Table III. Equilibrium Composition of Reaction Mixture

Oxidation mixture: Analysis in Table I
Temperature: 2300°F
Pressure: 20 atm

Specie	Fuel I, mol frac	Fuel II, mol frac
N_2	0.3614	0.4339
CO	0.3080	0.3325
H_2	0.2640	0.1620
H_2O	0.0412	0.0371
CO_2	0.0177	0.0280
H_2S	0.0072	0.0061
COS	0.0002	0.0004
CH_4	0.0002	0.0001
NH_3	3×10^{-5}	2×10^{-5}

Composition at equilibrium of all other species was less than 10^{-5}.

bines directly with sulfur to form carbon disulfide. In fact, 17.5% of the total sulfur is present as CS_2 under these conditions. However, at 55% oxygen more carbon combines with oxygen and only 1.2% of the total sulfur appears as CS_2. This "liberated" sulfur initially forms H_2S corresponding to the H_2S peak at 55% oxygen. As the amount of oxygen is further increased, H_2S is gradually replaced by oxygen–sulfur species such as COS and SO_2.

Let us now inquire further into the effect of decreasing hydrogen on the distribution of sulfur species. An important function of the steam used in gasification is temperature control since the carbon–steam reaction is endothermic. Future gasification research will undoubtedly aim at higher exit gas temperature. Thus it is logical to assume that the amount of steam used in gasification will decrease in the future. Since steam is the primary source of hydrogen, this decrease will significantly reduce the pro-

portion of H_2S in the fuel gas with increasing amounts of COS and $S_2(g)$. Figure 4 indicates the combined effect of hydrogen availability and temperature. All of the results are reported at a constant quantity of oxygen equal to 59% of stoichiometric. Thus, decreased steam is compensated by increased air to maintain the constant oxygen level.

In Figure 4, the fraction of the total sulfur contributed by the three major sulfur species is plotted as a function of temperature at four different steam/air ratios from zero to 0.36. Hydrogen sulfide, it will be noticed, decreases with increasing temperature and decreasing availability of hydrogen. The concentration of carbonyl sulfide is relatively independent of temperature except at the lowest hydrogen levels. S_2 increases rapidly with increasing temperature and with decreasing hydrogen. However, the S_2 concentration is quite small near the reference case temperature of 2300°F except at the lowest hydrogen levels.

Literature Cited

del Valle, E. G., April G. C., Pike, R. W., Final Rept. CR-79677, National Aeronautics and Space Administration, 1967.
McBride, B. J., Hermel, S., Ebberes, J. G., Gordon, S., Rept. NASA-SP-3001, National Aeronautics and Space Administration, 1963.
Robson, F. L., Giramonti, A. J., Lewis, G. P. Gruber, G., Final Report CPA 22-69-114, National Air Pollution Control Administration, 1970.
Squires, A. M., *Science*, 169, 821 (1970).
Stull, D. R., JANAF Thermochemical Tables, Dow Chemical Co., 1965.
Van Zeggeren, F., Storey, S. H., "The Computation of Chemical Equilibria," Cambridge Press, London, 1970.

Theoretical Model for Relating Indoor Pollutant Concentrations to Those Outside

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■ A general ventilation model, which relates indoor pollutant concentrations to those outside, is discussed in detail. When the time interval associated with changes in the outdoor concentration is long compared to that required either to change the air within the building or to remove the pollutant by internal means, the indoor concentration of pollutant can be related to the outdoor concentration by means of a simple expression. In the case of indoor ozone associated with buildings located in photochemically smoggy regions, there is good agreement between theory and experiment. Theoretical considerations suggest that the indoor levels of ozone in many commercial buildings located in Los Angeles could be substantially reduced rather quickly and possibly with relatively little effort.

Establishing clean indoor air can immediately improve the environment for certain groups, as well as significantly reduce the impact of air pollution upon the general population. One attractive feature about considering indoor air quality is that the decision to make improvements within a particular structure requires the involvement of relatively few persons, and need not wait for the development of the proper legislation and enforcement needed to improve the air quality outdoors. The work up to 1972 was reviewed by Benson et al. (1972). Wallick (1973) has stressed the importance of indoor air quality among other factors associated with the indoor environment experienced within American factories.

To provide a framework useful in understanding the dependence of indoor pollutant levels upon ventilation parameters, geometric factors, and outdoor pollutant levels, a dynamic theoretical model which allows rapid calculation of indoor pollutant levels is needed. Turk (1963),

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Hunt et al. (1971), and Cote and Holcombe (1971) have used the well-mixed chemical reactor in their investigations. Sabersky et al. (1973) reported that the model of a well-mixed chemical reactor, involving an outdoor concentration which varied sinusoidally in time and a first-order heterogeneous decomposition step, gave qualitative agreement with data for indoor concentrations of ozone. However, there is a need to develop a dynamic model for reactive pollutants that permits rapid concise calculations useful in developing design guidelines. This work was aimed at the development of such a model.

Theoretical Development

General Aspects. We shall use the model of a well-mixed chemical reactor equation as a statement of mass balance for the airborne toxic substance. Concentration gradients throughout the system are neglected, and consequently the output concentration is equal to that throughout the system at any particular time. In our ventilation model for a structure of volume V, makeup air enters from the outside and passes through a filter at a rate q_0, air is recirculated through another filter at a rate q_1, and air infiltrates the structure (from the outside) at a rate q_2. The indoor and outdoor concentrations of toxin at time t are C_i and C_o, respectively. The net rate at which toxin is added to the indoor air owing to internal sources, s, and internal sinks, R, is $s - R$. The filter, through which the makeup stream is passed, is characterized by a factor $F_0 = (C_{inlet} - C_{outlet})/C_{inlet}$, where C_{inlet} is the pollutant concentration in the air stream just prior to the filter, and C_{outlet} that in the air stream leaving the filter. The recirculated air passes through a filter characterized by F_1.

For typical ventilation systems, the appropriate starting equation is

$$V \frac{dC_i}{dt} = q_0 C_o (1 - F_0) + q_1 C_i (1 - F_1) + q_2 C_o - (q_0 + q_1 + q_2)C_i + s - R \quad (1)$$

The first three terms on the right-hand side of Equation 1 represent the rate at which the toxin enters the structure via input streams; the fourth term represents the rate at which the toxin leaves the structure via output streams. Air exits the structure either through exfiltration or exhaust ducts. The sum of the rates of exfiltration plus exhaust is, of course, equal to the sum of the rates of infiltration plus makeup. A graphic description of the model is shown in Figure I. Quite often both the makeup air and the recirculated air are passed through the same filter, in which case $F_0 = F_1 \equiv F$. In general, the filter factors will be a function of pollutant, flow rate, and extent of use. The value of the filter factor and the rate at which it decreases with time must be determined a priori by experimental means. The infiltration rate should be determined a priori for any given operation of any given ventilation system. Generally, the source term will reflect emissions from equipment operated within the structure, and/or the product of chemical reactions. Usually the sink term will originate from either a homogeneous or a heterogeneous chemical reaction; it is likely that many cases of interest will involve either first-order or pseudo first-order kinetics as a result of the low concentrations (i.e., parts per million or less) at which most toxins are generally present. In the case of ozone, the main mechanism of decomposition indoors has been found to involve a first-order heterogeneous mechanism (Mueller et al., 1973; Sabersky et al., 1973); that is, $R = \Sigma_j k_j A_j C$ where k_j is the decomposition rate on the jth surface with area A_j.

For convenience we shall nondimensionalize Equation 1 to yield

$$\frac{d\theta_i}{d\tau} + \delta\theta_i = \epsilon\theta_o + \sigma \quad (2)$$

where $\theta_i = C_i/C_{ref}$, $\tau = q_0 t/V$, $\alpha = q_1/q_0$, $\beta = q_2/q_0$, $\gamma = \Sigma_j k_j A_j/q_0$, $\delta = 1 + \alpha F_1 + \beta + \gamma$, $\epsilon = 1 + \beta - F_0$, $\theta_o = C_o/C_{ref}$, and $\sigma = s/q_0 C_{ref}$. The reference concentration, C_{ref}, is any fixed concentration chosen for convenience.

The general solution to Equation 2 is simply

$$\theta_i = \epsilon e^{-\delta\tau} \int_0^\tau e^{\delta\tau}\theta_o d\tau + e^{-\delta\tau}\int_0^\tau e^{\delta\tau}\sigma d\tau + \theta_{io}e^{-\delta\tau} \quad (3)$$

where $\theta_{io} = C_{io}/C_{ref}$ and C_{io} is the indoor concentration at $t = 0$. Equation 3 relates the indoor concentration of pollutant to that outside. Although the outdoor concentration θ_o generally cannot be predicted accurately for any specific day, air monitoring stations can provide typical daily profiles of air contaminates for many regions throughout the nation. Although internal sources which vary in time can be treated, for convenience we shall take σ to be constant.

Nondimensional quantities are used throughout the presentation that follows in order to provide a more concise discussion than would otherwise be possible. It is also worthwhile to note that there are five separate time scales associated with this problem. First, there is a characteristic time, t_1, associated with changes in the outdoor concentration. Next, there are four time scales associated with the quantity $\delta\tau$; these are V/q_0, $V/q_1 F_1$, V/q_2, and $V/\Sigma_j k_j A_j$, which represents the characteristic time to exchange the building air with makeup air, the characteristic time to remove the pollutant via the recirculation filter, the characteristic time to exchange the building air with infiltrated air, and the characteristic time to remove the pollutant via a first-order decomposition mechanism, respectively. When the value of t_1 is either small or the same order of magnitude of the inverse of the sum of the inverses of the latter four characteristic times, then the complete solution (Equation 3) should be used in
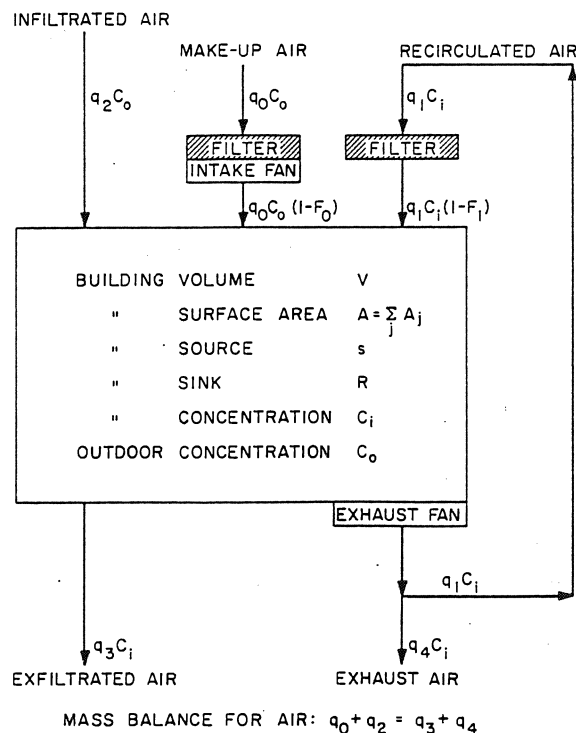

MASS BALANCE FOR AIR: $q_0 + q_2 = q_3 + q_4$

Figure 1. Schematic diagram of ventilation model
Generally, makeup air and recirculated air both pass through the same filter and intake fan system

ventilation design calculations. However when t_1 is large compared to the inverse of the sum of the inverses of the other characteristic times, the last term in Equation 3 may be neglected, and when C_o can be represented by a straight line during t_1, a useful approximate expression can be developed.

We shall now consider two specific cases; each case involves a different approximation to the time dependence of the outdoor concentration. The sinusoidal case is used to discuss briefly phase lags associated with the indoor concentrations as compared to those outside. The linear case is then analyzed in great detail because it provides an approximate expression which gives excellent agreement with data and provides a technique for very rapid calculation of indoor air quality for a variety of ventilation conditions and systems.

Sinusoidal Input. The outdoor concentration of a toxin may sometimes be approximated by a sinusoidal function. The typical daily increase of ozone in some photochemically smoggy areas appears roughly to follow a sine wave; in Pasadena the ozone concentration rises from zero at about 8:00 a.m. to some maximum value at about 1:00 p.m., and then decreases to zero at about 7:00 p.m. during a typical smoggy day. In this case $\theta_o = \sin \omega \tau$, C_{ref} is the maximum pollutant concentration outdoors, $\omega = 2 \pi f V / q_0$, f is the frequency associated with the sinusoidal behavior of the outdoor concentration of pollutant. It should be noted that the representation of θ_o is valid only for values of $\omega \tau$ such that $\theta_o > 0$. Sometimes a better representation for θ_o is $\theta_o = 1 - \cos \omega \tau$ where C_{ref} is one half of the maximum pollutant concentration outside. In either case, the general aspects of the following discussion are the same. When $C_i = 0$ at $t = 0$ and for a constant source, the indoor concentration of pollutant is given by

$$\theta_i = \frac{\sigma}{\delta} + \left(\frac{\epsilon}{\delta^2 + \omega^2}\right)(\delta \sin \omega \tau - \omega \cos \omega \tau) + \left(\frac{\omega \epsilon}{\delta^2 + \omega^2} - \frac{\sigma}{\delta}\right) e^{-\delta \tau} \quad (4)$$

The first term on the right-hand side of Equation 4 represents the contribution due to internal sources, the second term indicates the possibility of phase lags developing between the indoor and outdoor concentrations, and the third term represents the usual transient part which, in the case of most ventilation systems, decays quite rapidly. In this case, $t_1 = (1/2)\pi f$ and the other characteristic times are the same as those defined previously. Consequently, during most of the day the indoor concentration is given by the first two terms of Equation 4. It is of interest to note the behavior of Equation 4 in the two limiting cases $\delta >> \omega$ and $\delta << \omega$.

When the outdoor concentration of pollutant changes slowly compared to the time either to change the air within the building or to remove the pollutant by internal means, $\delta >> \omega$ and the phase lag is small since $\theta_i \sim \sin \omega \tau$; apparently this is generally the case with most commercial buildings.

When the outdoor concentration of pollutant changes rapidly compared to the time to either change the air within the building or to remove the pollutant by internal means, $\delta << \omega$ and the phase lag can approach $\pi/2$ radians or half the time period of the interval associated with the outdoor concentration. In this case $\theta_i \sim - \cos \omega \tau$ after t is such that $\omega \tau >> \pi/2$ radians (i.e., $\theta_i > 0$). In general, the indoor concentration can lag the outdoor values up to ¼ of the period associated with the outdoor change.

Ramp Input. Many cases of practical interest involve an input function which does not warrant the use of a sophisticated interpolation procedure in order to predict the pol-

lutant concentration within a time interval defined by two successive data points. When such is the case it would appear that a linear interpolation between two successive data points would be appropriate. It should also be noted that a more sophisticated interpolation procedure does not appear justified in view of the more dominant uncertainties associated with other parameters such as building volume, decomposition rate, and surface area. When such is the case, we shall represent the outdoor concentration by the expression $C_o = C_{oo} + at$ where a is positive during periods of increasing outdoor concentration and negative during periods of decreasing concentration; the quantity C_{oo} represents the outdoor concentration at the beginning of the period and C_{o1} that at the end. The quantity t_1 represents the length of the time period. The value of C_{o1} associated with one time interval becomes the value of C_{oo} for the next. When the initial indoor concentration is C_{io} and the internal source is constant, the indoor concentration of pollutant is given by

$$\theta_i = \frac{\epsilon \theta_{oo} + \sigma}{\delta} + \frac{b \epsilon}{\delta^2} (\delta \tau - 1) + \left[\theta_{io} + \frac{\epsilon b}{\delta^2} - \left(\frac{\epsilon \theta_{oo} + \sigma}{\delta}\right)\right] e^{-\delta \tau} \quad (5)$$

where $\theta_{oo} = C_{oo}/C_{ref}$, $b = aV/C_{ref}q_0$, $a = (C_{o1} - C_{oo})/t_1$ and the rest of the terms are the same as those defined previously.

When there is a constant outdoor concentration of pollutant, a constant internal source, a single filter such that $F_0 = F_1$, and no sink, the steady state solution reduces to $\theta_i = (\epsilon + \sigma)/\delta = (1 + \beta - F + \sigma)/(1 + \alpha F + \beta)$ which is the same as that used by Cote and Holcombe (1971) in their discussion of indoor pollutant concentrations of particulate matter and carbon monoxide. When there is a constant outdoor concentration of pollutant, a constant internal source, a single filter such that $F_0 = 0$ but $F_1 > 0$, then Equation 5 reduces to that used by Turk (1963) in his investigations of models suitable for describing the transient concentration of odors within enclosures.

By solving Equation 5 for each of m time intervals of length t_1, it can easily be shown that the indoor pollutant concentration after the mth time interval of length t_1 is equal to

$$C_{i(m)} = S + [AC_{o(m-1)} + BC_{o(m)}] +$$
$$[A(C_{o(m-2)} - C_{o(m-1)}) + B(C_{o(m-1)} - C_{o(m)})]e^{-\delta \tau_1} +$$
$$[A(C_{o(m-3)} - C_{o(m-2)}) + B(C_{o(m-2)} - C_{o(m-1)})]e^{-2\delta \tau_1} \ldots +$$
$$[A(C_{o(0)} - C_{o(1)}) + B(C_{o(1)} - C_{o(2)})]e^{-(m-1)\delta \tau_1} +$$
$$[C_{i(0)} - S - AC_{o(0)} - BC_{o(1)}]e^{-m\delta \tau_1} \quad (6)$$

where $C_{i(m)}$ is the indoor pollutant concentration after the mth time interval of length t_1, $C_{o(m)}$ is the outdoor pollutant concentration measured at the end of the mth time interval of length t_1, $S = s/q_o\delta$, $A = \epsilon/^2\tau_1$, $B = (\epsilon/\delta^2\tau_1)(\delta\tau_1 - 1)$, $\tau_1 = q_0 t_1/V$, and the rest of the terms are the same as those defined previously.

In many cases of interest the time interval, t_1, associated with the outdoor concentration is quite long compared to the time required either to change the air within the building or to remove the pollutant by internal means. In such cases, exponential terms in Equation 6 rapidly decay and can be neglected during most of interval, t_1. During a typical smoggy day in Los Angeles, the outdoor concentrations of ozone may be approximated by a series of straight lines connecting the ozone concentration at each hour, whereas the average commercial air-conditioning system changes the air in a room five to six times per hour (Wohlers, 1971). Operating rooms are recommended to have

15 air changes per hour, and specialized rooms may have up to 20 air changes per hour (Wohlers, 1971). When the outdoor concentration can be approximated by a series of straight lines, and when exponential terms in Equation 6 can be neglected for most of the time, the indoor concentration at the end of the time interval can be calculated from the expression

$$C_{i1} = S + AC_{o0} + BC_{o1} \qquad (7)$$

For convenience we shall drop the subscripted parentheses during the rest of the discussion; thus $C_{i(1)} = C_{i1}$, and so forth. Consequently, the indoor concentration consists of source term plus a linear combination of the outdoor concentrations at the beginning and end of the current linear segment time period. In the following discussion, Equation 7 is referred to as the linear-combination theory.

Presentation and Discussion of Results

The indoor concentrations of ozone, measured by a Dasbi Corp. Model 1003 monitor, were recorded in two connected rooms during each of five days in the summer of 1973. The rooms, 312 and 314 Dabney Hall of the Caltech campus, are a conference room and office, respectively; they have a combined volume of 7390 ft³, a combined surface area of 3600 ft², and are air conditioned by the same ventilation system. The makeup and recirculated air streams are passed through a glass fiber filter so that $F_0 = F_1 = F$, and for ozone $F \sim 0$. Duct measurements involving usual anemometry techniques were used to determine the value of q_0 and q_1. Once the values of q_0 and q_1 were obtained, an exponential dilution test, similar to that described by Drivas et al. (1972) was conducted with a carbon monoxide tracer in order to determine the value of q_2 by difference. The outdoor concentrations of ozone (Hunticker, 1973) were measured on the roof of the Keck Laboratory by a similar Dasibi monitor, located about 100 yards downwind of Dabney Hall.

When the air-conditioning system was adjusted to maximize the rate of makeup air, $q_0 = 680$ ft³/min, $q_1 = 770$ ft³/min, and $q_2 \sim 0$. On the other hand, when the air-conditioning system was adjusted to minimize the rate of makeup air, $q_0 = 148$ ft³/min, $q_1 = 1150$ ft³/min, and $q_2 = 289$ ft³/min. Fans placed within the room provided good mixing, and the mixing factor (Brief, 1960; Turk, 1963; Constance, 1970) was close to unity. It is especially important to note that increasing the recirculation rate of air significantly increased the infiltration rate. The increase in q_2 associated with an increase in q_1 is thought to be related to a decrease in the pressure difference between the inside and the outside of the building; in both cases, the building pressure was thought to be slightly above the outside static pressure. The infiltration rate should be

measured for any given ventilation system; however, when measurements are impractical, the rates of infiltration for some structures may be estimated by either of two general methods ("ASHRAE Handbook of Fundamentals," 1972). Mueller et al. (1973) found the ozone decay constant for an office to be 0.073 ft³/ft²-min, and that for a bedroom to be 0.122 ft³/ft² - min. In the calculations discussed below, we shall use a value of $k = 0.1$ ft³/ft² - min.

Nominal values of q_0, q_1, q_2, k, A_b, and V were used in the following calculations in the comparison between theory and data. A better fit of the data could have been obtained by changing the value of one or more parameters, but that was thought not worthwhile.

Figures 2 and 3 show the data obtained with operation at the maximum rate of makeup air. The dashed lines represent the line segments connecting the outdoor concentrations of ozone measured each hour on the hour. The solid lines are the predicted indoor concentrations predicted by the linear-combination theory for $\alpha = 1.1$, $\beta = 0$, $\gamma = 0.53$, $\delta = 1.53$, $\epsilon = 1$, in this case and $\sigma = 0$; $C_{i1} = 0.077 \, C_{o1} + 0.58 \, C_{o1}$ which is in good agreement with the indoor data. The 1971 threshold limit value, TLV, of 0.1 ppm for ozone ("Documentation of the Threshold Limit Value," 1971) is indicated by the dotted line. As indicated, the linear-combination theory also predicts that filters with values of F greater than about 0.7 would have kept the indoor levels of ozone well below the TLV.

Figures 4 and 5 show the data obtained with operation at the maximum rate of makeup air but with the glass fiber filter replaced with a filter having a value of F between 0.1 and 0.2. In this case $\alpha = 1.1$, $\beta = 0$, $\gamma = 5.3$, $\delta = 2.6$, $\epsilon = 0.8$, $F \simeq 0.2$, $\sigma = 0$; and $C_{i1} = 0.047 \, C_{o0} + 0.41 \, C_{o1}$ which is in agreement with the indoor data.

Figure 6 shows the data for the case of minimum makeup rate with the glass fiber filter in use. In this case $\alpha = 7.8$, $\beta = 2.0$, $\gamma = 2.4$, $\delta = 5.38$, $\epsilon = 2.9$, $F = 0$, and $\sigma = 0$; and $C_{i1} = 0.084 \, C_{o0} + 0.46 \, C_{o1}$ which is again in agreement with the indoor data.

Design of Ventilation Systems

As has been indicated above, by adjusting the makeup rate, the recirculation rate, and the filter factor, it may be possible to either design systems for new buildings or to modify existing ventilation systems in order to keep the ozone concentration from reaching 0.1 ppm.

For several cases of wide public interest, the "problem" of indoor air quality corresponds to economically treating the indoor air in such a manner to maintain $C_i/C_o \leq 0.2$. Since 1955, when the smog alert system was adopted in Los Angeles, about 85 first-stage smog alerts have been declared; and all but 3 or 4 have been due to the outdoor
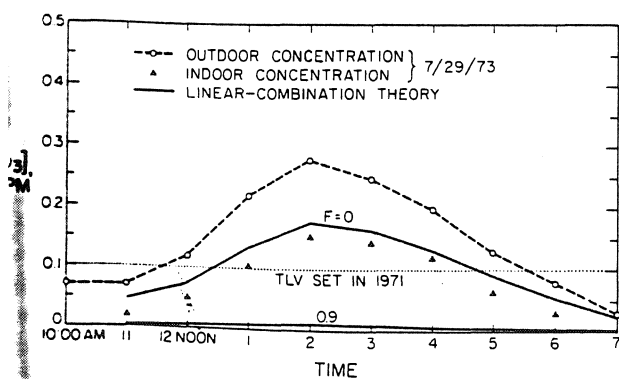

Figure 2. Indoor-outdoor concentrations of ozone for rooms 312 and 314 of Dabney Hall. Theoretical curves for $F = 0$ and $F = 0.9$ ventilation system operated at maximum makeup rate during 7/29/73. Filter factor $\simeq 0$ for ozone

Figure 3. Indoor-outdoor concentrations of ozone for rooms 312 plus 314 of Dabney Hall. Theoretical curves for $F = 0$, $F = 0.7$, and $F = 0.9$
Ventilation system operated at maximum makeup rate during 8/18/73. Filter factor $\simeq 0$ for ozone
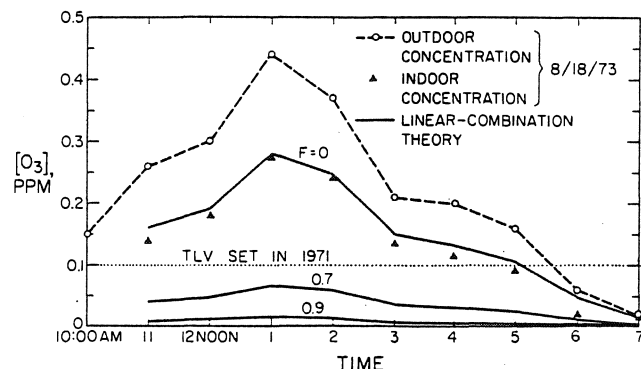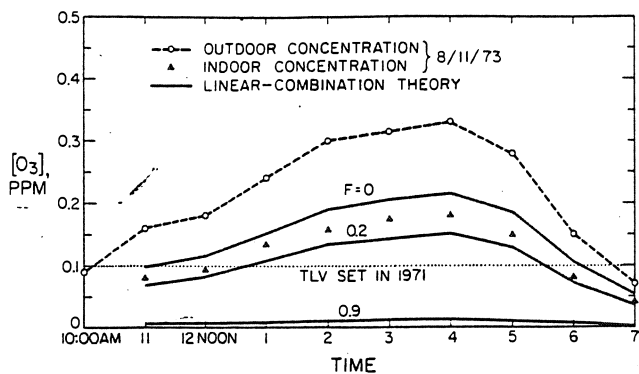
Figure 4. Indoor-outdoor concentrations of ozone for rooms 312 plus 314 of Dabney Hall. Theoretical curves for $F = 0$, $F = 0.2$, and $F = 0.9$
Ventilation system operated at maximum makeup rate during 8/11/73. Filter factor $\simeq 0.1-0.2$ for ozone

Figure 5. Indoor-outdoor concentrations of ozone for rooms 312 plus 314 of Dabney Hall. Theoretical curves for $F = 0$ and $F = 0.9$ Ventilation system operated at maximum makeup rate during 8/19/73. Filter factor $\simeq 0.1-0.2$ for ozone
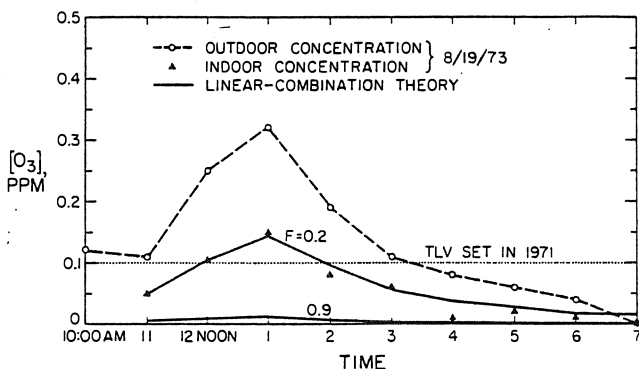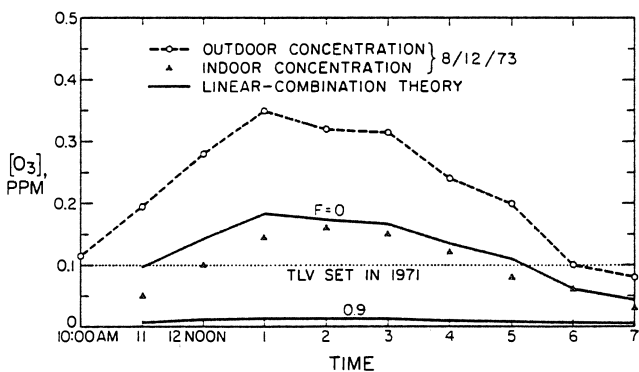

Figure 6. Indoor-outdoor concentrations of ozone for rooms 312 plus 314 of Dabney Hall. Theoretical curves for $F = 0$ and $F = 0.9$ Ventilation system operated at minimum makeup rate during 8/12/73. Filter factor $\simeq 0$ for ozone
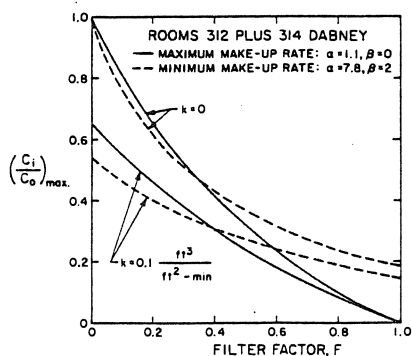

Figure 7. Predicted maximum value of ratio of indoor-outdoor concentrations of ozone as a function of the filter factor

level of ozone reaching 0.5 ppm. Consequently, ventilation systems which maintain $C_i/C_o \leq 0.2$ would have permitted $C_i > $ TLV for ozone only four or five days per year at the worst. In special cases, involving for example the elderly, the ill, and young school children, it may be desirable to maintain the indoor air quality such that $C_i/C_o \leq 0.1$; for such systems located in Los Angeles, the indoor concentrations of ozone during the last 18 years would seldom, if ever, have reached the threshold limit value (i.e., the value of C_o has never been observed to reach the second stage alert level of 1 ppm).

To demonstrate how the linear-combination theory can be used in designing ventilation systems, Equation 7 was used to construct the performance curves shown in Figure 7. For these calculations, the outdoor concentration of
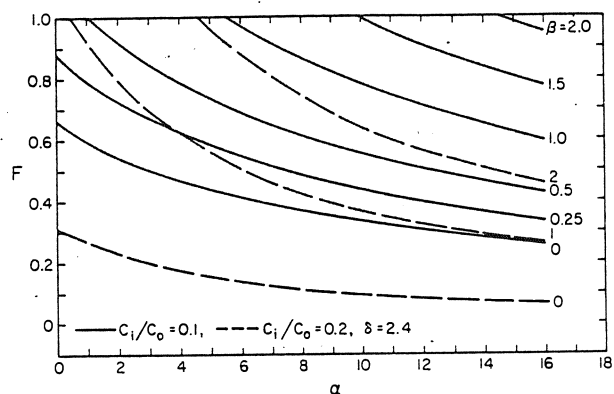
Figure 8. Predicted value of filter factor required to maintain values of indoor/outdoor concentration ratio of ozone for room 312 plus 314 of Dabney Hall
Values of the filter factor vs. recirculation rates of various infiltration rates

Figure 9. Values of filter factor required to maintain value of indoor/outdoor concentration ratio = 0.2
Sources and sinks neglected

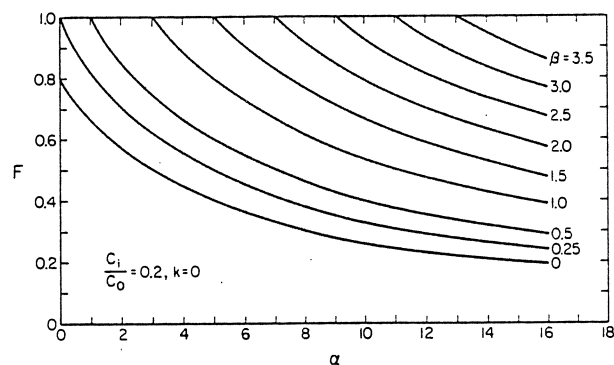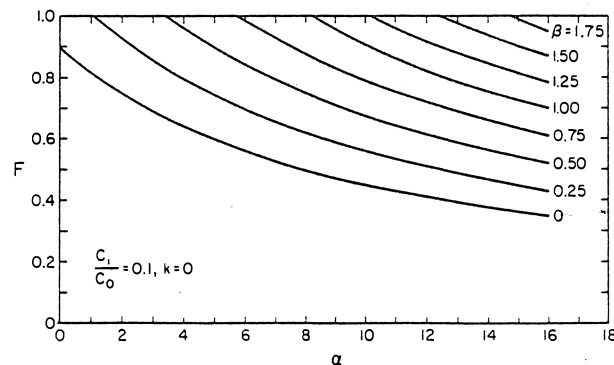**Figure 10.** Values of filter factor required to maintain value of indoor/outdoor concentration ratio = 0.1
Sources and sinks neglected

pollutant was taken to be constant over the time period t_1, and no internal sources were considered (i.e., $C_{oo} = C_{o1}$ and $\sigma = 0$). The values of α and β were those measured. The bottom two curves were those calculated for the actual system. With filters with $F < 0.4$, the indoor concentration of ozone would be lower with the maximum makeup rate as compared to that with the minimum makeup rate; this effect is due to the increased infiltration rate associated with the minimum makeup rate (i.e., maximum recirculation rate). In this particular case $(C_i/C_o) < 0.2$ for $F \simeq 0.5$ for the maximum makeup rate, and F needs to be ~ 1.0 for the minimum makeup rate. To show the contribution of the heterogeneous decomposition term, the two upper curves, for which $k = 0$, are also presented.

The influence of the ventilation variables for the Dabney Hall rooms is clearly shown in Figure 8. Equation 7 was used to calculate the value of F needed to give $C_i/C_o = 0.1$ and $C_i/C_o = 0.2$, as a function of recirculation rate and infiltration rate. It should again be emphasized that for this case, and probably in general, the value of β will increase with increasing value of α, and should be measured. It is expected that the frequency and cost of either reactivating or replacing the filter to maintain the value of F greater than that indicated in Figure 8 will be important factors in determining the economic desirability of proposed changes in the design of ventilation systems.

If the heterogeneous decomposition is neglected then, for buildings without sources, a general set of curves can be drawn for various values of recirculation and infiltration rates. Values of F obtained from such curves will be somewhat higher than actually needed, and represent an upper bound required to produce the desired ratio of the indoor-outdoor concentrations. Figure 9 indicates the minimum value F, neglecting heterogeneous decomposition, required to establish $C_i/C_o = 0.2$ for various rates of recirculation and infiltration; Figure 10 is for $C_i/C_o = 0.1$.

To indicate typical values of the parameters used in Equation 7, several buildings (or portions thereof) on the Caltech campus were analyzed. The ventilation and geometric quantities are given in Table I. Each case involves a single ventilation system. The makeup rates for the Noyes Lab, and for the two systems in the Keith Spalding building are fixed. The other systems have makeup rates which change with changes in the outdoor temperature; to minimize the load on the air-conditioners, the makeup rates decrease with increasing outdoor temperature. Except in the case of Dabney Hall the surface areas "A_b" are those associated with floors, ceilings, and partition walls. For the room in Dabney Hall, the total surface area was actually measured; for all the other cases the surface area of furniture, books, and so forth was omitted and the "A_b" listings in Table I are minimum values of the surface area available for ozone decomposition. Except for the Dabney

Table I. Listing of Ventilation and Geometric Quantities

Case	Building	q_0, cfm	q_1, cfm	q_2,[a] cfm	s, cfm	V, ft³	A_b, ft²	A_b/V, ft⁻¹	F_0	F_1	Remarks
1	Arms	34,000	0	0	0	475,200	169,100	0.36	0	0	Fixed q_0
2a	East Bridge	28,000	0	0	0	363,500	127,400	0.35	0	0	"
2b	West Bridge	33,000	0	0	0	379,000	140,000	0.37	0	0	"
3a	East Church	50,300	0	0	0	475,000	184,900	0.39	0	0	"
3b	West Church	41,200	0	0	0	384,000	142,000	0.37	0	0	"
4	Crellin	48,000	0	0	0	435,700	159,400	0.37	0	0	"
5a	Dabney Hall, 312 and 314	680	770	0	0	7,390	3,600	0.49	0	0	Max q_0
5b	Dabney Hall, 312 and 314	148	1,150	289	0	7,390	3,600	0.49	0	0	Min q_0
6a	Keith Spalding, basement and 1st floor	11,400	18,600	0	0	406,000	148,000	0.36	0	0	Fixed q_0
6b	Keith Spalding, 2nd, 3rd, and penthouse	6,500	31,700	0	0	376,000	155,000	0.41	0	0	"
7	Kellogg	7,000	0	0	0	218,000	74,800	0.34	0	0	"
8a	Lauritsen-Downs, subbasement	11,700	0	0	0	160,000	47,900	0.30	0	0	"
8b	Lauritsen-Downs, 1–4	8,500	0	0	0	775,000	252,500	0.33	0	0	"
9a	Millikan Library, 10 floors	53,500	0	0	0	673,000	214,000	0.32	0	0	Max q_0
9b	Millikan Library	11,270	42,230	0	0	673,000	214,000	0.23	0	0	Min q_0
11	Noyes Lab (west wing) 5 floors	49,350	94,600	0	0	1,120,000	308,000	0.26	0	0	Fixed q_0
12	Robinson	24,570	0	0	0	413,000	168,700	0.41	0	0	"
13	Sloan Lab	54,000	0	0	0	620,000	161,000	0.26	0	0	"
14a	Spalding, subbasement	19,400	0	0	0	127,500	41,600	0.33	0	0	"
14b	Spalding, basement	16,000	0	0	0	127,500	48,400	0.38	0	0	"
14c	Spalding, 1–3 floors	90,000	0	0	0	473,000	161,500	0.34	0	0	Max q_0
14d	Spalding, 1–3 floors	50,000	40,000	0	0	473,000	161,500	0.34	0	0	Min q_0
15a	Steele Lab, 5 floors	90,000	0	0	0	533,000	254,000	0.48	0	0	Max q_0
15b	Steele Lab, 5 floors	18,000	72,000	0	0	533,000	254,000	0.48	0	0	Min q_0

[a] In cases where not measured $q_2 = 0$ for purpose of calculation. In actual design calculations, the value of q_2 should be measured or properly estimated.

Hall experiments the infiltration rates were not measured, and were taken to be negligible for the purposes of calculation. The nondimensional parameters associated with Equation 7 are listed in Table II. For commercial size ventilation systems, values of several nondimensional parameters ranged as follows: $0 < \alpha < 5$, $0 < \gamma < 2.5$, $0 < \delta < 4$, $0 < A < 0.2$, $0.2 < B < 0.8$.

The challenge to improve indoor air quality can be translated to that of reducing the values of A and B under the constraints of overall safety, comfort and economics. For the cases discussed in Table II the relatively large values of recirculation rates, which can be obtained during hot smoggy days, suggests that the values of A and B can be easily lowered by inserting filters such that $F > 0$. This conclusion is in agreement with those based upon a previous preliminary investigation conducted by Bush and Segall (1970).

In Table III are listed the values of F needed to ensure that the indoor concentrations of ozone do not rise above 0.2 times the outdoor concentrations. It is important to note that, for all of the buildings we studied which had a recirculation stream, insert filters with $F \geq 0.5$ would ensure that all the indoor levels of ozone would not exceed the TLV of 0.1 ppm during more than four or five days a year. For the buildings which we studied which did not

have a recirculating stream, the corresponding values of F ranged upward to near 0.75; for buildings having negligible rates of infiltration, the maximum value of F required would be 0.8.

It should be noted that, except for the rooms in Dabney Hall, the calculations listed in the tables are for building averages. For any specific room of interest, the ventilation and geometric quantities for that room should be measured if accurate predictions are to be made using Equation 7.

It would appear that a substantial improvement in indoor air quality might be accomplished in the Los Angeles region without greatly sacrificing the other considerations involved in the design and operation of air-conditioning systems.

The example of indoor ozone, associated with buildings located in photochemically smoggy regions, was discussed in some detail. However, the linear-combination model may also be applied to other pollutants.

Summary and Conclusions

A dynamic model for relating indoor pollutant concentrations to those outside was developed and tested. There is good agreement between theory and experiment.

In certain instances the outdoor concentration changes

Table II. Indoor Air Quality Table of Nondimensional Parameters

Case	Building	α	β	γ	δ	ϵ	τ_1	S	A	B	$A + B$
1	Arms	0	0	0.49	1.49	1.0	4.30	0	0.104	0.57	0.67
2a	East Bridge	0	0	0.45	1.45	1.0	4.63	0	0.10	0.58	0.68
2b	West Bridge	0	0	0.42	1.42	1.0	5.22	0	0.094	0.61	0.70
3a	East Church	0	0	0.36	1.36	1.0	6.35	0	0.084	0.65	0.74
3b	West Church	0	0	0.34	1.34	1.0	6.45	0	0.086	0.66	0.74
4	Crellin	0	0	0.33	1.33	1.0	6.62	0	0.085	0.67	0.75
5a	Dabney Hall, 312 and 314	1.1	0	0.53	1.53	1.0	5.52	0	0.077	0.58	0.66
5b	Dabney Hall, 312 and 314	7.8	2	2.43	5.38	2.9	1.20	0	0.084	0.46	0.54
6a	Keith Spalding, basement and 1st floor	1.6	0	1.30	2.30	1.0	1.7	0	0.11	0.32	0.43
6b	Keith Spalding, 2nd, 3rd, and penthouse	4.9	0	2.40	3.40	1.0	1.0	0	0.21	0.21	0.30
7	Kellogg	0	0	1.07	2.07	1.0	1.93	0	0.12	0.36	0.48
8a	Lauritsen-Downs, subbasement	0	0	0.41	1.41	1.0	4.38	0	0.11	0.60	0.71
8b	Lauritsen-Downs, 1–4	0	0	2.96	3.96	1.0	0.65	0	0.097	0.15	0.25
9a	Millikan Library, 10 floors	0	0	0.40	1.40	1.0	4.8	0	0.11	0.63	0.74
9b	Millikan Library, 10 floors	3.7	0	1.90	2.90	1.0	1.0	0	0.12	0.23	0.35
10	Mudd	0	0	0.72	1.72	1.0	3.17	0	0.11	0.47	0.58
11	Noyes Lab, (west wing) 5 floors	1.9	0	0.62	1.62	1.0	2.6	0	0.15	0.48	0.63
12	Robinson	0	0	0.68	1.68	1.0	3.56	0	0.099	0.49	0.59
13	Sloan Lab	0	0	0.29	1.29	1.0	5.22	0	0.12	0.66	0.78
14a	Spalding, subbasement	0	0	0.26	1.26	1.0	7.55	0	0.084	0.71	0.80
14b	Spalding, basement	0	0	0.24	1.24	1.0	9.17	0	0.07	0.74	0.81
14c	Spalding 1–3 floors	0	0	0.32	1.32	1.0	6.35	0	0.091	0.67	0.76
14d	Spalding, 1–3 floors	4	0	1.62	2.62	1.0	1.27	0	0.115	0.27	0.38
15a	Steele Lab, 5 floors	0	0	0.28	1.28	1.0	10.1	0	0.060	0.72	0.78
15b	Steele Lab, 5 floors	4.0	0	1.40	2.40	1.0	2.0	0	0.087	0.33	0.42

$\alpha = q_1/q_0$, $\beta = q_2/q_0$, $\gamma = \Sigma_j l_j A_j / q_0$, $\delta = 1 + \alpha F_1 + \beta + \gamma$, $\epsilon = 1 + \beta - F_0$, $\tau_1 = q_0 t_1 / V$

$S = s/q_0$, $A = \epsilon/\delta^2 \tau_1$, $B = A(\delta \tau_1 - 1)$

$C_{i1} = S + A C_{o0} + B C_{o1}$

Table III. Filter Factor Required to Establish (C_o/C_i) = 0.2 Assuming Building Is Well Mixed

Case	Building	F for C_i/C_o = 0.2
1	Arms	0.70
2a	East Bridge	0.71
2b	West Bridge	0.72
3a	East Church	0.73
3b	West Church	0.73
4	Crellin	0.73
5a	Dabney	0.57
5b	Dabney	0.12
6a	Keith Spalding	0.41
6b	Keith Spalding	0.16
7	Kellogg	0.59
8a	Lauritsen-Downs	0.72
8b	Lauritsen-Downs	0.21
9a	Millikan Library	0.72
9b	Millikan Library	0.24
10	Mudd	0.66
11	Noyes Lab	0.49
12	Robinson	0.66
13	Sloan Lab	0.74
14a	Spalding	0.74
14b	Spalding	0.75
14c	Spalding	0.74
14d	Spalding	0.26
15a	Steele Lab	0.74
15b	Steele Lab	0.29

$F = (0.8 - 0.2\gamma)/(1 + 0.2\alpha)$

rather slowly and can be adequately approximated by a straight line within a time interval which is long compared to the time required either to remove the air within the structure or to remove the pollutant by internal means. This is true for ozone pollution associated with buildings located in photochemically smoggy areas such as the Los Angeles region. In such cases the indoor pollutant concentration at the end of any given time interval is equal to the sum of three terms; the first term represents the contribution due to internal sources, and the other two terms represent a linear combination of the outdoor concentrations at the beginning and end of the time interval. Nondimensional coefficients involve the makeup rate, recirculation rate, infiltration rate, filter efficiencies, and first-order chemical reaction terms.

Based upon an analysis of several buildings on the Caltech campus, it appears that for air-conditioned buildings it would be rather easy to reduce the indoor ozone levels to 0.2 of those outside. If this were done, the indoor levels of ozone would exceed the threshold limit value of 0.1 ppm probably no more than four or five days a year, whereas the outdoor concentrations and current indoor concentrations typically exceed this value over 200 days each year.

References

"ASHRAE Handbook of Fundamentals," Published by The American Society of Heating, Refrigeration and Air-Conditioning Engineers, Inc., 345 East 47th St., New York, N.Y. 10017 (1972).

Benson, F. B., Henderson, J. J., Caldwell, D. W., "Indoor-Outdoor Air Pollution Relationships: A Literature Review," Environmental Protection Agency, National Environmental Research Center, Research Triangle Park, N.C. 27709 (1972).

Brief, R. S., *Air Eng.*, 2, 39 (1960).

Bush, A. F., Segall, M., "Reduction of Smog Effects in California Institute of Technology Buildings," ASHRAE Semiannual Meeting (January 1970).

Constance, J. D., *Power*, 114, 56 (February 1970).

Cote, W. A., Holcombe, J. K., "The Influence of Air Conditioning Systems on Indoor Pollutant Levels," Proceedings of Second Conference on Natural Gas Research and Technology, IGT/AGA, J. W. White, Ed., Information Services IGT, 3424 S. State St., Chicago, Ill. 60616 (March 1971).

"Documentation of the Threshold Limit Values for Substances in Workroom Air," Published by the American Conference of Governmental Industrial Hygenists, 3rd ed. P.O. Box 1937, Cincinnati, Ohio 45201 (1971).

Drivas, P. J., Simmonds, P. G., Shair, F. H., *Environ. Sci. Technol.*, 6, 609 (1972).

Hunt, C. M., Cadoff, B. C., Powell, F. J., "Indoor Air Pollution Status Report," NBS Rept. 10591, U.S. Dept. of Commerce, NBS, Washington, D.C. 20234 (April 19, 1971).

Huntzicker, J. J., Calif. Inst. Tech., 1201 E. Calif., Pasadena, Calif. 91109 (1973).

Kalika, P. W., Holcombe, J. K., Cote, W. A., *ASHRAE J.*, 12, 44 (1970).

Mueller, F. X., Loeb, L., Mapes, W. H., *Environ. Sci. Technol.*, 7, 342 (1973).

"Profile of Air Pollution Control, " County of Los Angeles Air Pollut. Contr. Distr., 434 South San Pedro Street, Los Angeles, Calif. 90013 (1971).

Sabersky, R. H., Sinema, D. A., Shair, F. H., *Environ. Sci. Technol.*, 7, 347 (1973).

Segall, M., Calif. Inst. Tech., 1201 E. Calif., Pasadena, Calif. 91109 (1973).

Turk, A., *ASHRAE J.*, 5, 55 (1963).

Wallick, F., "The American Worker: An Endangered Species," Ballantine Books, Inc., New York, N.Y. (1973).

Wohlers, H. C., Suffet, I. H., Blakemore, W. S., Kenepp, D., Coriell, L. L., McGarrity, G. J., *Am. Ind. Hyg. Ass. J.*, 32, 831 (1971).

Yocom, J. E., Clink, W. L., Cote, W. A., J. Air Pollut. Contr. Ass., 21, 251 (1971).