Limitations of Models for Characterizing Indoor Particle Concentrations from Cigarette Smoking in an Office Environment

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1. ABSTRACT

Mathematical models have been used by various researchers to provide both a fundamental understanding of indoor air quality dynamics and a platform for estimation of IAQ constituents in lieu of experimental measurements. Due to the diverse nature of these applications the complexity and hence applicability and accuracy of the models varies tremendously. Some models have been specifically developed for evaluation of the impact of a broad range of environmental conditions on IAQ constituents. Cigarette smoking has been included as a source in many of these models since the contribution of smoking to particle and gas concentrations is measurable in many locations.

Part one of this paper uses results from tests that accurately measured particle and gas concentrations during smoking in a real world office environment reported by Curl[1] at IAQ95. The test was conducted in a 511 square meter office space with ventilation and smoking controlled and measured. The smoking rate was held constant throughout the test under both integrated and segregated smoking conditions. Ventilation of the office space was controlled to two rates; no mechanically delivered outside air and full economizer.

Part two of this paper explores a more detailed and controlled test of particle concentration from cigarette smoking that was conducted in a single office setting. This test measured and recorded activities on a real time basis. The information gathered from this real-time single office observation is much more detailed than that from the large office space.

Single compartment models are evaluated using the experimental data from the large office space and from the more detailed single office. The site factors associated with both the comfort cooling system and the air exchange variation were expected to be challenges to the performance of the available models. The theoretical foundation for each model is similar but each model contains slightly different mathematical terms and treatments for ventilation effectiveness, deposition, and filtration. The computed values were compared to the actual data measured in the test. Each model's performance is evaluated using the criteria suggested in ASTM D5157-91 *Standard Guide for Statistical Evaluation of Indoor Air Quality Models*[2]. All of the models have limited use in a real world environment where conditions are not represented by perfect mixing and uniform distribution.

2. INTRODUCTION

2.1. Evaluation Criteria

ASTM D5157-91 *Standard Guide for Statistical Evaluation of Indoor Air Quality Models* "provides quantitative and qualitative tools for evaluation of indoor air quality (IAQ) models"[2]. The tools to be used in assessing the models compare the predicted value *Cp* to the observed value *Co*. They include:

1. The correlation coefficient ***r*** that ranges from -1 to 1. This coefficient indicates the strength of the relationship of the model to the data. The formula for ***r*** is:

$$r = \sum_{i=1}^{n}\left[(Coi-\overline{C}o)(Cpi-\overline{C}p)\right] \Big/ \sqrt{\sum_{i=1}^{n}\left[(Coi-\overline{C}o)^2\right]\left[\sum_{i=1}^{n}(Cpi-\overline{C}p)^2\right]} \quad (1)$$

2. The slope ***b*** of the regression line. This slope is calculated by:

$$b = \sum_{i=1}^{n}\left[(Coi-\overline{C}o)(Cpi-\overline{C}p)\right] \Big/ \sum_{i=1}^{n}\left[(Coi-\overline{C}o)^2\right] \quad (2)$$

3. The intercept ***a*** of the regression line. The intercept is calculated by:

$$a = \overline{C}p - \left[(b)(\overline{C}o)\right] \quad (3)$$

4. The normalized mean square error ***NMSE*** which is a measure of the magnitude of prediction error. This calculation is:

$$NMSE = \overline{(Cp-Co)^2} \Big/ \left[(\overline{C}o)(\overline{C}p)\right] \quad \text{where} \quad \overline{(Cp-Co)^2} = \sum_{i=1}^{n}(Cpi-Coi)^2/n \quad (4)$$

5. The fractional bias ***FB*** of the mean concentrations. This result will be in the range of -2 to 2. ***FB*** is calculated by:

$$FB = 2\cdot(\overline{C}p-\overline{C}o)/(\overline{C}p+\overline{C}o) \quad (5)$$

6. The index of bias ***FS*** of the variance σ^2 of the concentrations. This result will be in the range of -2 to 2. ***FS*** is calculated by:

$$FS = 2\cdot(\sigma^2 Cp - \sigma^2 Co)/(\sigma^2 Cp + \sigma^2 Co) \quad (6)$$

2.2. Models applied to the Large Office Space

EPA issued a draft document "Air Quality Criteria for Particulate Matter" in April 1995[3]. In this document, a 140 page chapter addresses exposure to particulate matter (PM) in ambient and indoor concentrations. "Since major modeling efforts have been aimed specifically at cigarette smoking, a special section is devoted to these models."[3] Many proposed models for estimating indoor air particle concentrations are listed. Most contain a ventilation (outside air or air exchange) component.

Data from a test that accurately measured particle concentrations during smoking in a real world environment was used as input for the models[1]. The test was conducted in an office space with measured and controlled ventilation and smoking. The smoking rate was held constant. The ventilation was controlled to two rates; 0.35 ACH (air changes per hour) and 7.78 ACH. How do the models respond to this variation?

2.3. Models applied to Single Offices

In addition to evaluation of model performance applied to a large office space we tested the performance of a time-dependent single compartment model applied to two moderate-size single occupant offices. These smaller indoor environments enable a more detailed evaluation, both experimentally and theoretically. For this evaluation, both time-integrated and real-time measurements of respirable suspended particles (RSP) were made. Ventilation was also monitored in real-time using two different approaches; (1) conventional measurements using

Pitot tubes placed in the supply air ducts and (2) tracer gas dilution measurements using SF_6. A detailed record of all smoking activity in the offices, including the particular brand smoked and the time, was maintained by the occupant. All inputs to the model were either monitored in the particular office space or measured in controlled chamber experiments.

3. PART 1- LARGE OFFICE SPACE

3.1. Literature Review

Fourteen of the papers referenced in the EPA draft document "Air Quality Criteria for Particulate Matter"[2] contained environmental tobacco smoke (ETS) particle models. The models can be separated into three categories; fundamental physical models (9 papers referenced here), empirical models (3 papers that focused on residences), and exposure attribution models (2 papers). The fundamental physical models are the only ones that can be used for prediction in an office setting. The equations proposed by the papers are similar but contain slightly different terms and treatments for mixing factors, deposition, and filtration.

Most authors discussed more than one equation. The equation selected for evaluation is either the one used by the authors for their data set, or is the form that is appropriate for this application. The equations are numbered for reference purposes and are listed by author. The equation number from the original paper is included in braces { }.

[M1] Ishizu[4] {3} $$C = C_0 e^{-m(Q_i+EQ_r)t/V} + \frac{mC_iQ_i + G}{m(Q_i+EQ_r)}(1-e^{-m(Q_i+EQ_r)t/V}) \quad (7)$$

[M2] Bridge[5] {4} $$C = C_0 e^{-(Q_i+EQ_r)mt/V} + \frac{C_iQ_i + G}{(Q_i+EQ_r)}(1-e^{-(Q_i+EQ_r)mt/V}) \quad (8)$$

[M3] Turk[6] {10} $$C_\infty = \frac{IC_0(1-\eta)+(s_1+s_2)/V}{I+k+\eta R} \quad (9)$$

[M4] Leaderer[7] {3} $$C = C_0 e^{-m(Q_a+Qv+EQ_t)t/V} + \frac{mC_vQ_v + G}{m(Q_a+Q_v+EQ_t)}(1-e^{-m(Q_a+Q_v+EQ_t)t/V}) \quad (10)$$

[M5] Repace[8] {1} $$A_{eq} = 650D_s / C_{eff} \quad (11)$$

[M6] Repace[9] {1,3} $$p(t) = p_{eq}(1-e^{-t_v C_a}), \quad C_a = m(C_v + C_d) \quad (12)$$

[M7] Ott[10] {32} $$\bar{z} = \frac{g_\delta}{\phi_{CO}\nu} \cdot \frac{mfs}{60} \quad (13)$$

[M8] Nazaroff[11] {1} $$dC_{ijk}/dt = S_{ijk} - L_{ijk}C_{ijk} \quad (14)$$

[M9] Koutrakis[12] {10,5} $$C_i = (P\alpha C_0 + Q_{is}/V)/(\alpha + \sigma u_d), \quad Q_{is} = cS/t \quad (15)$$

Table 1 lists the variables used by the authors. This table allows for comparison of the terms used by each author's approach. C is concentration. Equation (14) of Nazaroff[11] is a

general form of the mass balance equation. In total, Nazaroff[11] lists 57 different variables for use in the aerosol dynamic model. We have no basis for estimating the input values for most of the 57 variables so this model is not evaluated.

Table 1 - Variables included in models

Reference Variable	[M1] Ishizu	[M2] Bridge	[M3] Turk	[M4] Leaderer	[M5] Repace	[M6] Repace	[M7] Ott	[M9] Koutrakis	Units
Volume	V	V	V	V			V	V	m^3
Time	t	t		t				t	min
C f(t)	C	C		C		p			$\mu g/m^3$
C equilibrium			C∞		Aeq	p_{eq}		Ci	$\mu g/m^3$
C mean							z		$\mu g/m^3$
C initial	Co	Co		Co	=0				$\mu g/m^3$
C outdoor	Ci	Ci	Co	Cv				Co	$\mu g/m^3$
Air Exchange Outdoor	Qi	Qi	I	Qv		Cv	Φ	α	hr^{-1} or m^3/min
Air Exchange recirculation	Qr	Qr	R	Qt					hr^{-1} or m^3/min
Air Exchange					Ceff	Ca			hr^{-1}
Air Filter	E	E	η	E					none
Mixing factor	m	m		m		m			none
Deposition			k	Qa		Cd			none
Generation	G	G	s_1	G			go		μg/min
Smoker density					Ds				cig /$100m^2$
Smokers							m		people
Cig/hr/person							f		
Duration of cigarette							s		hr
Surface/Volume								σ	m^{-1}
Particle penetration								P	none
Cigarettes								c	cig
Emission rate								S	mg/cig

3.2. Methodology

In the test reported by Curl[1], the particle concentrations were measured by gravimetric sampling and represent the average over the eight hour period. In this test, the concentrations of respirable suspended particles (RSP) indoors was almost the same as the outdoor concentrations. In order to minimize interference from ambient particles, UVPM (ultraviolet particulate matter) is used as the measure of particles from smoking. This marker is more specific to ETS as a source of particles[13], and is at low levels in the outdoor air.

Calculated concentrations were obtained from each model. For the time dependent models, the functions were integrated with respect to time in order to obtain the average concentration over the eight hour period. For the models that are not time dependent the

concentration values were calculated. These values represent the steady state condition. The calculated values were then compared to the observed values.

Table 2 - Values used as input for the models

Relates to:	Reference Variable	Source	Value	Units
Room	Volume	measured	1332	m^3
Room	Area	measured	511	m^2
Room	Surface/Volume	estimated	<0.75	m^{-1}
Time	Time	measured	8	hr
Concentration	Concentration f(t)	model	----------	$\mu g/m^3$
Concentration	Concentration equilibrium	model	----------	$\mu g/m^3$
Concentration	Concentration mean	measured	data	$\mu g/m^3$
Concentration	Concentration initial	assumed	=outdoor	$\mu g/m^3$
Concentration.	Concentration outdoor	measured	data	$\mu g/m^3$
Vent	Air Exchange Outdoor - Low	measured	0.35	hr^{-1}
Vent	Air Exchange Outdoor - High	measured	7.78	hr^{-1}
Vent	Supply Air	measured	9.62	hr^{-1}
Vent	Air Exchange recirculation	calculated		hr^{-1}
Vent	Air Exchange General term	calculated		hr^{-1}
Removal	Particle penetration	estimated	100%	none
Removal	Air Filter	estimated	<5%	none
Removal	Mixing factor	estimated	0.3	none
Removal	Deposition	calculated	0.2025	hr^{-1}
Generation	Cigarettes	measured	160	cig
Generation	Emission rate	estimated	16900	µg/cig
Generation	Cigarettes/hr/person	estimated	2	
Generation	Duration of cigarette	estimated	0.1	hr
Generation	Generation	calculated	338000	µg/hr
Generation	Smokers	calculated	10	people

The values of variables input into the models are given in Table 2. The units used are meters (m), hours (hr), and micrograms (µg). Appropriate conversions were made for each model equation to normalize to these units.

The room area was measured from scale drawings. The volume was computed by multiplying by the ceiling height. The volume was then multiplied by 0.95 in order to adjust for space occupied by furnishings. The surface to volume ratio is estimated to be similar to the measured surface to volume ratio of the single offices reported in part two of this paper. The value of 0.75 was used in the computations. The tests were conducted over an eight hour period each day.

The concentrations are either the output of the models or the measured values. The initial indoor concentration is assumed to be the same as the outdoor concentration. The air exchange terms for outdoor air and supply air were measured. The recirculation air is the difference of the supply air minus the outdoor air. The general air exchange term is defined by the models that use it as the sum of the outdoor air exchange rate plus the deposition rate.

The removal term particle penetration, the proportion of particles introduced from the outdoor air is estimated at 100% (no removal is assumed). The air filtration term is estimated by determining the ETS particle size[13] and then determining the efficiency of the filter on the HVAC system (30% nominal) for that specific particle size[14]. The efficiency is <5% so 5% is used. For the models that use a mixing factor 0.3 is used. This factor is either the number used by the authors of the papers[4,5,7] or is approximately in the middle of the range for the author[9] citing a range of values. The deposition value 0.2025 hr^{-1} is determined by multiplying the measured deposition velocity (from Part 2) times the surface to volume ratio.

The cigarettes smoked were controlled to 160 per day. The emission rate per cigarette is estimated[13] at 16900 µg. The other factors in the models, duration of cigarettes, number of smokers, and cigarettes per hour per person, are used by the models to estimate the number of cigarettes smoked when the actual smoking rate is not measured. The values input into these models are consistent with 160 cigarettes per day.

3.3. Discussion

The calculated values and the observed values were compared using the ASTM equations. The ASTM standard suggests ranges of values that a model should exhibit in order to be judged adequate in describing the observed situation[2]. These values are listed in the third line of Table 3.

Table 3 Resulting Values from Model Performance Assessment

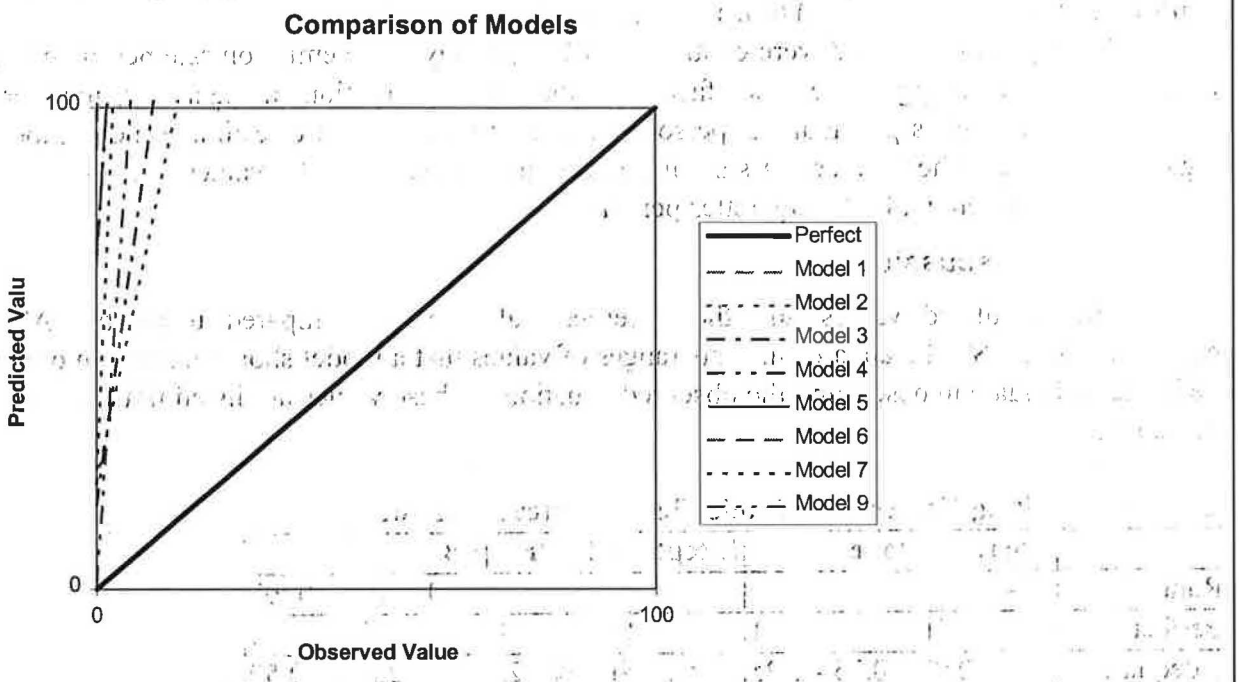
	Corr.	Slope	Intcpt.	NMSE	FB	FS
Range	-1 to 1				0 to 2	0 to2
Perfect	1	1	0	0	0	0
Adequate	> 0.9	0.75 - 1.25	< 25%	< 0.25	< 0.25	< 0.50
Model 1	0.8416	18.17	429%	30.10	1.83	1.99
Model 2	0.8428	5.43	143%	7.31	1.49	1.91
Model 3	0.8424	8.21	111%	11.69	1.61	1.96
Model 4	0.8417	15.91	443%	26.42	1.81	1.99
Model 5	0.8410	90.42	-64%	151.18	1.96	2.00
Model 6	0.8410	36.84	582%	62.32	1.91	2.00
Model 7	0.8410	26.38	140%	41.68	1.85	2.00
Model 9	0.8417	16.20	9%	24.76	1.77	1.99

The ASTM guidance includes quantitative and qualitative criteria. None of the models can be judged to be adequate by either ASTM criteria. The correlation coefficients in the range of 0.84 are likely because of the variance in the observed data and would not be a justification for rejection of the models. However, the regression lines demonstrate a very poor fit and are both quantitative and qualitative rationale for rejecting these models. The slopes indicate that the models over predict by a factor ranging from 5 to 90. This error is illustrated in Graph 1.

There are several possible explanations for the poor performance of the models as applied to this office space. The models are developed using the assumption that the room air is well mixed. Some of the chamber validation studies report the use of mixing fans in order to approach completely mixed conditions. In this office space there were no mixing fans present. The air mixing was only that of the HVAC system diffusers. The mixing factor used (0.3) is

based upon the assumption that the particles are only partly displaced by the outside air introduced into the space. In this case, there was a component of plug flow from the non-smoking area to the smoking area. This characteristic tends to remove particles rather than imperfectly mixing them. The well mixed assumption implicitly assumes that room concentrations are equal (to the average concentration). All of the measurements were taken in the workplaces of nonsmokers. The concentrations were probably higher in the workplaces of the smokers but were not measured, since the test was designed to determine possible nonsmoker exposure in the workplace.

Graph 1 - Comparison of Predicted Value to Observed Value



4. PART 2 - SINGLE OFFICES

Theoretical models of indoor air quality can be used as efficient, cost-effective methods for estimating human exposure to indoor air contaminants. The quality and complexity of these models span from simple single compartment models[4,15,16,17] to complex models based upon computational fluid dynamics.[18,19] Models applied to evaluation of environmental tobacco smoke (ETS) in both experimental chamber and field environments typically have been of the single compartment type. This is primarily due to the chemical complexity of ETS, the dynamic nature of the smoke matrix, and the use of time-integrated area sampling devices for the experimental measurements to which the model estimates are compared. In any case, the model chosen to represent the evolution of a contaminant in an indoor environment should be sufficiently complex to reproduce the salient features of the inherently dynamic environment.

4.1. Formulation of the Single Compartment Model

The mass balance equation is the basis for many indoor air quality models[11,17,20,21,22] and for the model evaluated here. Single compartment models all contain the basic assumption that within a specified region of space, i.e., the core of the model compartment, the modeled contaminants are instantaneously and uniformly distributed. The single compartment model we will use is defined by the following equation:

$$V\frac{dC(t)}{dt} = g(t) - l(t)C(t) \tag{16}$$

$C(t)$ represents the concentration of a particular contaminant within the compartment. $g(t)$ is the generation rate of the component from all sources both within the compartment and introduced into the compartment from outside the defined boundaries. $l(t)$ represents all losses or sinks of the component and V is the volume.

The source generation term, $g(t)$, and the sink term, $l(t)$, are equal to the sum of all such processes:

$$g(t) = \sum_{i=1}^{m} g_i(t) + \sum_{j=1}^{n} q_j(t)\,C_j(t)\ , \quad l(t) = \sum_{j=1}^{n} q_j(t) + v_d\,A_s\ . \tag{17}$$

In equations (17), $g_i(t)$ represents the generation rate of a contaminant due to the i^{th} source at time t with m total sources. $q_j(t)$ is the volumetric ventilation rate for the j^{th} HVAC supply duct with n total supply ducts. Leakage of outside air directly into the test space can be included as a supply duct. $C_j(t)$ is the concentration of the component in the supply air of the j^{th} HVAC supply. v_d is the deposition velocity for the component and A_S is the total exposed surface area within the compartment for deposition. This last term, v_dA_S, represents adsorptive losses for the component. For RSP this term can be a substantial sink whereas for carbon monoxide and sulfur hexaflouride it is virtually zero. There are additional processes which for a particular component may be a source or sink. For instance, gas phase reactions are sinks for the reactants and sources for the products. We will not attempt to simulate aerosol dynamics or chemical reaction. However, evaporation, condensation, and agglomeration can have a substantial effect upon the temporal and spatial evolution of RSP. Particle agglomeration and a detailed treatment of particle deposition have been included in a model of ETS RSP by Nazaroff[11].

Application of equation (16) to a field environment requires component source emissions characterization for each component and source. In addition, any sink phenomena, such as the deposition velocity, which may be properly scaled for use in simulating field environments should be measured experimentally. For our purposes we wish to characterize the ETS emissions of RSP from a variety of common market brand cigarettes. Since smoking behavior can have significant impact upon total ETS generation rates we will determine only the sidestream smoke component using machine smoked cigarettes.

4.2. Measurement of the Source Generation Rates and the Deposition Velocity

The controlled test chamber used for the measurement of the RSP generation rate and the deposition velocity has gross dimensions of 4.20m x 3.91m x 2.69m (l x w x h) for a total volume of 42.21m^3. A supply/recirculation air plenum contains a single makeup air supply

which is combined with a recirculation loop into a single supply vent. Makeup air flow rates are adjustable between 4.7 and 330 L/s. Temperature is controlled both by the recirculation loop and makeup air. Humidity is controlled by dehumidifying the makeup air followed by steam humidification of the total supply air, makeup plus recirculation. Air is exhausted through two 0.20m diameter vents which are combined into a single exhaust duct. For all experiments the chamber conditions were maintained at 22.2° C and 50% R.H. Ventilation in the test chamber was monitored using tracer gas dilution and the system controller (hot wire anemometer).

The deposition velocity is determined from experiments in which the chamber is loaded with ETS RSP and v_d is extracted from the measured RSP decay rate, the measured ventilation rate, and the surface area of the chamber, A_s in equation (17). In these experiments the ventilation rate is measured by the tracer gas method. The recirculation loop of the HVAC system is sealed in order to remove that loss mechanism. ETS RSP is measured in real time using a TEOM Series 1400 PM-10 Monitor (Rupprecht & Patashnick). The TEOM is operated such that the ETS RSP mass concentration is recorded every 2 seconds.

For the measurement of the deposition velocity, only the portion of the decay curve which contained log-linear behavior was used. This results in approximately a five-minute delay between the time the cigarette is extinguished and the time at which linear behavior begins. A linear relationship between the logarithm of the RSP concentration and time indicates a first order loss rate, i.e., the cumulative loss rates in the system are constant in time. Results of these measurements are shown in the table below.

Table 4. Average deposition velocity for ETS RSP.

Average Ventilation Rate (L/s), $\overline{q}_t$	Average Deposition Velocity (10^{-6} m/s), $\overline{v}_d$
22.00 ± 0.38	47.7 ± 4.5
21.91 ± 0.35	84.3 ± 5.1
21.27 ± 0.40	91.4 ± 5.1

The average of the three measurements of $\overline{v}_d$ is 7.5 ± 2.5 x 10^{-5} m/s. This lies in the range of deposition velocities reported by Nazaroff[18] for 0.72 μm ($\overline{v}_d$ = 1.51 x 10^{-5} m/s) to 0.91 μm ($\overline{v}_d$ = 13 x 10^{-5} m/s) diameter smoke particles. It is important to note that we have computed an average deposition velocity which does not explicitly take into account surface orientation and temperature.

Time dependent generation functions for ETS components from machine smoked cigarettes can be extracted from real-time concentration data in controlled chamber experiments by fitting the components' growth-decay curve to an empirical model function and using this representation for the concentration in equation (16). The experiment consists of machine smoking a cigarette every thirty minutes until six cigarettes total have been smoked. The smoking machine is set to draw one 35 ml puff of two seconds duration once per minute. Cigarettes are smoked to a mark located 3 mm from the tipping paper. Mainstream smoke is exhausted outside the test chamber. The TEOM is set to record the RSP mass concentration once per minute. Each experiment is conducted twice. In these experiments humidity, temperature and ventilation rate are held constant at 50% RH, 22.2° C and 9.4 L/s. The ventilation rate is recorded from the system controller and estimated from the carbon monoxide decay rate.

Ventilation rates computed using carbon monoxide decay rates agree within 0.5 L/s to the system controller recorded ventilation rate.

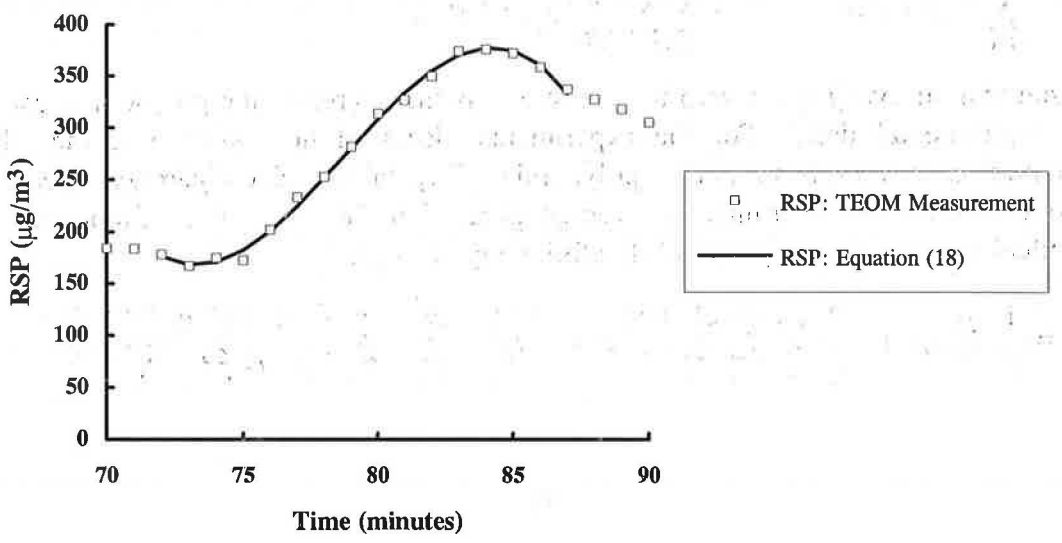
Computation of the generation function is accomplished using equations (16) and (17). Since only one cigarette is smoked at a time the summation in equation (17) over the source generation functions, $g_i(t)$, contains but one term. It is assumed that the filtered makeup airstream contains only small amounts of RSP and that the fluctuations of the RSP concentration in this airstream are also small. These assumptions are based upon real-time RSP concentration measurements made within the test chamber using the TEOM during periods of no cigarette smoking. The RSP deposition rate, $v_d A_s$, is computed from the RSP decay rate after each cigarette has been extinguished. The deposition velocity calculated above cannot be used in evaluating this data due to use of the HVAC recirculation loop which substantially alters the air flow in the test chamber. Computing the loss terms after each cigarette is smoked compensates for fluctuations in the system on a per cigarette basis.

The procedure for determining the total RSP generation function involves fitting the real time RSP measurements from the TEOM analyzer to an empirical function, $C(t)$. More than thirty different functions were fit to the experimental data in an attempt to find the best representation. Simple polynomials were found to reproduce the experimental RSP concentrations better than transcendental functions or combinations of polynomials with transcendental functions (see Graph 2). The following analysis is therefore in terms of polynomial functional representations of the RSP concentration.

$$C_{RSP,i}(t) = \sum_{j=0}^{m} a_{ij}\, t^j \qquad (18)$$

The subscript i refers to i^{th} cigarette smoked in an experiment, j is the polynomial expansion coefficient index, m is the degree of the polynomial, and a_{ij} is the expansion coefficient.

Graph 2. Example of linear regression fit of equation (3) with m = 3 to TEOM measurement of ETS RSP. Regression fit parameters: R^2 = 0.9965, χ^2 = 16.145, start time = 72 minutes, stop time = 87 minutes.



Substituting $C_{RSP,i}(t)$ in equation (16) and solving for $g_i(t)$ yields:

$$g_i(t) = \sum_{j=0}^{m} a_{ij} \left(j V t^{j-1} + l(t) t^j \right) \tag{19}$$

In order to compute the time dependent generation function the sink term, $l(t)$, must be calculated.

$$l(t) = q(t) + v_d A_s + q_r(t)\varepsilon_r \tag{20}$$

where $q(t)$ is the makeup air volumetric ventilation rate, $v_d A_s$ the particle deposition rate, $q_r(t)$ the volumetric recirculation air rate, and ε_r the particle removal efficiency in the HVAC recirculation loop. The makeup air ventilation rate and the recirculation rate are measured throughout the experiment and average values are used for these variables. Experiments were conducted to measure the removal efficiency in the recirculation loop but the magnitude of this parameter was too small to be resolved in our system. Thus, the removal efficiency was set to zero. The deposition losses for RSP were measured in the same fashion as described above using the portion of the decay curve five minutes after the cigarette has been extinguished.The loss rate, $l(t)$, in equation (5) may then be replaced by an average loss rate:

$$\bar{l} = \bar{q} + v_d A_s \tag{21}$$

Having computed the sink terms for the experiment, a simple expression for the generation rate may be derived by collecting terms in t^j, shifting the summation index, and noting that $a_{i,m+1}$ is identically zero:EMBED $g_i(t) = \sum_{j=0}^{m} c_{ij} t^j$ $c_{ij} = (j+1) V a_{ij+1} + (\bar{q} + v_d A_s) a_{ij}$

(22)

$g_i(t)$ represents a time dependent generation function extracted from a single experiment. Combination of all the generation functions for a given cigarette brand requires initializing the individual generation functions such that $g_i(t = 0) = 0$ for all i. This is necessary due to the method used to fit the raw data to the empirical function. A temporal shift, t_i', is determined for each of the individual generation functions such that the generation rate is zero at time zero. Given this temporal shift the expression for $g_i(t)$ is:

$$g_i(t) = \sum_{j=0}^{m} c_{ij} (t + t_i')^j = \sum_{j=0}^{m} \sum_{k=0}^{j} \binom{j}{k} c_{ij} t^{j-k} t_i'^{k} . \tag{23}$$

The summation over j spans zero to m where m is the degree of the polynomial used to fit the RSP experimental data. For the experiments discussed here m=3, i.e., the TEOM RSP concentration data are fit to a cubic polynomial. Typically twelve cigarettes of each brand are smoked in order to determine an average generation function $G(t)$. Combination of each individual generation function yields the following average:

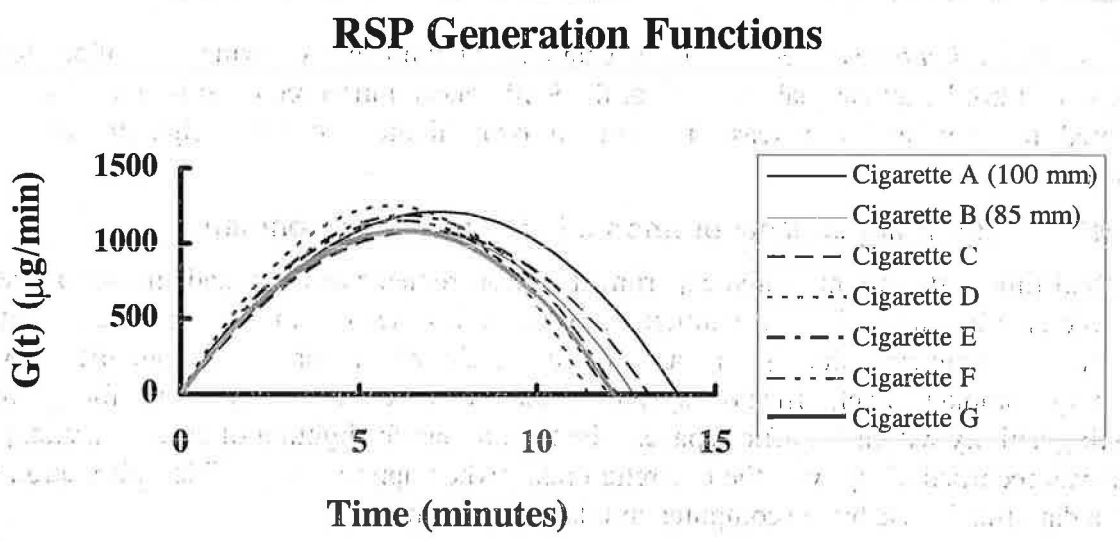
$$G(t) = \frac{1}{N} \sum_{i=1}^{N} g_i(t) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=0}^{m} \sum_{k=0}^{j} \binom{j}{k} c_{ij} t^{j-k} t_i'^{k} = \sum_{l=0}^{m} t^l \sum_{j=l}^{m} \binom{j}{j-l} \sum_{i=1}^{N} \frac{c_{ij} t_i'^{j-l}}{N} . \tag{24}$$

where N is the total number of cigarettes smoked. The terms in brackets are the binomial coefficients. The last equation results from setting the summation variable $k = j\text{-}l$ and summing over the l index first. This index shift enables computation of average polynomial expansion coefficients, A_l.

$$A_l = \sum_{j=l}^{m} \binom{j}{j-l} \sum_{i=1}^{N} \frac{c_{ij}\, t_i'^{\,j-l}}{N} \quad \text{and} \quad G(t) = \sum_{l=0}^{m} A_l\, t^l. \tag{25}$$

Generation functions for seven market brand cigarettes are shown in Graph 3.

Graph 3. ETS RSP generation functions for selected market brand cigarettes.



Integration of $G(t)$ over the domain of interest, the start and stop times for smoking the cigarette, yields the average total RSP yield per cigarette. The total RSP yield ($\overline{G}$) is:

$$\overline{G} = \int_{t_0}^{t_f} G(t)\,dt = \int_{t_0}^{t_f} \left(\sum_{l=0}^{m} A_l\, t^l \right) dt = \sum_{l=0}^{m} \frac{A_l\,(t_f^{\,l+1} - t_0^{\,l+1})}{l+1} \tag{26}$$

Total RSP (sidestream) yields for the seven cigarettes tested are listed in Table 5.

The cigarette burn times in Table 5 are approximately two to four minutes longer than the normal burn time of these cigarettes. This is of some concern since it is the temporal evolution of ETS RSP we wish to simulate in the field environments. During sidestream smoke measurements of cigarette A, an average of 11.2 puffs per cigarette (approximately 11 minute burn time) has been measured under the same machine smoking regime used above versus a burn time of approximately 14 minutes extracted from this data set. The difference lies in (1) the uncertainties involved in determining the generation functions and its zero roots and (2) in a basic assumption of the model, instantaneous uniform dispersion of the smoke components.

Table 5. Total RSP yields for seven market brand cigarettes. Total yields computed from equation (26). The cigarette burn time (Δt_s) is the smoking time calculated from the zeros of $G(t)$, i.e., $\Delta t_s = t_f - t_0$.

Cigarette Brand	Total RSP (μg/cig)	Calculated Cigarette Burn Time (Δt_s)
Cigarette A 100 mm	11253 ± 1290	13.98
Cigarette B 85 mm	9206 ± 1027	12.78
Cigarette C	9488 ± 1100	13.15
Cigarette D	9548 ± 1022	11.47
Cigarette E	9655 ± 6444	12.23
Cigarette F	9181 ± 986	11.99
Cigarette G	8763 ± 957	12.15

The *dispersion time* of RSP in the test chamber is unknown. A mixing time of one to two minutes would not be unreasonable. Indeed, the RSP concentration recorded by the TEOM has been noted to continue to increase for one to two minutes after the cigarette has been extinguished.

4.3. Experimental Measurements in the Field Environments

Real-time and time-integrated experimental measurements of were made in two offices of comparable size but with different ventilation systems. The net volume and surface area (total volume minus furniture volume) for each office are shown in Table 6. Both offices were occupied by a smoker. Each office occupant was supplied on each test day a form for recording all smoking activity within the office space. The time of day for lighting of each cigarette, pipe, or cigar was recorded along with the cigarette brand (when appropriate). This information was input to a data file for use by the computer simulation program.

Table 6. Net volume and surface area for test offices.

	Building #1 Office	Building #2 Office
Volume (m^3)	48.36	34.26
Surface Area (m^2)	117.7	94.18

To fully test the performance of the single compartment model real-time measurements of both ventilation and IAQ contaminants are needed. A mobile system was constructed for this purpose. A Brüel and Kjær (B&K) model 1303 multipoint sampling system in conjunction with a B&K model 1302 infrared absorption photoacoustic detector was used to quantify SF_6 at five locations within the Building #1 office and in the HVAC supply duct. In the Building #2 office this system was used to sample at four locations within the office plus one sampling line in the HVAC supply to the office and one sampling line in the outside air supply. The system was capable of recording the SF_6 concentration approximately every 1.6 minutes or once every 9.6 minutes at a single sampling location. A Rupprecht and Patashnik TEOM Series 1400 PM-10 Monitor was used for real-time measurement of respirable suspended particulate matter (RSP). The RSP mass concentration was recorded once per minute.

Time integrated RSP measurements were also made over the same sampling period as the real-time measurements. Duplicate samples were taken for each measurement. Gravimetric, measurements of RSP were made in the center of the office spaces and in the HVAC supply ducts. The RSP concentrations from the TEOM real time measurements averaged 20% less than the gravimetric samples. This indicates that the measurement techniques are comparable for the conditions present in the offices. The difference does not impact the real time model calculations since both the particle generation function and the field concentration were measured with the same real time instrumentation.

The Building #1 office is supplied outside air through a constant air volume (CAV) induction system. One hundred percent outside air is supplied to induction units around the perimeter of the building by a main air handling unit located on the roof. The interior of the building is served by fan coil units which operate with 100% recirculated air and provide filtration and cooling only. The office used in this investigation is located on the north side perimeter of the building and receives 100% outside air by the mechanical HVAC system. The air is exhausted into the interior of the building either through the open door or, in the case of the door closed, through a transfer duct located in the ceiling in the center of the room.

The Building #2 office is ventilated by a variable air volume (VAV) HVAC system. The main air handling unit serving this office is located on the ground level of the building and serves the lower floors. This system delivers constant temperature air and varies the flow to maintain room air temperature. The total air flow to the office is controlled by a thermostat located within the room which is connected to a damper located in the HVAC duct serving the office. This damper only controls air flow to the test office. All other ducts downstream of the damper were disconnected and sealed. Outside air supplied to the test office is controlled mechanically through a damper system in the main air handling unit which mixes outside air and recirculated air. The outside air flow to the office can be computed by combining the measurement of total air flow of the main air handling unit with the measurements of the total flow of outside air supplied. Air to this office is exhausted either through the above ceiling return or through the open doorway.

Ventilation rates were continuously monitored for both test offices using conventional measurements. Since the Building #1 office is ventilated through a single HVAC duct with 100% outside air only a single monitoring location was necessary. The flow rate to the office is based upon measurement of velocity pressure in the supply duct.[23] The total air flow to the Building #2 office was monitored in a manner similar to that in the Building #1 office. However, since this HVAC system uses recirculated air, additional measurements were needed to quantify the outside air flow to the test space. The fraction of outside air in the office supply air is calculated as the ratio of the outside air flow to the total HVAC system flow. Both of these flows were recorded by permanently installed pitot tube grids and were recorded every ten minutes.

The air supply to the Building #1 office was essentially constant within the uncertainty of the measurement, which is estimated to be approximately 10% of the measured flow. For many of the test days the VAV system in Building #2 also operated in what amounted to a constant air supply mode. There is some variation over the two-week period of the study. This system varies the outside air flow to the building relative to outdoor temperature and indoor thermal demand. For the time period of this test outside air temperatures were mild and therefore the system operated in economizer mode for most of the test. Economizer mode is a condition in which the

system utilizes outside air for its cooling demands. For all but one test day the calculated fraction of outside air in the supply air to the test office was above 0.8.

Tracer gas techniques were also employed to evaluate the ventilation of the test office spaces. The tracer gas measurements were made using sulfur hexaflouride and the B&K multipoint sampling and quantitation system. For the Building #1 office the entire building could be dosed with tracer gas through a single HVAC intake located on the roof of the ninth floor. The building was dosed with sufficient tracer gas to reach a peak concentration in the test office of approximately 10 ppm. The Building #2 office was dosed by adding tracer gas within the outside air/recirculated air mixing chamber located within the main air handling unit. For these tests the B&K system was set to record the tracer gas concentration every 1.6 minutes and every 6.93 minutes at a particular sampling location. The daily average ventilation rates in Building #1 varied from 54.7 to 55.7 L/s conventional measurement, and 21.7 to 27.8 L/s using the tracer gas measurement. Interestingly, on one afternoon the door to this office was closed and the tracer gas measurement of the ventilation rate increased to 53.3 L/s. Daily average outside air ventilation rates in the Building #2 office varied from 72.7 to 177 L/s as measured using conventional techniques and from 25 to 35 L/s using the tracer gas technique.

Possible explanations for the differences in the ventilation measurement techniques focus on the tracer gas measures. It is likely that the tracer was imperfectly mixed in the test buildings by the HVAC supply air. It is also possible for the tracer gas to flow back into the rooms through the open doors, or the above ceiling returns. For the model analysis here, the conventional techniques are viewed to be more appropriate. This is because the airflow quantities are large and easily measurable by pitot traverse techniques and both buildings were positively pressurized by the HVAC system operation thereby minimizing any effects of infiltration.

4.4. Application of the Single Compartment Model to Field Environments

The time dependent generation functions determined in the experiments described in Section 4.2 were represented by cubic polynomials. However, equation (16) may be solved for the contaminant concentration in the modeled space, $C(t)$, for a generation function represented by any simple polynomial of arbitrary degree, p. The general expression for the time dependent generation rate for a particular component, particle or gas, is:

$$g_i(t) = \sum_{j=0}^{p} A_{ij}(t + t_i')^j = \sum_{j=0}^{p} A_{ij} \sum_{k=0}^{j} \binom{j}{k} t^{j-k} t_i'^k \qquad (27)$$

where $g_i(t)$ represents the time dependent generation rate. t_i' is a temporal offset and is the solution to $g_i(t=0) = 0$. The A_{ij} are polynomial expansion coefficients and have been determined for a series of market brand cigarettes. The subscript i refers to a particular cigarette brand smoked at a specific time as recorded by the test office occupants. This cigarette brand and time information are recorded in an input file which the computer simulation program accesses. In addition to the generation rate measurements, the deposition velocity for RSP was extracted from its measured decay rate and tracer gas measurements of the ventilation rate.

In order to solve equation (16) analytically some assumptions regarding the ventilation rate and the concentration of a contaminant in the HVAC supply airstream must be made. If, over the time period $t_1 \le t \le t_2$, the HVAC supply air flow and concentration of the contaminant species in that air flow are constant then equation (16) using equations (17) and (27) becomes:

$$V\frac{dC(t)}{dt} = \bar{q}C_s + \sum_{i=1}^{m}\sum_{j=0}^{p} A_{ij}\sum_{k=0}^{j}\binom{j}{k} t^{j-k} t_i'^{k} - (\bar{q} + v_d A_s)C(t), \qquad (28)$$

where $\bar{q} = q(t_2)$, $C_s = C_s(t_2)$ .and m is the total number of cigarettes burning at time t. Since experimental measurements are used for the ventilation rate and concentration of the contaminant in the supply air stream the values at time t_2 will be used. The solution for the contaminant concentration, $C(t)$, in a room with one HVAC supply vent, $n = 1$ in equations (17), at any time in the interval $t_1 \le t \le t_2$ is:

$$C(t) = C(t_1)\, e^{-(\bar{q}+v_d A_s)(t-t_1)/V} + \frac{\bar{q}\, C_s}{\bar{q} + v_d A_s}(1 - e^{-(\bar{q}+v_d A_s)(t-t_1)/V})$$

$$+ \frac{1}{\bar{q} + v_d A_s}\sum_{i=1}^{m}\sum_{j=0}^{p}(-\frac{V}{\bar{q} + v_d A_s})^j \sum_{k=j}^{p} A_{ik}\sum_{l=0}^{k-j}\frac{k!\, t_i'^{l}}{l!(k-l-j)!}(t^{k-l-j} - t_1^{k-l-j} e^{-(\bar{q}+v_d A_s)(t-t_1)/V}). \qquad (29)$$

The first term represents the evolution of the contaminant in the room air at time t_1 on the time interval t_1 to t. The second term is the introduction and evolution of the contaminant from the HVAC supply and the third term is the generation and evolution of the contaminant due to smoking. No other sources are considered. For instance, leakage of a contaminant from the outside through a window is not included in this treatment. If knowledge of the outside air leak rate and the effective transport probability of a contaminant through that orifice were available, an additional term could be added to represent this process. This addition would appear as another ventilation term.

A computer program that incorporates the experimental measurements of ventilation and contaminant levels in the supply airstream was developed for the calculation of equation (29). Conventional measurements of the office ventilation rate were made in real time and the computer program reads this data directly. Computer simulations were also run using the average tracer gas results for the ventilation rate. Gravimetric RSP measurements were used as an estimate of the concentration of this component in the HVAC supply.

4.5. Computer Simulations of RSP in the Test Offices

Computer simulations of RSP in the two office environments were conducted using the simple single compartment model described above, equation (16). The simulations were run for each experimental test day, ten days in each office, over the time period 8:00 to 16:30. To simplify evaluation of the model performance, the computer simulation program generates a calculated concentration at each point in time for which an experimental measurement was recorded. Time dependent generation rates, equation (25) for each cigarette brand smoked in the test offices were used. Each simulation is initialized to the experimental measurement closest to 8:00.

One real-time plot of the TEOM measurement and computer simulation of the RSP concentration in the office in Building 1 is shown in Graph 4. Comparison of the simulation results shows that the time dependent and constant RSP generation rates essentially yield the same predicted concentrations. The trace labeled Simulation: Pitot Tube Ventilation Rate was generated using the time dependent generation function.

Results of the computer simulations for RSP in the test offices are given in Tables 7 and 8 below. The integrated average RSP concentrations for the TEOM measurement and the computer model prediction are given in the second and third columns, respectively. Comparison of these average values indicates that the computer model is capable of adequately predicting the RSP concentration for the simulations in which the conventional measurements of the ventilation rate and the time dependent RSP generation functions are used. However, the model fails all the statistical evaluation tests (ASTM D5157-91)[2]. The disagreement between the time-resolved experimental measurement of RSP and the model prediction is probably due to non-uniform, non-instantaneous distribution of the contaminant in the test space. Remember, two primary assumptions for this particular model are that the contaminants *are* instantaneously and uniformly dispersed within the core of the model compartment. Baughman et al. have addressed the mixing of a point source contaminant, SF_6, in an unventilated room.[24] These experiments show concentration gradients existing for over 100 minutes.

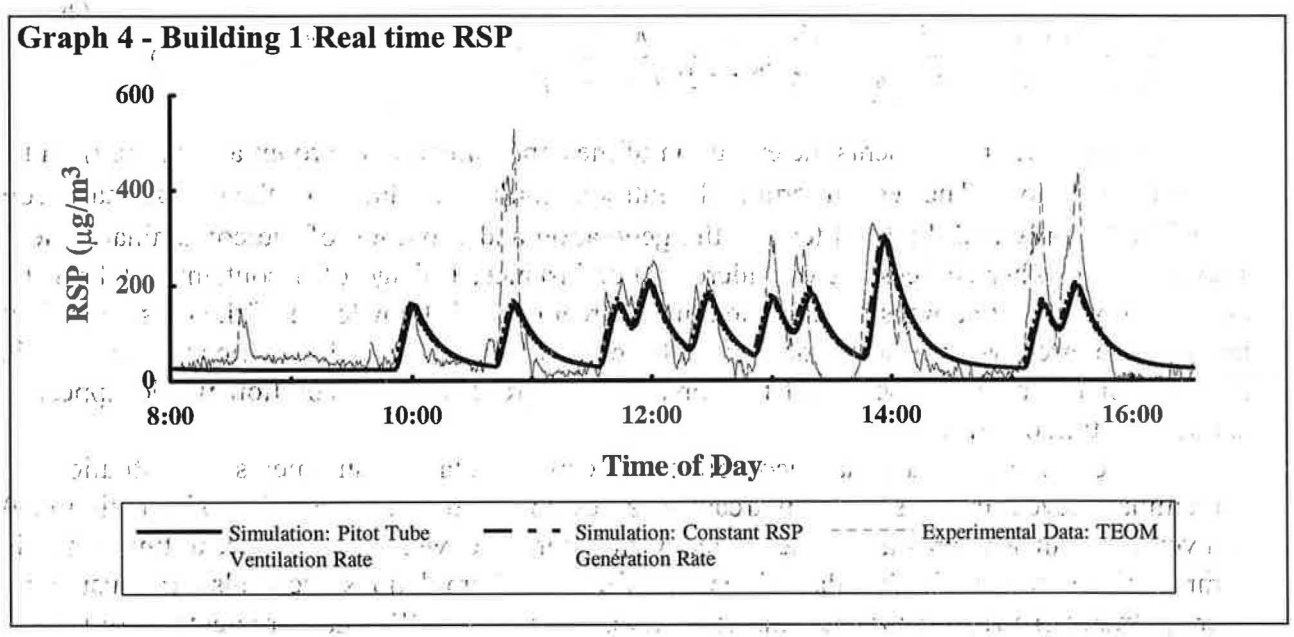


Table 7 - Model evaluation parameters for RSP in the Building #1 Office. Time dependent RSP generation functions determined in test chamber experiments and conventional measurements of the office volumetric ventilation rate were used in the model simulation.

Date	RSP - TEOM ($\mu g/m^3$)	RSP - Simulation ($\mu g/m^3$)	Correlation Coefficient	Slope	Intercept ($\mu g/m^3$)	NMSE	Fractional Bias	Fractional Bias Variance
April 23	53.3 ± 2.7	55.8 ± 3.5	0.55	0.35	37.4	2.03	0.05	-0.82
April 27	37.3 ± 1.9	34.0 ± 3.1	0.79	0.56	13.0	1.23	-0.09	-0.75
May 4	42.4 ± 2.1	44.8 ± 3.7	0.72	0.56	21.2	2.14	0.05	-0.46
May 5	61.5 ± 3.1	63.9 ± 4.0	0.70	0.49	33.5	1.71	0.04	-0.63
May 6	10.5 ± 0.5	10.0 ± 0.1	-0.41	-0.04	10.4	1.33	-0.05	-1.96
May 11	62.6 ± 3.1	44.7 ± 3.0	0.69	0.31	25.1	2.41	-0.33	-1.49
May 12	46.9 ± 2.3	44.5 ± 2.5	0.48	0.27	32.0	2.73	-0.05	-1.09
May 13	85.5 ± 4.3	74.7 ± 3.7	0.54	0.28	50.8	2.04	-0.13	-1.25
May 14	17.5 ± 0.9	31.0 ± 0.2	0.74	0.27	26.3	0.66	0.56	-1.22
May 15	86.2 ± 4.3	77.8 ± 4.3	0.69	0.42	41.8	0.73	-0.10	-1.00

Table 8 - Model evaluation parameters for RSP in the Building #2 Office. Time dependent RSP generation functions determined in test chamber experiments and conventional measurements of the office volumetric ventilation rate were used in the model simulation.

Date	RSP - TEOM ($\mu g/m^3$)	RSP - Simulation ($\mu g/m^3$)	Correlation Coefficient	Slope	Intercept ($\mu g/m^3$)	NMSE	Fractional Bias	Fractional Bias Variance
May 26	30.2 ± 1.5	19.7 ± 1.8	0.65	0.32	10.0	4.50	-0.42	-1.45
May 27	34.4 ± 1.7	50.9 ± 2.2	0.55	0.45	35.4	1.89	0.39	-0.002
May 28	28.0 ± 1.4	26.2 ± 1.8	0.39	0.18	21.1	5.70	-0.07	-1.33
May 29	28.8 ± 1.4	27.1 ± 1.7	0.59	0.27	19.2	3.83	-0.06	-1.34
June 2	28.0 ± 1.4	19.2 ± 2.2	0.55	0.30	10.7	5.63	-0.37	-1.31
June 3	38.1 ± 1.9	43.9 ± 1.9	0.77	0.46	26.3	0.58	0.14	-0.83
June 5	29.2 ± 1.5	27.1 ± 2.1	0.68	0.46	13.7	1.90	-0.08	-0.08
June 8	41.9 ± 2.1	49.1 ± 2.9	0.69	0.51	27.7	1.03	0.16	-0.44
June 9	48.2 ± 2.4	48.1 ± 3.2	0.75	0.45	26.5	0.94	-0.002	-0.95
June 10	48.5 ± 2.4	41.8 ± 2.7	0.68	0.37	24.0	1.0	-0.15	-1.19

5. CONCLUSIONS

A single compartment real time predictive model for particle concentration from cigarette smoking was developed from fundamental physical principles. The particle generation functions were determined by testing different brands and styles of cigarettes in a chamber and fitting to the measured data. These generation functions were inputs into the models coincident with the recorded smoking activity in the single offices. Deposition factors were determined by the chamber data. Ventilation for each office was carefully measured and monitored in real time. The real time particle concentrations were measured in multiple locations in each room. Two primary assumptions for the model are that the particles are instantaneously and uniformly dispersed within the model compartment. The resulting model based upon the instantaneous and

uniform dispersal assumptions fails to replicate the observations when judged by the ASTM criteria[2].

Published single compartment models were tested using data from a measured and controlled test of smoking in an office space. None of the models can be judged adequate by the ASTM criteria[2].

The simple single compartment models have limited utility in locations where perfect mixing and uniform distribution do not resemble the actual environmental conditions. Few if any office spaces, restaurants, and other commercial building spaces fit the assumptions used in deriving the models. Most of the models were validated in environmental chambers or in a single rooms of a house. In the case of the large office space, the models would over predict the observed concentrations by one to two orders of magnitude.

6. ACKNOWLEDGEMENTS

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