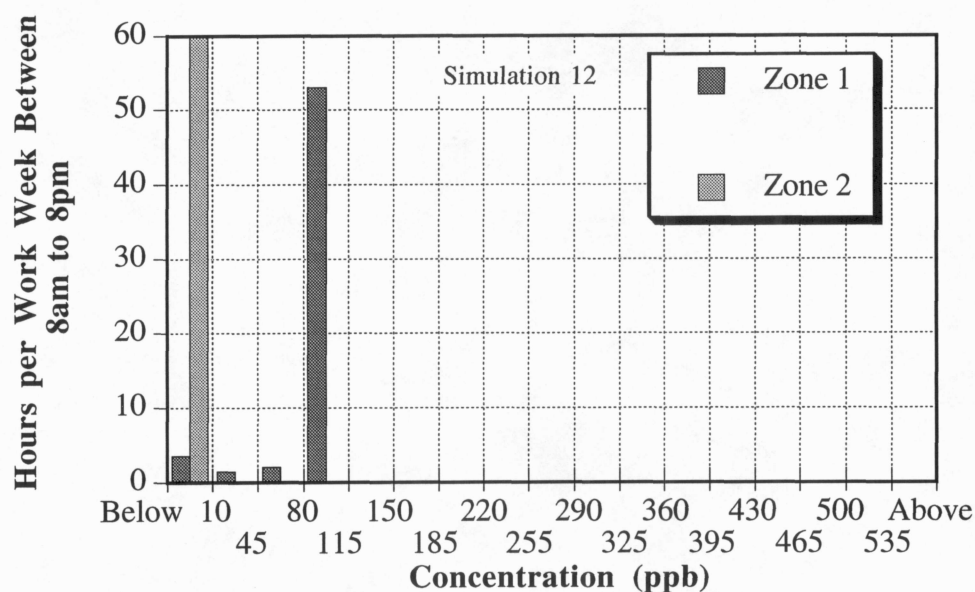
**Figure 5.5.21:** Zone concentrations for no filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.



**Figure 5.5.22:** Zone concentrations for a perfect filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.



**Figure 5.5.23:** Zone concentration histogram for no filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.

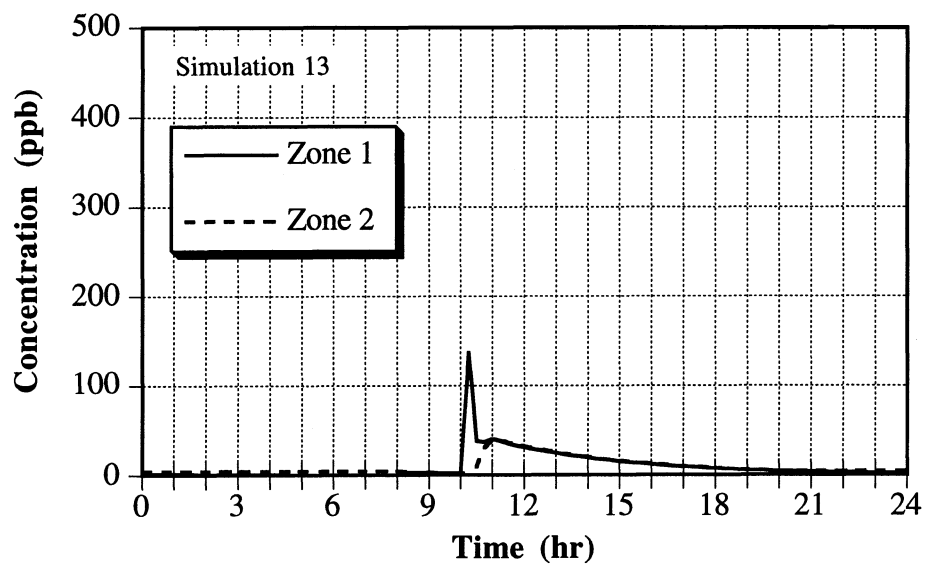


**Figure 5.5.24:** Zone concentration histogram for a perfect filter, 24 hour ventilation, and occupant pollutant generation from 8am to 7pm.

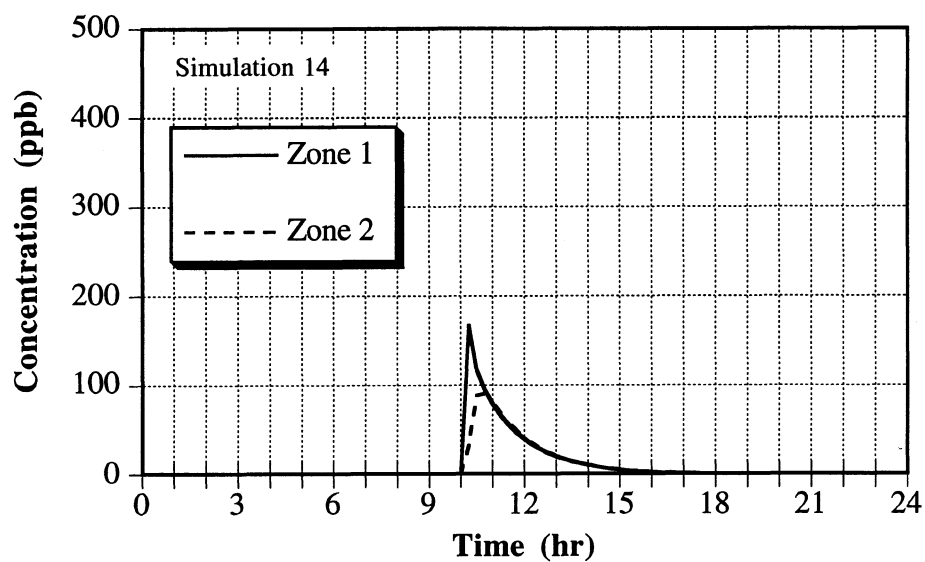
#### **5.5.4 Short Term Large Event of Pollutant Generation with 12 Hour Ventilation.**

The concentration trends for the short term large event case consisted of a rapid increase of the zone concentrations at the initiation of the event followed by an asymptotic decrease of the contaminant levels towards zero concentration.

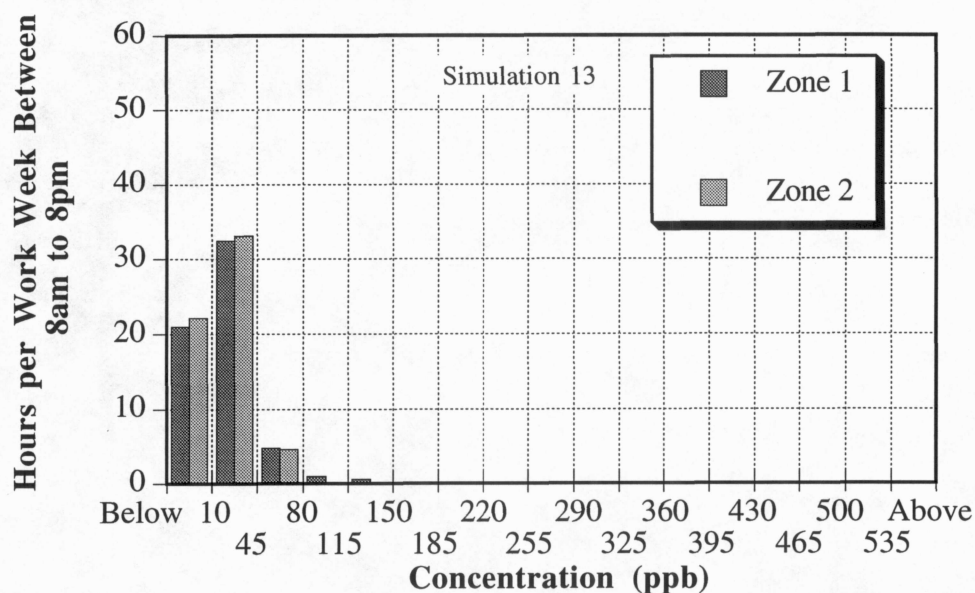
The large filter case, shown in Figure 5.5.25, experienced an initial increase in the zone concentrations followed by a rapid decrease of the concentrations towards zero. The concentration in Zone 1 for the smaller filter, shown in Figure 5.5.26, did not exhibit the same rapid initial decrease because of its smaller capacity. The contaminant broke through more quickly and the concentration decreased to zero more rapidly than in the large filter case because the smaller filter did not store as much contaminant to desorb back into the zone. The lesser capacity of the small filter created a higher concentration for a shorter period than the large filter case. The histograms for the large and small filter cases shown in Figures 5.5.27 and 5.5.28 indicate the distributive effect of the filter on a short pollutant generation event. The large filter case underwent more hours at a lower concentration than the small filter case. The no filter case, shown in Figure 5.5.29, further increased the concentration over a shorter period. The perfect filter case, shown in Figures 5.5.30, completely adsorbed the contaminant producing only a small concentration spike at the time of the event. The histograms for the no filter and perfect filter cases are shown in Figures 5.5.31 and 5.5.32. The histograms follow the trends of the small and large filter cases where the perfect filter case experienced lower concentrations for a longer period than the large filter case and the no filter case experienced more hours at higher concentrations than the small filter case.



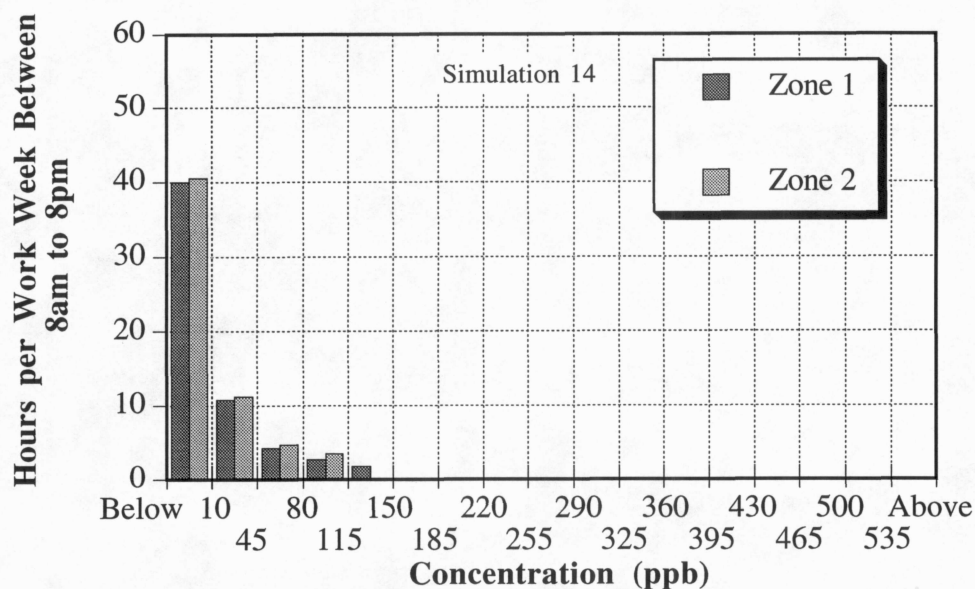
**Figure 5.5.25:** Zone concentrations for the large filter, 12 hour ventilation, and a short large volume event of pollutant generation.



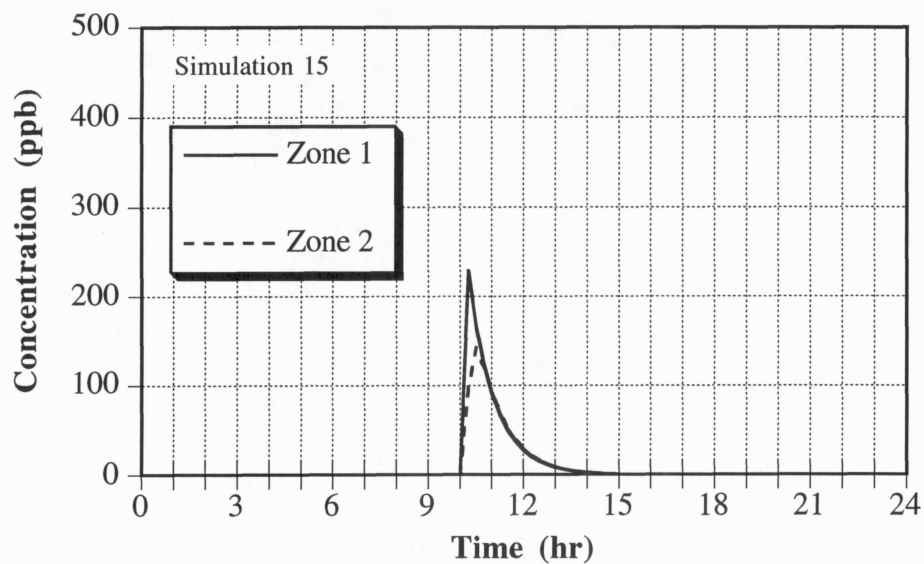
**Figure 5.5.26:** Zone concentrations for the small filter, 12 hour ventilation, and a short large volume event of pollutant generation.



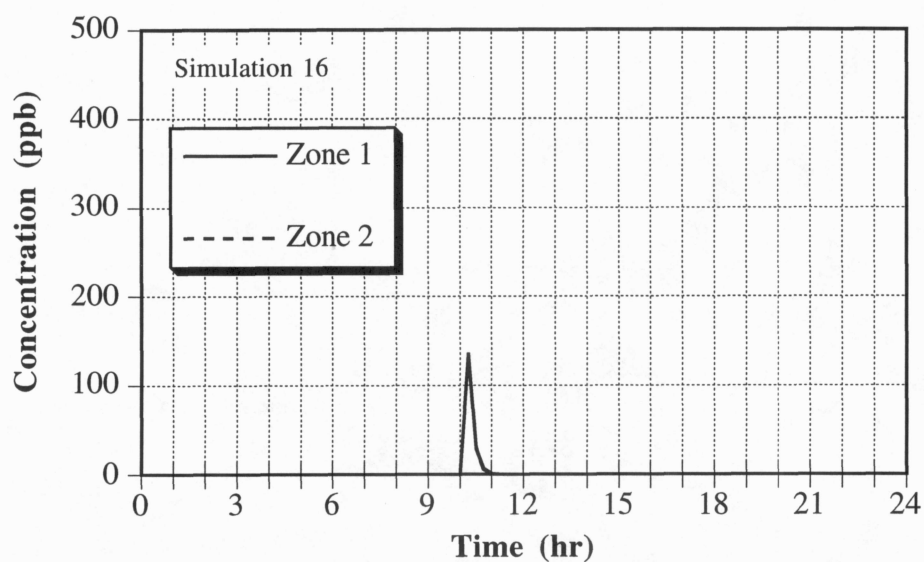
**Figure 5.5.27:** Zone concentration histogram for the large filter, 12 hour ventilation, and a short large volume event of pollutant generation.



**Figure 5.5.28:** Zone concentration histogram for the small filter, 12 hour ventilation, and a short large volume event of pollutant generation.

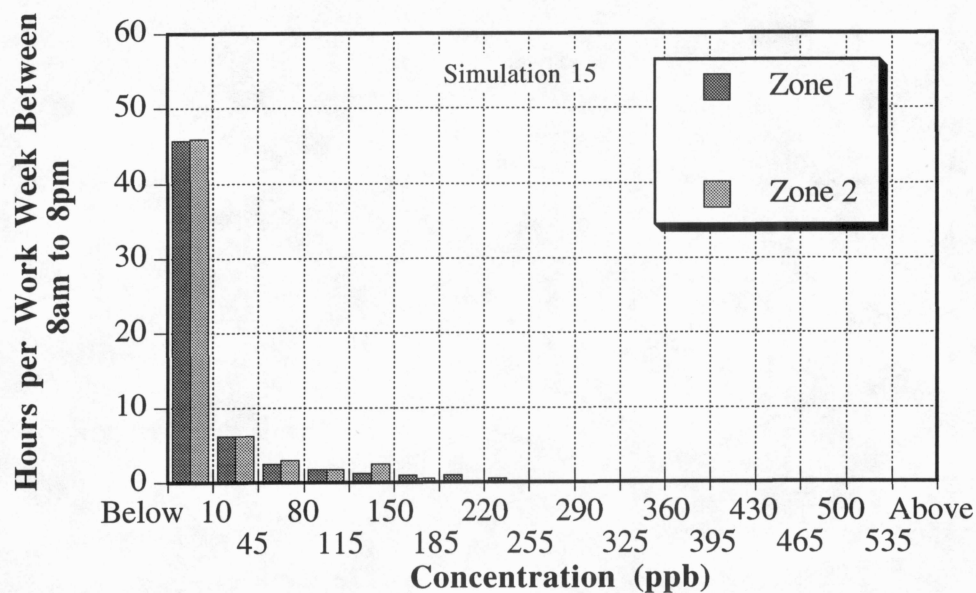


**Figure 5.5.29:** Zone concentrations for no filter, 12 hour ventilation, and a short large volume event of pollutant generation.

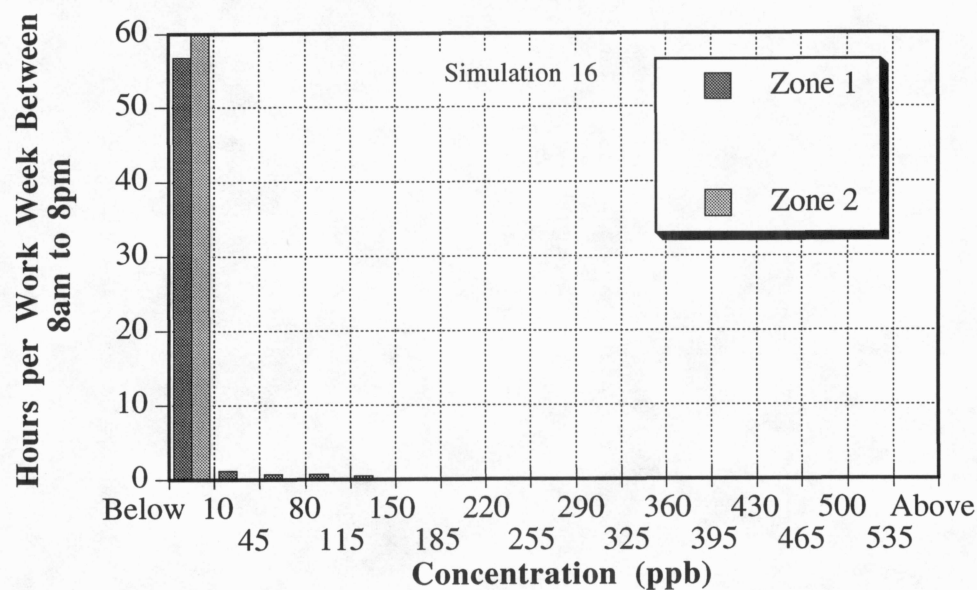


**Figure 5.5.30:** Zone concentrations for a perfect filter, 12 hour ventilation, and a short large volume event of pollutant generation.





**Figure 5.5.31:** Zone concentration histogram for no filter, 12 hour ventilation, and a short large volume event of pollutant generation.



**Figure 5.5.32:** Zone concentration histogram for a perfect filter, 12 hour ventilation, and a short large volume event of pollutant generation.



The energy costs differed only between the two ventilation strategies. The annual energy use for each ventilation scheme is listed in Table 5.5.1. The total energy use is the sum of the heating, cooling, and reheat energy. The 24 hour operation total energy use is not simply twice as much as the 12 hour energy use is because the ambient temperature and humidity during the additional 12 hours of operation were not the same as the initial 12 hours of operation.

**Table 5.5.1:** Comparison of two ventilation strategies effect on the heating and cooling loads for one year in Madison, Wisconsin

Ventilation Strategy	Total Energy Use (GJ)
12 Hour Operation	1810
24 Hour Operation	3017

## 5.6 Summary

Because of the carbon filter's limited capacity and the high volumetric flow rates associated with HVAC systems it is not feasible to attempt to remove indoor air contaminants with a fixed filter. The filter's utility lies in its ability to shift high contaminant levels from occupied to unoccupied times and to distribute high concentration events over longer periods of time at lower concentrations.

## **CONCLUSIONS AND RECOMMENDATIONS**

### **6.1 Conclusions**

The impact of activated carbon filters on the concentration of VOCs present in the indoor environment was the focus of this investigation. The issue was approached first by measurement of the equilibrium capacity of an activated carbon bonded filter for propane over a range of low concentrations. The kinetic adsorption behavior was also recorded and applied to existing breakthrough models capable of predicting the outlet concentration for step inputs. The results were then applied to a more complex transient simulation model of a building where the effects of ventilation control and pollutant generation on energy use and zone concentration levels were examined. Conclusions drawn from the results of the simulations and measurements as well as recommendations for further research are presented in the following remarks.

#### **6.1.1 Propane Isotherm Measurement**

The methods used to measure the propane isotherm produced results with a relatively high degree of precision as was also concluded by Boor (1992). However, the results yield an isotherm slope for propane on activated carbon bonded filters almost half that of

Boor and other investigators, Forsythe (1988) on granular activated carbon. The discrepancy may be due to a decrease in available capacity of the activated carbon during the bonding process. It is also possible that because the carbon weight of the filter was measured indirectly, as a fraction of the filter weight based on the manufactures specifications, the carbon weight used in the calculation may have been incorrect. Fortunately, this inconsistency would not affect the kinetic information derived from the capacity measurements because such data were collected as a fraction of the breakthrough versus time basis and as such were insensitive to the quantity of pollutant adsorbed per gram of carbon provided that the capacity values were used consistently throughout the analysis.

### **6.1.2 Building Zone Pollutant Removal Modeling**

It is apparent that the filters have limited utility for the 24 hour pollutant generation case for even the large filter did not lower contaminant concentrations significantly more than no filter at all when compared to the perfect filter. The concentrations determined in the perfect filter case were calculated by setting the supply concentration to zero. To approach the performance of the perfect filter case, a fixed filter would be too large to be practical. One solution to the relatively low capacity of fixed filters is a rotary wheel filter as described in chapter 1. The rotary wheel addresses the capacity limitations by simultaneously desorbing contaminants from one part of the filter as the other part is adsorbing contaminants by rotating a circular filter through both the supply air stream and an exhaust air stream.

The occupant generated cases demonstrated that the 24 hour ventilation could desorb the filters of occupant generated contaminants during unoccupied periods. However, the

24 hour ventilation significantly almost doubled the energy costs. It may not be necessary to increase the ventilation to completely to 24 hours to benefit from the filter desorption. The filter size and ventilation schedule could be optimized to achieve significant increases in indoor air quality and minimize energy costs.

The short term large event pollutant generation was the case in which the filters were able to approach the performance of the perfect filter because of the small amount of contaminant generated. The filters were able to spread the contaminant over a longer period at a lower concentration than the high short term concentration experienced in the no filter case.

## **6.2 Recommendations For Future Work**

- The collection of kinetic adsorption data at higher velocities such as those that would be experienced in typical air handling units would provide kinetic information to improve and validate the filter model.
- Multiple contaminant experiments would provide the data necessary to assess if and how contaminant mixtures at typical indoor concentrations affect the adsorption of each of the components.
- The measurement of the affect of relative humidity as discussed in chapter 2 would yield important information because of the large changes in relative humidity experienced in different components of a building HVAC system.

- Creation of a scaled zone model where contaminant concentrations could be measured would enable the simulation model to be verified with experimental results.

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## APPENDIX A

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### CALGON TYPE PCB GRANULAR CARBON SPECIFICATIONS

#### Physical Properties

Total Surface Area .....	1150-1250 m <sup>2</sup> /g
Apparent Density .....	0.44 g/cc
Particle Density .....	0.85 g/cc
Real Density .....	2.2 g/cc
Pore Volume .....	0.72 cc/g
Voids in Dense Packed Column .....	50 %
Specific Heat at 100 °C .....	0.25

#### Specifications

Iodine Number, mg/g Minimum .....	1200
Carbon Tetrachloride Adsorption, Weight, % Minimum .....	60
Ash, Maximum, % .....	6.0
Moisture, Maximum, % as Packed .....	3.0
Hardness Number, Minimum .....	92

---

## APPENDIX B

---

### EES Worksheet

```
{ Analysis Worksheet}
{ Atm. Pressure 98508 pa}
{ Temperature 295K}
```

```
DensityN2{mole/m^3}=98508{Pa}/8.3143{J/moleK}/295{K}
```

```
q{mg/g}=A*B/C
```

```
A=FlowRate{mL/min}*DensityN2{mol/m^3}*
1.67E-08{m^3.min/s.mL}*Area{ppm.sec}
```

```
B=1000*MW
```

```
C=Carbonwt{g}*1E+06
```

```
FPM=FlowRate{mL/min}*(1/1E+6){m^3/mL}*35.315{ft^3/m^3}/TubeArea
```

```
TubeArea=pi*(D/12)^2/4{ft^2}
```

```
ConcPolt{mol/m^3}=ppm/1e6*DensityN2
```

```
Cap{mol/m^3}=q/1000/MW*Densitycarb
```

```
Densitycarb{g/m^3}=0.47{g/cc}*1e6
```

```
K=Cap/ConcPolt
```

---

## APPENDIX C

---

### TYPE 61 CARBON FILTER MODEL FORTRAN LISTING

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C ACTIVATED CARBON FILTER MODEL
C
C CREATED BY:
C      MICHAEL SKOLNICK
C CREATED ON:
C      JULY 6, 1993
C VARIABLE LISTING
C
C I - INPUT VALUE      C - CALCULATED VALUE
C
C AREA      I      CROSS-SECTIONAL AREA OF THE FILTER BED {m^2}
C DLA      I      ADSORPTION COEFFICIENT FOR MODEL {m^2/s} OR {1/s}
C DLD      I      DESORPTION COEFFICIENT FOR MODEL {m^2/s} OR {1/s}
C DELTA    C      DIMENSIONLESS COEFFICIENT
C E      I      VOID FRACTION OF THE FILTER
C F      C      FRACTION OF CONCENTRATION STEP BREAKTHROUGH
C I      C      INDEX
C INTC     C      STORAGE USED TO STORE BROKEN THROUGH CURVES
C INLETC   I      INLET CONCENTRATION FROM ZONE
C J      C      INDEX
C K      I      ISOTHERM COEFFICIENT FOR CONTAMINANT
C LENGTH   I      LENGTH OF THE FILTER {m}
C LASTC    C      LAST CONCENTRATION STEP CHANGE VALUE
C MOD      I      TYPE OF MODEL, 1 FOR DIFFUSION, 2 FOR MASS TRANSFER
C NI      C      NUMBER OF INPUTS
C NP      C      NUMBER OF PARAMETERS
C OUTLETC  C      OUTLET CONCENTRATION INTO ZONE
C PPMSTEP  I      MINIMUM CONCENTRATION STEP FOR FILTER CALC.
C QASB     I      FLOW RATE THROUGH FILTER DURING ADSORPTION {m^3}
C QDSB     I      FLOW RATE THROUGH FILTER DURING DESORPTION {m^3/s}
C SMINUS   C      BREAKTHROUGH CALCULATION COEFFICIENT
C SPLUS    C      BREAKTHROUGH CALCULATION COEFFICIENT
C STEP     C      THE MAGNITUDE OF THE CONCENTRATION STEP FOR A WAVE
C STATUS   I      INDICATES IF VENTILATION SYSTEM IS ON OR OFF
C TANDC    C      STORES THE TIME AND CONCENTRATION OF A WAVE
C TIMES    C      TIME IN SECONDS OF THE SIMULATION {s}
C TINIT    C      TIME AT BEGINING OF THE SIMULATION {hr}
C TIMSTP   I      TIMESTEP {hr}
C TP      C      FILTER PROPAGATION TIME {s}
C U      C      INTERSTITIAL FLUID VELOCITY IN FILTER {m/s}
C X      C      TIME STORAGE INDEX COUNTER
C

```

```

SUBROUTINE TYPE61(TIME,XIN,OUT,T,DTDT,PAR,INFO)
C
C      DIMENSION AND DECLARE VARIABLES
C
INTEGER INFO(10),I,K,Z,N,NI,NP,MOD,X,ARRAY
REAL *8 TIMES,F,LASTC,INITC,INLETC,OUTLETC,PPMSTEP,STATUS
REAL *8 LASTEXIT,TIMSTP
REAL *8 TP,E,AREA,TANDC(1000,3),C,DLD,DLA
REAL *8 ERFCA,ERFCB,SMINUS,SPLUS,DELTA,U,LENGTH,Q,QASB,QDSB
REAL  XIN(2),OUT(1),PAR(13),TIME

C  SET PARAMETERS, DO CHECKS, SET INITIAL CONCENTRATIONS, ON
C  FIRST CALL OF THE SIMULATION. CHOOSE MODEL TYPE.

IF (INFO(7).EQ.-1) THEN
  INFO(6)=1
  CALL TYPECK(1,INFO,2,13,0)
  DLA=PAR(1)
  DLD=PAR(2)
  E=PAR(3)
  LENGTH=PAR(4)
  AREA=PAR(5)
  K=PAR(6)
  PPMSTEP=PAR(7)
  QASB=PAR(8)
  QDSB=PAR(9)
  INITC=PAR(10)
  MOD=PAR(11)
  TIMSTP=PAR(12)
  ARRAY=PAR(13)
  INLETC=XIN(1)
  OUT(1)=OUTLETC
  LASTC=INITC
  OUTLETC=INITC
  X=0
  Z=1
  I=1
  RETURN
ENDIF

C  SET THE INPUTS

INLETC=XIN(1)
STATUS=XIN(2)

C
C  IF USING THE FILTER WITH A BUILDING VENTILATION SYSTEM CHECK TO SEE
C  IF THE BUILDINGS SYSTEM IS ON OR OFF. IF IT IS OFF SUBTRACT THE TIME
C  OFF FROM THE FILTER OPERATION TIME AND RETURN TO MAIN TRNSYS
C  PROGRAM.
C
IF (STATUS.EQ.0.0) THEN

  IF (X.GT.0) THEN

```

```

DO 5 N=1,X
  TANDC(N,1)=TANDC(N,1) + TIMSTP
  OUT(1)=0.0
5  CONTINUE
  RETURN
  ELSE
  RETURN
ENDIF
ENDIF

C CHECK TO SEE IF THERE IS A CHANGE IN THE INLET CONCENTRATION
C THAT IS GREATER THAN THE MINIMUM STEP INCREMENT. IF THERE IS, THEN
C THE STEP AND THE TIME OF THE STEP ARE STORED. THEY ARE STORED IN THE C
C ARRAY AND SUPERIMPOSED AS A WAVE FOR THAT STEP ON THE TOTAL
C CONCENTRATION BREAKING THROUGH.

IF (ABS(INLETC-LASTC).GT.PPMSTEP) THEN
  X=X+1
  TANDC(X,1)=TIME - (TIMSTP/2.0)
  TANDC(X,2)=(INLETC-LASTC)
  LASTC=INLETC
  LASTEXIT=OUTLETC
ENDIF

C WHEN USING MODELS 1 AND 2 THE OUTLET CONCENTRATION IS
C CALCULATED AS THE SUM OF THE SUPERIMPOSED BREAKTHROUGH CURVES
C WHERE THE TIMES AND STEPS ARE STORED IN AN ARRAY

OUTLETC=INITC

C THE OUTLETC IS RESET SO THAT IT CAN BE SUMMED UP FROM THE INITIAL
C STATE AFTER EACH TIME STEP. THUS THE SOLUTION IS SOLVED EXPLICITLY
C FOR EACH TIME STEP IT IS NOT A FINITE DIFFERENCE APPROACH. EACH TIMESTEP
C IS INDEPENDENT.

DO 10 N=1,X
  TIMES=(TIME - TANDC(N,1))*3600.0 + 0.01
  IF (TANDC(N,2).LT.0) THEN
    C=DLD
    Q=QDSB
  ELSE
    K=PAR(6)
    C=DLA
    Q=QASB
  ENDIF

  U=(Q)/(AREA*E)
  IF (MOD.EQ.1) THEN
    TP=((1.0-E)*(K/E)+1.0)*(LENGTH/U)
    DELTA=C/(U*LENGTH)
    SPLUS=(1.0/(2.0*DELTA**0.5))*((TP/TIMES)**
    . 0.5+(TIMES/TP)**0.5)

```

```

    SMINUS=(1.0/(2.0*DELTA**0.5))*((TP/TIMES)**
    0.5-(TIMES/TP)**0.5)
    CALL ERRORF(SPLUS,ERFCA)
    CALL ERRORF(SMINUS,ERFCB)
    F=(0.5*(EXP(1.0/DELTA))*(ERFCA))+0.5*(ERFCB)
ELSE
    SPLUS=C*K*LENGTH/U*((1-E)/E)
    IF (SPLUS.LT.1) THEN
        CALL TYPECK(2,INFO,0,0,0)
    ENDIF
    SMINUS=C*(TIMES-LENGTH/U)
    IF (SMINUS.GT.0) THEN
        DELTA=SPLUS**0.5-SMINUS**0.5-(1/8)*SPLUS**0.5-
        (1/8)*SMINUS**0.5
        CALL ERRORF(DELTA,ERFCA)
        F=0.5*ERFCA
    ELSE
        F=0
    ENDIF
ENDIF

TANDC(N,3)=F
CONC=F*TANDC(N,2)
OUTLETC=OUTLETC + CONC

10    CONTINUE

C    AFTER THE ARRAY IS FULL, CHECK THE BREAKTHROUGH CURVE TIME AND
C    CONCENTRATION INFORMATION IN THE STORAGE ARRAY TO SEE IF THEY HAVE
C    PASSED THROUGH THE FILTER YET. IF THEY HAVE, ADD THEM TO THE OUTLETC.
C    WRITE THE DATA AFTER THE LAST CURVE BROKEN THRU, TO THE BEGINING OF
C    THE ARRAY AND CONTINUE WRITING FROM THERE.

    IF (X.GE.ARRAY) THEN
        IF(TANDC(1,3).LT.0.998) THEN
            CALL TYPECK(2,INFO,0,0,0)
            RETURN
        ENDIF

125    IF (TANDC(Z,3).GT.0.998) THEN
        INITC=INITC + TANDC(Z,2)
        Z=Z+1
        GOTO 125
129    ENDIF

    DO 136 W=Z,ARRAY
        DO 134 Q=1,3
            TANDC(I,Q)=TANDC(W,Q)
134        CONTINUE
        I=I+1
136    CONTINUE

    X=ARRAY-Z+1
    Z=1

```

I=1

ENDIF

C SET THE OUTPUTS

OUT(1)=OUTLETC  
RETURN  
END

C SUBROUTINE ERRORF USES A POLYNOMIAL APPROXIMATION TO  
C CALCULATE THE ERROR FUNCTION USED IN THE BREAKTHROUGH  
C CURVE CALCULATION.

SUBROUTINE ERRORF(M,ERFC)

REAL\*8 A1,A2,A3,A4,A5,A6,ERFC,M,A,J  
A1=0.0705230784  
A2=0.0422820123  
A3=0.0092705272  
A4=0.0001520143  
A5=0.0002765672  
A6=0.0000430638  
A=1.0

IF (M.LT.0.0) THEN  
A=-1.0  
ENDIF

J=ABS(M)  
ERFC=1.0-A\*(1.0-(1.0/((1.0+A1\*J+A2\*J\*\*2.0+A3\*J\*\*3.0+A4\*  
J\*\*4.0+ A5\*J\*\*5.0+A6\*J\*\*6.0)\*\*16.0)))

IF (ERFC.LT.1.0E-7) THEN  
ERFC=0.0  
ENDIF

RETURN  
END

```

C CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C TYPE 60 - MULTIPLE ZONE CONTAMINANT FLOW MODEL
C
C CALCULATES THE CONCENTRATION OF A CONTAMINANT IN A MULTIPLE ZONE
C VENTILATED VOLUME AS A FUNCTION OF SIMULATION TIME
C
C CREATED BY:
C   PAUL KNOESPEL
C
C CREATED ON:
C   MAR  2, 1990
C
C MODIFIED ON / BY / REASON:
C OCT 26, 1992 / SJ EMMERICH / TO CALCULATE BREATHING ZONE AND WALL
C CONCENTRATIONS
C
C
C SUBROUTINE TYPE60 CALLS:
C   SUBROUTINE SHORTCALC
C   SUBROUTINE CALC
C
C VARIABLE LISTING
C
C I - INPUT VALUE
C C - CALCULATED VALUE
C
C   A1           C ZONE SOURCES INDEPENDENT OF ZONE CONCENTRATION
C   A2           C ZONE SOURCES DEPENDENT ON ZONE CONCENTRATION
C   A3           C ZONE SINKS DEPENDENT ON ROOM RETURN DUCT
C               C CONCENTRATION
C   BZ           C RATIO OF BREATHING ZONE CONC. TO ZONE AVERAGE CONC.
C   C            C ZONE AVERAGE CONTAMINANT VOLUME CONCENTRATION
C   C1           C ITERATIVE CONCENTRATION VALUE AT TIME STEP I+1
C   CAHU         C COMBINED RETURN CONTAMINANT CONCENTRATION AT THE
C               C AHU
C   FLTSWT       I ON/OFF SWITCH TO INDICATE IF THERE IS A CARBON FILTER
C   CBZ          C BREATHING ZONE CONTAMINANT CONCENTRATION
C   COA          I CONTAMINANT CONCENTRATION IN OUTSIDE AIR
C   CRET         C RETURN DUCT CONTAMINANT CONCENTRATION AT THE
C               C ZONE
C   CSUP         C SUPPLY DUCT CONTAMINANT CONCENTRATION
C   CWALL        C CONTAMINANT CONCENTRATION NEAR WALL
C   DELTAT       I TRNSYS SIMULATION TIME STEP
C   DT           I TIME STEP FOR EACH CALCULATION (S)
C   DTDt         C TRNSYS VARIABLE - NOT USED
C   ERR          C ERROR TOLERANCE FOR CHANGE BETWEEN ITERATION
C               C STEPS
C   ERRFLAG      C ERROR FLAG SET WHEN ERROR TOLERANCE IS NOT MET
C   F            C FUNCTION FOR RHS OF CONCENTRATION DIFFERENTIAL
C               C EQUATION

```



C	FILTEFF	I	FRACTIONAL FILTER EFFICIENCY
C	FLTINT	C	THE POLLUTANT CONCENTRATION ENTERING THE CARBON FILTER
C			
C	HOD	C	CURRENT HOUR OF THE DAY BASED ON SIMULATION TIME
C	HOW	C	CURRENT HOUR OF THE WEEK BASED ON SIMULATION TIME
C	I	C	TIME STEP INDEX
C	IDELAY	C	NUMBER OF TIME STEPS FOR AIR TO FLOW THROUGH RETURN PATH
C			
C	INFO	C	TRNSYS TYPE INFORMATION
C	IZF	I	INTER-ZONE FLOW (KG/HR, LBM/HR)
C	J	C	ZONE NUMBER INDEX
C	K	C	SOURCE SCHEDULE INDEX
C	L	C	ZONE NUMBER INDEX IN 2D IZF(J,L) ARRAY
C	LUB	I	FORTTRAN LOGICAL UNIT FOR BUILDING DATA FILE
C	LUS	I	FORTTRAN LOGICAL UNIT FOR SOURCE DATA FILE
C	ND	C	NUMBER OF DERIVATIVES
C	NI	C	NUMBER OF INPUTS
C	NP	C	NUMBER OF PARAMETERS
C	NSTEPS	C	NUMBER OF TIME STEPS
C	NZONES	I	NUMBER OF ZONES
C	OUT	C	OUTPUT ARRAY TO TRNSYS
C	PAR	I	CONSTANT INPUT ARRAY FROM TRNSYS
C	QCIZF	C	TOTAL INTER-ZONE CONTAMINANT FLOW INTO A ZONE (ACS)
C	QIZF	C	INTER-ZONE AIR FLOW (M3/S, FT3/S)
C	QIZFNET	C	NET INTER-ZONE FLOW FOR A ZONE (M3/S, FT3/S)
C	QZIFOUT	C	INTER-ZONE FLOW LEAVING A ZONE (M3/S, FT3/S)
C	QOA	I	OUTSIDE AIR VOLUME FLOW RATE INTO A ZONE (M3/S, FT3/S)
C	QOAPU	C	ZONE FLOW RATE OF OUTSIDE AIR PER SOURCE UNIT (L3/S-U, FT3/MIN-U)
C			
C	QOATOT	C	TOTAL OUTSIDE AIR VOLUME FLOW RATE (M3/S, FT3/S)
C	QRET	C	VENTILATION VOLUME FLOW RATE LEAVING A ZONE (M3/S, FT3/S)
C			
C	QRETTOT	C	TOTAL RETURN DUCT VOLUME FLOW RATE (M3/S, FT3/S)
C	QSUP	I	CIRCULATION AIR VOLUME FLOW RATE INTO A ZONE (M3/S, FT3/S)
C			
C	QCIRC	C	TOTAL CIRCULATION AIR VOLUME FLOW RATE (M3/S, FT3/S)
C	RE	I	ZONE POLLUTANT REMOVAL EFFECTIVENESS WITH HVAC ON
C	REMEFF	C	ZONE REMOVAL EFFECTIVENESS USED IN CALCULATIONS
C	RETVOL	I	VOLUME OF THE ZONE'S RETURN AIR PATH TO THE AHU (M3, FT3)
C			
C	RHOAIR	C	CONSTANT AIR DENSITY (KG/M3, LBM/FT3)
C	SOURCE	I	CONTAMINANT SOURCE VOLUME FLOW RATE IN A ZONE (M3/S, FT3/S)
C			
C	SMULT	C	SOURCE MULTIPLIER FOR THE CURRENT TIME STEP
C	SMULTWD	I	WEEKDAY SCHEDULED SOURCE MULTIPLIER
C	STIMEWD	I	WEEKDAY SCHEDULE TIME THAT SOURCE MULTIPLIER IS APPLIED
C			
C	SMULTWE	I	WEEKEND SCHEDULED SOURCE MULTIPLIER
C	STIMEWE	I	WEEKEND SCHEDULE TIME THAT SOURCE MULTIPLIER IS APPLIED
C			
C	SUNIT	I	UNIT CONTAMINANT SOURCE VOLUME FLOW RATE (M3/S, FT3/S)
C			
C	T	C	TRNSYS VARIABLE - NOT USED
C	TIME	C	SIMULATION TIME (HR)

C	TIMEPREV	C	TIME OF THE PREVIOUS SIMULATION STEP
C	UNITFLAG	I	FLAG TO INDICATE SI OR ENGLISH UNITS (1=SI, 2=ENGLISH)
C	VENTST	C	INDICATE TO FILTER IF VENTILATION SYSTEM IS ON OR OFF
C	CRBOUT	I	CONCENTRATION POLLUTANTS AT OUTLET OF CARBON
C			FILTER
C	WALL	C	RATIO OF WALL CONC. TO ZONE AVERAGE CONC.
C	XIN	I	INPUT ARRAY FROM TRNSYS
C	ZONEVOL	C	ZONE VOLUME (M3, FT3)
C			

SUBROUTINE TYPE60(TIME,XIN,OUT,T,DTDT,PAR,INFO)

IMPLICIT NONE

INTEGER INFO(10), NI, NP, ND, LUB, LUS

INTEGER NSTEPS, NZONES, IDELAY(25), I, J, K, L, UNITFLAG

REAL TIME, XIN(51), OUT(104), T, DTDT, PAR(11), FLTSWT, VENTST  
 REAL C(-60:60,25), CAHU, CSUP, COA, FILTEFF(3), CRBOUT  
 REAL SOURCE(25), SUNIT(25), SMULT(25), RHOAIR, FLTINT  
 REAL STIMEWD(25,6), SMULTWD(25,6), STIMEWE(25,6), SMULTWE(25,6)  
 REAL ZONEVOL(25), RE(25), REMEFF(25), RETVOL(25), DT, DELTAT  
 REAL QSUP(25), QRET(25), QOA(25), INFILT(25), IZF(25,25)  
 REAL QCIRC, QOATOT, QRETTOT, QCRETOT, QOAPU  
 REAL QIZF(25,25), QIZFNET, QIZFOUT, TIMEPREV, HOW, HOD  
 REAL F, A1(25), A2(25), A3(25)  
 REAL CBZ(25), CWALL(25), BZ(25), WALL(25)

COMMON A1, A2, A3

C  
 C SET PARAMETERS, DO CHECKS, SET ALL INITIAL ZONE CONCENTRATIONS EQUAL  
 C TO THE OUTSIDE AIR CONCENTRATION, AND READ IN SOURCE AND ZONE  
 C INFORMATION  
 C ON THE FIRST CALL OF THE SIMULATION  
 C

IF(INFO(7).EQ.-1)THEN  
 NZONES = NINT(PAR(1))  
 DT = PAR(2)  
 DELTAT = PAR(3)  
 COA = PAR(4)  
 LUS = NINT(PAR(5))  
 LUB = NINT(PAR(6))  
 FILTEFF(1) = PAR(7)  
 FILTEFF(2) = PAR(8)  
 FILTEFF(3) = PAR(9)  
 UNITFLAG = NINT(PAR(10))  
 FLTSWT = PAR(11)  
  
 NSTEPS = NINT(DELTAT\*3600.0/DT)  
 TIMEPREV = -1.0

C

```

C USE ENGLISH UNITS IF THE UNITS FLAG IS SET; OTHERWISE USE SI UNITS
C

```

```

      IF (UNITFLAG .EQ. 2) THEN
        RHOAIR = 0.07517
      ELSE
        RHOAIR = 1.204
      ENDIF

```

```

C
C STOP THE SIMULATION IF NSTEPS IS GREATER THAN 60
C

```

```

      IF ((NSTEPS .LT. 1) .OR. (NSTEPS .GT. 60)) THEN
        WRITE (6,*) 'THE TRNSYS SIMULATION TIME STEP PAR(3) IN'
        WRITE (6,*) 'TYPE 60 MUST BE BETWEEN 1 AND 60 TIMES THE'
        WRITE (6,*) 'TYPE 60 TIME STEP PAR(2)'
        WRITE (6,*) '-- SIMULATION STOPPED --'
        STOP
      ENDIF

```

```

      NI = 2*NZONES + 1
      NP = 11
      ND = 0
      INFO(6) = 3*NZONES+10
      INFO(9) = 1
      CALL TYPECK(1,INFO,NI,NP,ND)

```

```

      DO 5 J = 1, NZONES
        DO 5 I = -60, 60
          C(I,J) = COA
5      CONTINUE

```

```

C
C READ INPUT VALUES FOR THE SOURCE AND ZONE PHYSICAL DATA
C

```

```

      OPEN (LUS, STATUS = 'OLD')
      REWIND (LUS)
      DO 10 J = 1, NZONES
        READ (LUS,*) SUNIT(J)
        READ (LUS,*) (STIMEWD(J,K), K = 1, 6)
        READ (LUS,*) (SMULTWD(J,K), K = 1, 6)
        READ (LUS,*) (STIMEWE(J,K), K = 1, 6)
        READ (LUS,*) (SMULTWE(J,K), K = 1, 6)
10     CONTINUE
      CLOSE (LUS)

```

```

      OPEN (LUB, STATUS = 'OLD')
      REWIND (LUB)
      READ (LUB,*) (ZONEVOL(J), J = 1, NZONES)
      READ (LUB,*) (RE(J), J = 1, NZONES)
      READ (LUB,*) (RETVOL(J), J = 1, NZONES)
      READ (LUB,*) (INFILT(J), J = 1, NZONES)

```

```

      READ (LUB,*) (BZ(J), J = 1, NZONES)
      READ (LUB,*) (WALL(J), J = 1, NZONES)

      DO 20 J = 1, NZONES
        READ (LUB,*) (IZF(J,L), L = 1, NZONES)
        DO 15 L = 1, NZONES
          QIZF(J,L) = IZF(J,L) / (3600.0 * RHOAIR)
15      CONTINUE
20      CONTINUE
        CLOSE (LUB)

      ENDIF

C
C IF THE TIME HAS NOT CHANGED SINCE THE PREVIOUS SUBROUTINE CALL, RETURN
C TO TRNSYS TO PREVENT CHANGING THE CONCENTRATIONS TWICE DURING A
C SINGLE TIME STEP
C
      IF (TIME .EQ. TIMEPREV) THEN
        RETURN
      ELSE
        TIMEPREV = TIME
      ENDIF

C
C FIND THE CURRENT SOURCE VALUE BASED ON THE SOURCE MULTIPLIER
C APPROPRIATE FOR THE CURRENT SIMULATION TIME; IF THERE IS NO SOURCE IN A
C ZONE, SET THE ZONE REMOVAL EFFECTIVENESS TO 1.0
C
      HOW = AMOD(TIME,168.0)
      HOD = AMOD(HOW,24.0)
      OUT(5*NZONES+5)=0.0
      DO 25 J = 1, NZONES

        IF (HOW .LE. 120.0) THEN
          SMULT(J) = SMULTWD(J,6)
          DO 22 K = 1, 5
            IF ((HOD .GT. STIMEWD(J,K)) . AND.
& (HOD .LE. STIMEWD(J,K+1))) THEN
              SMULT(J) = SMULTWD(J,K)
              GOTO 24
            ENDIF
22          CONTINUE

          ELSE
            SMULT(J) = SMULTWE(J,6)
            DO 23 K = 1, 5
              IF ((HOD .GT. STIMEWE(J,K)) . AND.
& (HOD .LE. STIMEWE(J,K+1))) THEN
                SMULT(J) = SMULTWE(J,K)
                GOTO 24
              ENDIF

```

```

23    CONTINUE

      ENDIF

24    SOURCE(J) = SUNIT(J)*SMULT(J)
      OUT(5*NZONES+5)=SOURCE(J)*3600 + OUT(5*NZONES+5)
      IF (SOURCE(J) .EQ. 0.0) THEN
        REMEFF(J) = 1.0
      ELSE
        REMEFF(J) = RE(J)
      ENDIF

25    CONTINUE

      QCIRC = 0.0
      QOATOT = 0.0

      DO 30 J = 1, NZONES

C
C READ INPUT DATA; AIR FLOWS ARE CONVERTED FROM AIR CHANGES PER HOUR
C TO M3/S (OR FT3/S)
C

      QSUP(J) = XIN(J)*ZONEVOL(J) / 3600.0
      QCIRC = QCIRC + QSUP(J)
      QOA(J) = XIN(J+NZONES)*ZONEVOL(J) / 3600.0
      QOATOT = QOATOT + QOA(J)

C
C CALCULATE THE RETURN AIR TIME STEP DELAY
C

      IF (QSUP(J) .EQ. 0.0) THEN
        IDELAY(J) = 0
      ELSE
        IDELAY(J) = 0
      ENDIF

      IF (IDELAY(J) .GT. 60) IDELAY(J) = 60

30    CONTINUE

      QRETTOT = 0.0

      DO 35 J = 1, NZONES

C
C CALCULATE THE RETURN AIR FLOW BY A FLOW BALANCE; IF THE VENTILATION
C SYSTEM IS OFF, INFILTRATION CONTINUES BUT INTER-ZONE FLOW IS ASSUMED
C TO BE ZERO
C

      QIZFNET = 0.0

```

```

QIZFOUT = 0.0

IF (QCIRC .EQ. 0.0) THEN
  QRET(J) = INFILT(J)*ZONEVOL(J) / 3600.0
ELSE
  DO 33 L = 1, NZONES
    QIZFNET = QIZFNET + QIZF(L,J) - QIZF(J,L)
    QIZFOUT = QIZFOUT + QIZF(J,L)
33  CONTINUE
    QRET(J) = QSUP(J) + QIZFNET + INFILT(J)*ZONEVOL(J) / 3600.0
  ENDIF

  QRETTOT = QRETTOT + QRET(J)

C
C CALCULATE CONSTANTS FOR THE dC/dT FUNCTION F
C

  A1(J) = SOURCE(J) / ZONEVOL(J) + ( INFILT(J) * COA ) / 3600.0
  A2(J) = QSUP(J) / ZONEVOL(J)

  IF (QCIRC .EQ. 0.0) THEN
    A3(J) = QRET(J) * REMEFF(J) / ZONEVOL(J)
  ELSE
    A3(J) = ( QRET(J) * REMEFF(J) + QIZFOUT ) / ZONEVOL(J)
  ENDIF

35  CONTINUE

C
C CALL THE MAIN CALCULATION SUBROUTINE; IF THE VENTILATION SYSTEM IS OFF,
C A SHORTENED CALCULATION WITHOUT RECIRCULATION IS PERFORMED
C

  OUT(5*NZONES+6)=0.0
  CRBOUT=XIN(2*NZONES+1)

  IF (QCIRC .EQ. 0.0) THEN
    CALL SHORTCALC (C,COA,DT,NSTEPS,NZONES)
    VENTST=0.0
    OUT(5*NZONES+3)=VENTST
    OUT(5*NZONES+6)=0.0
    OUT(5*NZONES+4)=0.0
  ELSE
    CALL CALC (C,COA,DT,IDELEY,QRET,QRETTOT,QCIRC,QOATOT,
      QIZF,REMEFF,NSTEPS,NZONES,ZONEVOL,FILTEFF,
      CRBOUT,FLTINT,FLTSWT,CAHU)
    VENTST=1.0
    OUT(5*NZONES+4)=FLTINT
    OUT(5*NZONES+3)=VENTST
    OUT(5*NZONES+6)=QOATOT*CAHU*3600
  ENDIF

C
C CALCULATE VALUES FOR OUTPUT; AIR FLOWS ARE CONVERTED BACK TO AIR

```

C CHANGES PER HOUR  
C

QCRETTOT = 0.0

DO 40 J = 1, NZONES

C  
C CALCULATE THE VOLUME FLOW RATE OF OUTSIDE AIR PER SOURCE UNIT;  
C ENGLISH UNITS IN FT<sup>3</sup>/MIN, SI UNITS IN L/S  
C

IF (SMULT(J) .LE. 0.0) THEN  
  QOAPU = 0.0  
ELSEIF (UNITFLAG .EQ. 2) THEN  
  QOAPU = QOA(J)\*60.0/SMULT(J)  
ELSE  
  QOAPU = QOA(J)\*1000.0/SMULT(J)  
ENDIF

QCRETTOT = QCRETTOT + QRET(J)\*C(-IDELAY(J),J)\*REMEFF(J)

C  
C CALCULATE BREATHING ZONE AND WALL CONTAMINANT CONCENTRATIONS  
C

CBZ(J) = C(0,J)\*BZ(J)  
CWALL(J) = C(0,J)\*WALL(J)

OUT(J) = QOAPU  
OUT(NZONES+J) = C(0,J)  
OUT(2\*NZONES+J) = C(0,J)\*REMEFF(J)  
OUT(3\*NZONES+J) = CBZ(J)  
OUT(4\*NZONES+J) = CWALL(J)

40 CONTINUE

CAHU = QCRETTOT/QRETTOT

OUT(5\*NZONES+1) = CAHU

IF (QCIRC .NE. 0.0) THEN

& OUT(5\*NZONES+2) = ((QCIRC-QOATOT)\*CAHU\*(1-FILTEFF(1))+  
& QOATOT\*COA\*(1-FILTEFF(2)))\*  
& (1-FILTEFF(3))/QCIRC

ENDIF

RETURN  
END

CC  
CCCCCCCCCCCCCCCCCCCCCCCC  
C  
C SUBROUTINE SHORTCALC  
C  
C USES AN ITERATIVE MODIFIED EULER (SECOND-ORDER RUNGE-KUTTA)

C METHOD FOR SOLVING THE CONCENTRATION DIFFERENTIAL EQUATION WHEN  
C THE VENTILATION SYSTEM IS OFF

C  
C SUBROUTINE SHORTCALC IS CALLED BY:  
C SUBROUTINE TYPE60

C  
C SUBROUTINE SHORTCALC CALLS:  
C FUNCTION F  
C

SUBROUTINE SHORTCALC (C,COA,DT,NSTEPS,NZONES)

IMPLICIT NONE  
INTEGER I, J, NSTEPS, NZONES, ERRFLAG  
REAL F, C(-60:60,NZONES), COA, DT, C1, ERR

DO 30 I = 0, NSTEPS - 1

C  
C ESTIMATE CONCENTRATION AT STEP I+1  
C

DO 10 J = 1, NZONES  
C(I+1,J) = C(I,J) + DT\*F(0.0,C(I,J),0.0,J)  
10 CONTINUE

C  
C CALCULATE CONCENTRATION AT STEP I+1 USING THE SLOPE ESTIMATE AT STEP  
I+1/2  
C

15 ERRFLAG = 0  
DO 20 J = 1, NZONES  
C1 = C(I,J) + DT\*F(0.0,(C(I,J)+C(I+1,J))/2.0,0.0,J)  
ERR = ABS( C1 - C(I+1,J) )  
IF (ERR .GE. 1.0E-8) ERRFLAG = 1  
C(I+1,J) = C1  
20 CONTINUE  
IF (ERRFLAG .EQ. 1) GOTO 15

30 CONTINUE

C  
C RESET THE CURRENT CONCENTRATION TIME STEP TO 0 TO GET READY FOR THE  
NEXT  
C ENTRY INTO THIS SUBROUTINE  
C

DO 40 J = 1, NZONES  
DO 40 I = -60+NSTEPS, NSTEPS  
C(I-NSTEPS,J) = C(I,J)  
40 CONTINUE



RETURN  
END

CC

C

C SUBROUTINE CALC

C

C USES AN ITERATIVE MODIFIED EULER (SECOND-ORDER RUNGE-KUTTA)

C METHOD FOR SOLVING THE CONCENTRATION DIFFERENTIAL EQUATION AND

C INCLUDES A TIME DELAY IN THE HVAC AIR PATH FOR EACH ZONE.

C

C SUBROUTINE CALC IS CALLED BY:

C SUBROUTINE TYPE60

C

C SUBROUTINE CALC CALLS:

C FUNCTION F

C

SUBROUTINE CALC (C,COA,DT,IDELAY,QRET,QRETTOT,QCIRC,QOATOT,  
QIZF,REMEFF,NSTEPS,NZONES,ZONEVOL,FILTEFF,  
CRBOUT,FLTINT,FLTSWT,CAHU)

IMPLICIT NONE

INTEGER I, J, L, NSTEPS, NZONES

INTEGER IDELAY(NZONES), ERRFLAG

REAL F, C(-60:60,NZONES), COA, DT, QRET(NZONES), QRETTOT, QCRETTOT

REAL QCIRC, QOATOT, QIZF(25,NZONES), REMEFF(NZONES)

REAL ZONEVOL(NZONES), FILTEFF(3), CRBOUT, FLTINT

REAL QCIZF(25), CSUP, CAHU, C1, ERR, FLTSWT

C

C BEGIN THE MAIN CALCULATION LOOP BY CALCULATING A NEW CONCENTRATION

C FOR EACH ROOM AND THEN PROCEEDING TO THE NEXT TIME STEP

C

DO 50 I = 0, NSTEPS-1

C

C CALCULATE THE SUPPLY AIR CONCENTRATION AND THE INTER-ZONE

C CONTAMINANT FLOWS FOR TIME STEP I

C

QCRETTOT = 0.0

DO 10 J = 1, NZONES

QCRETTOT = QCRETTOT + QRET(J)\*C(I-IDELAY(J),J)\*REMEFF(J)

QCIZF(J) = 0.0

DO 5 L = 1, NZONES

QCIZF(J) = QCIZF(J) + QIZF(L,J)\*C(I,L)/ZONEVOL(J)

5

CONTINUE

```

10    CONTINUE

      CAHU = QCRETTOT / QRETTOT
      CSUP = ((QCIRC-QOATOT)*CAHU*(1-FILTEFF(1))+
&          QOATOT*COA*(1-FILTEFF(2)))*(1-FILTEFF(3))/QCIRC

      IF (FLTSWT.EQ.0) THEN
        CSUP = CSUP
      ELSE
        FLTINT = CSUP
        CSUP = CRBOUT
      ENDIF

C  ESTIMATE CONCENTRATION AT STEP I+1
C
      DO 20 J = 1, NZONES
        C(I+1,J) = C(I,J) + DT*F(CSUP,C(I,J),QCIZF(J),J)
20    CONTINUE

C
C  CALCULATE THE SUPPLY AIR CONCENTRATION AND THE INTER-ZONE
C  CONTAMINANT FLOWS FOR TIME STEP I+1/2
C
22    QCRETTOT = 0.0

      DO 30 J = 1, NZONES
        IF (IDELAY(J) .LE. 0) THEN
          QCRETTOT = QCRETTOT + QRET(J)*REMEFF(J)*
&              (C(I,J)+C(I+1,J))/2.0
        ELSE
          QCRETTOT = QCRETTOT + QRET(J)*REMEFF(J)*
&              (C(I-IDELAY(J),J)+C(I-IDELAY(J)+1,J))/2.0
        ENDIF

        QCIZF(J) = 0.0

        DO 25 L = 1, NZONES
          QCIZF(J) = QCIZF(J) + QIZF(L,J)*(C(I,L)+C(I+1,L))/
&              (2.0*ZONEVOL(J))
25    CONTINUE
30    CONTINUE

      CAHU = QCRETTOT / QRETTOT
      CSUP = ((QCIRC-QOATOT)*CAHU*(1-FILTEFF(1))+
&          QOATOT*COA*(1-FILTEFF(2)))*(1-FILTEFF(3))/QCIRC

      IF (FLTSWT.EQ.0) THEN
        CSUP = CSUP
      ELSE
        FLTINT = CSUP
        CSUP = CRBOUT
      ENDIF

```

```

C
C CALCULATE CONCENTRATION AT STEP I+1 USING THE SLOPE ESTIMATE AT STEP
C I+1/2
C

```

```

      ERRFLAG = 0
      DO 40 J = 1, NZONES
        C1 = C(I,J) + DT*F(CSUP,(C(I,J)+C(I+1,J))/2.0, QCIZF(J),J)
        ERR = ABS( C1 - C(I+1,J) )
        IF (ERR .GE. 1.0E-8) ERRFLAG = 1
        C(I+1,J) = C1
40    CONTINUE
      IF (ERRFLAG .EQ. 1) GOTO 22

```

```

50    CONTINUE

```

```

C
C RESET THE CURRENT CONCENTRATION TIME STEP TO 0 TO GET READY FOR THE
C NEXT ENTRY INTO THIS SUBROUTINE
C

```

```

      DO 60 J = 1, NZONES
        DO 60 I = -60+NSTEPS, NSTEPS
          C(I-NSTEPS,J) = C(I,J)
60    CONTINUE

```

```

      RETURN
      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

```

```

C
C FUNCTION F
C
C THIS FUNCTION IS FOR A ZONE WITH A SOURCE TERM, A VENTILATION
C AIR TERM, AN INTER-ZONE AIR FLOW TERM, AND A REMOVAL TERM
C

```

```

      FUNCTION F (CSUP, C, QCIZF, J)

```

```

      IMPLICIT NONE

```

```

      INTEGER J, NZONES
      REAL F, A1(25), A2(25), A3(25), CSUP, C, QCIZF

```

```

      COMMON A1, A2, A3

```

```

      F = A1(J) + A2(J)*CSUP + QCIZF - A3(J)*C

```

```

      RETURN
      END

```

# **SAMPLE SIMULATION TRNSYS DECK**

ASSIGN WDATA.DAT 10  
 ASSIGN TM.OUT 6  
 ASSIGN SOURCE.DAT 13  
 ASSIGN CONTROL.DAT 15  
 ASSIGN OFF.BL1 11  
 ASSIGN OFF.TR1 12  
 ASSIGN BUILDING.DAT 19  
 ASSIGN BLD.DAT 14

```

*****
*
*   INDEPENDENT LIFE INSURANCE BUILDING
*   FLOOR MODEL
*   April 10, 1990
*
*****
  
```

EQUATIONS 3

START=0.0

STOP=288.0

STEP=0.05

TOLERANCES=-0.001 -0.001

SIMULATION START STOP STEP

\*

\*\*\*\*\*

UNIT 9 TYPE 54 WEATHER GENERATOR

\*\*\*\*\*

\* Convert to SI Units

\* 1 - INPUT UNITS, 2 - OUT UNITS, 3 - LUW, 4 - CITY, 5 - TEMP MODEL

\* 6 - HRC, 7 - RAND

PAR 7

1 1 10 127 1 1 1

\*

\*\*\*\*\*

UNIT 20 TYPE 33 PSYCHROMETRICS OUTSIDE AIR

\*\*\*\*\*

\*

PAR 2

\* Dry Bulb & Relative humidity, SI Units

2 1

INP 2

\* Toa RH

9,4 9,6

20.0 0.5

\*

\*\*\*\*\*

UNIT 16 TYPE 16 RADIATION PROCESSOR

\*\*\*\*\*

\*

PAR 9

\* Rnd1 Fix Rnd1 Day Lat Solc Shft Eng IE

5 1 3 1 43.1 428.0 0 1 -1

INP 14

\* Ih Toa RH Td1 Td2 rho N S E W

9,7 9,4 9,6 9,19 9,20 0,0 0,0 0,0 0,0 0,0 0,0 0,0 0,0  
0,0 71.6 0.5 0.0 0.0 0.2 90. -165. 90. 15. 90. -75. 90. 105.

\*

\*\*\*\*\*

UNIT 21 TYPE 33 PSYCHROMETRICS FLOOR9 AIR

\*\*\*\*\*

\*

PAR 2

\* Dry Bulb & Humidity Ratio, SI Units

4 1

INP 2

\* Tz1 Wz1

56,1 56,7  
72.0 0.008

\*

\*\*\*\*\*

UNIT 22 TYPE 33 PSYCHROMETRICS MTGROOM AIR

\*\*\*\*\*

\*

PAR 2

\* Dry Bulb & Humidity Ratio, SI Units

4 1

INP 2

\* Tz2 Wz2

56,2 56,8  
72.0 0.008

\*

\*\*\*\*\*

UNIT 56 TYPE 56 TWO-ZONE OFFICE

\*\*\*\*\*

\*

PAR 2

\* LU LU

11 12

INP 9

\* Toa Woa Ih N S E W Flow1 Flow2

9,4 20,1 16,4 16,6 16,11 16,14 16,17 65,3 65,4  
0,0 0,0 0,0 0,0 0,0 0,0 0,0 0,0 0,0

\*

\*\*\*\*\*

UNIT 65 TYPE 65 HVAC FLOW CONTROLLER

\*\*\*\*\*

PAR 11

\* FMode SMode VMode NZones THeat TCool LUB LUC CLimitH CLimitL Units

2 1 1 2 85.0 50.0 14 15 1.0 1.0 1

INP 21

0,0 0,0 0,0 0,0 56,1 56,2 56,3 56,4 21,3 22,3  
60,5 60,6 60,3 60,4 60,7 60,8 60,9 60,10

60,11 9,4 20,3  
 6.0 6.0 1.0 1.0 0.0 0.0 71.6 71.6 26.0 26.0  
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  
 0.0 71.6 26.0

\*\*\*\*\*

\*UNIT 63 TYPE 28 CONTAMINANT MASS BALANCE

\*\*\*\*\*

\* PAR 19  
 \* DTPR(HR) TOn TOFF LUnit Output  
 \* 24 START STOP 23 2  
 \* 0 -4 0 -4 0 -1 24480 1 -4 0 -1 24480 1 -4  
 \* INP 4  
 \* Source Gen. Cntmt.Exhaust FILTIN FILTOUT  
 \* 60,15 60,16 60,14 61,1  
 \* LABELS 4  
 \* Generation Exhaust IN OUT  
 \*

\*\*\*\*\*

UNIT 60 TYPE 60 CONTAMINANT MODULE

\*\*\*\*\*

PAR 11  
 \* NZones DT(s) DeltaT(hr) COA LUS LUB Filt1 Filt2 Filt3 Units CARBSWT  
 2 180 Step 0.0000 13 19 0.0 0.0 0.0 1 1  
 INP 5  
 65,1 65,2 65,3 65,4 61,1  
 0.0 0.0 0.0 0.0 0.0  
 \*

\*\*\*\*\*

UNIT 61 TYPE 61 CARBON FILTER MODEL

\*\*\*\*\*

PAR 13  
 \* ADS.CF. DSB.CF. VD LGTH AREA ISOTHRM PPMSTP AFLW(QSUP{M^3/S}) DFLW  
 \* INIT. MOD STP ARRAY  
 1.0E-02 1.0E-02 0.906 0.1 10.0 1.50E+05 1.0E-20 5.7516 5.7516  
 0.0 1 STEP 100  
 INP 2  
 60,14 60,13  
 0.0 0.0  
 \*

\*\*\*\*\*

UNIT 25 TYPE 25 OUTPUT FOR FLOW DATA TRACKING

\*\*\*\*\*

PAR 4  
 \* DTPR(hr) TOn TOFF LUnit  
 0.25 168.0 288.0 17  
 INP 7  
 60,3 60,7 60,4 60,8 60,9 60,10 60,11  
 czon1 cbz1 czon2 cbz2 cwall1 cwall2 CAHU  
 \*

\*\*\*\*\*

UNIT 51 TYPE 15 ZONE 1 CLG/HTG/VENT ENERGY CALCULATION

\*\*\*\*\*

PAR 14  
 0 8 -4 -11 7 8 -4 -12 8 -4 -12 7 8 -4  
 INP 2

```

* PZone1 QVent1
56,3 56,5
0.0 0.0 0.0
* Outputs +PZone1 -PZone1 +QVent1 -QVent1
*
*****
UNIT 52 TYPE 15 ZONE 2 CLG/HTG/VENT ENERGY CALCULATION
*****
PAR 14
0 8 -4 -11 7 8 -4 -12 8 -4 -12 7 8 -4
INP 2
* PZone2 QVent2
56,4 56,6
0.0 0.0 0.0
* Outputs +PZone2 -PZone2 +QVent2 -QVent2
*
*****
UNIT 50 TYPE 28 CLG/HTG/VENT ENERGY SUMMARY
*****
PAR 30
* Monthly Totals
* DTPR(Mo) TOn TOff LUnit Output
-1 START STOP 6 2
0 0 3 -3 0 0 3 -3 3 0 0 3 -3 3 -4 0 0 3 -3 0 0 3 -3 3 -4
INP 10
* +PZone1 +PZone2 -PZone1 -PZone2 QLat1 QLat2
51,1 52,1 51,2 52,2 56,9 56,10
* +QVent1 +QVent2 -QVent1 -QVent2
51,3 52,3 51,4 52,4
LABELS 7
ClgEng HtgEng LatEng TotCHL +QVent -QVent TotQVt
*
*****
UNIT 41 TYPE 15 ZONE 1 OUTSIDE AIR ENERGY CALCULATION
*****
PAR 19
0 -1 119000 1 -1 0.075 1 0 0 4 1 -21 -31 8 -4 -31 7 8 -4
INP 3
* OACHg1 Hoa HZone1
65,3 20,3 21,3
0.0 25.0 25.0
* Outputs +Qoa1 -Qoa1
*
*****
UNIT 42 TYPE 15 ZONE 2 OUTSIDE AIR ENERGY CALCULATION
*****
PAR 19
0 -1 2850 1 -1 0.075 1 0 0 4 1 -21 -31 8 -4 -31 7 8 -4
INP 3
* OACHg2 Hoa HZone2
65,4 20,3 22,3
0.0 25.0 25.0
* Outputs +Qoa2 -Qoa2
*

```

\*\*\*\*\*  
 UNIT 40 TYPE 28 OUTSIDE AIR ENERGY SUMMARY  
 \*\*\*\*\*

PAR 19  
 \* Monthly Totals  
 \* DTPr(Mo) TOn TOff LUnit Output  
 -1 168.0 288.0 17 2  
 0 -4 0 -4 0 0 3 -3 0 0 3 -3 3 -4  
 INP 6  
 \* CirTot OATot +Qoa1 +Qoa2 -Qoa1 -Qoa2  
 65,5 65,6 41,1 42,1 41,2 42,2  
 LABELS 5  
 CircFl OAirFl +QOAir -QOAir TotQOA  
 \*

\*\*\*\*\*  
 UNIT 31 TYPE 15 ZONE 1 REHEAT ENERGY CALCULATION  
 \*\*\*\*\*

PAR 24  
 0 -1 119000 1 -1 0.075 1 -1 0.241 1 0 -1 50.0 4 1 0 4 8  
 -13 -1 0.0 9 1 -4  
 INP 3  
 \* NChgs1 TZone1 PZone1  
 65,1 56,1 56,3  
 0.0 72.0 0.0  
 \*

\*\*\*\*\*  
 UNIT 32 TYPE 15 ZONE 2 REHEAT ENERGY CALCULATION  
 \*\*\*\*\*

PAR 24  
 0 -1 2850 1 -1 0.075 1 -1 0.241 1 0 -1 50.0 4 1 0 4 8  
 -13 -1 0.0 9 1 -4  
 INP 3  
 \* NChgs2 TZone2 PZone2  
 65,2 56,2 56,4  
 10.21 72.0 0.0  
 \*

\*\*\*\*\*  
 UNIT 30 TYPE 28 REHEAT ENERGY SUMMARY  
 \*\*\*\*\*

PAR 11  
 \* Monthly Totals  
 \* DTPr(Mo) TOn TOff LUnit Output  
 -1 168.0 288.0 17 2  
 0 -3 0 -3 3 -4  
 INP 2  
 \* ClgRH1 ClgRH2  
 31,1 32,1  
 LABELS 3  
 ClgRH1 ClgRH2 RHTot  
 \*

\*\*\*\*\*  
 UNIT 27 TYPE 17 ZONE CONCENTRATION BIN SORTER  
 \*\*\*\*\*

PAR 11



```
* TStart TEnd HOWOn HOWOff HODOn HODOff LUnit
168.0 288.0 0 120 8 19 17
* NVar LoLim HiLim NBin
4 1.0E-08 1.0E-06 10
INP 4
* CZone1 cbz1 c2 cbz2
60,3 60,7 60,4 60,8
0.0 0.0 0.0 0.0
*
END
```

# **SAMPLE TRNSYS BUILDING DATA FILE**

```

3370.0      81.0
1.0         1.0
615.9       14.4
0.2         0.0
1.1         1.0
0.72        1.0
0.0         0.0
60.0        0.0

```

Building Data File for TYPE 60

Enter the data above for each variable for J = 1, NZONES as follows:

```

ZONEVOL(1)...ZONEVOL(NZONES)
REMEFF(1)....REMEFF(NZONES)
RETVOL(1)....RETVOL(NZONES)
INFILT(1)....INFILT(NZONES)
BZRATIO(1)...BZRATIO(NZONES)
WALLRATIO(1).WALLRATIO(NZONES)

```

```

IZF(1,1).....IZF(1,NZONES)
.             .
.             .
.             .

```

```

IZF(NZONES,1)...IZF(NZONES,NZONES)

```

Where -

ZONEVOL is the zone volume in m<sup>3</sup> or ft<sup>3</sup>

REMEFF is the zone pollutant removal effectiveness

RETVOL is the zone HVAC return air path volume in m<sup>3</sup> or ft<sup>3</sup>

INFILT is the zone infiltration in air changes per hour

BZRATIO is the ratio of breathing zone to zone average  
contaminant concentration.

WALLRATIO is the ratio of near wall to zone average contaminant  
concentration.

IZF(A,B) is the inter-zone flow from zone A to zone B in kg/hr or lbm/hr

# **SAMPLE TRNSYS POLLUTANT GENERATION DATA FILE**

7.47E-08

0.0	8.0	12.0	17.0	19.0	24.0
1.0	1.0	1.0	1.0	1.0	1.0
0.0	9.0	12.0	13.0	16.0	24.0
1.0	1.0	1.0	1.0	1.0	1.0

0.0

0.0	9.0	12.0	13.0	16.0	24.0
1.0	1.0	1.0	1.0	1.0	1.0
0.0	9.0	12.0	13.0	16.0	24.0
1.0	1.0	1.0	1.0	1.0	1.0

Source Schedule Data File for TYPE60

Enter the data above for each variable for J = 1, NZONES as follows:

SUNIT(J)

STIMEWD(J,1)...STIMEWD(J,6)

SMULTWD(J,1)...SMULTWD(J,6)

STIMEWE(J,1)...STIMEWE(J,6)

SMULTWE(J,1)...SMULTWE(J,6)

Where -

SUNIT is the unit source volume flow rate in m<sup>3</sup>/s or ft<sup>3</sup>/s

STIMEWD is the schedule hour of the day for days 1 through 5

SMULTWD is the source multiplier for weekdays

STIMEWE is the schedule hour of the day for days 6 and 7

SMULTWE is the source multiplier for weekend days

# **SAMPLE TRNSYS VENTILATION CONTROL DATA FILE**

8.0  
20.0  
1.0

0.50  
70.0

5.0 11.0 12.0 16.0 18.0 20.0  
1.0 0.0 0.0 0.0 0.0 0.0

Control Schedule Data File for use with TYPE 65  
Enter the data above for each variable as follows:

TIMEON  
TIMEOFF  
CLIMITV

FCLH  
TOALH

STIME(1)...STIME(6)  
FOA(1).....FOA(6)

Where -

TIMEON is the hour of the day that the ventilation system is turned on  
TIMEOFF is the hour of the day that the ventilation system is turned off  
CLIMITV is the concentration limit below which turning off the  
ventilation system is permitted  
FCLH is the fraction of the high concentration limit above  
which the scheduled flow will be used  
TOALH is the outside air temperature above which the scheduled flow  
will be used in C or F  
STIME is the schedule hour of the day  
FOA is the fraction of outside air to be used