Modeling Indoor Concentrations and Exposures

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INTRODUCTION

Realistic conditions are especially important in the design of experiments to determine the effects from exposure to emissions from pollutant sources. The experiments should be conducted to mimic realistic exposures both in terms of concentration and duration of exposure to a given concentration.

Indoor air quality (IAQ) modeling provides a convenient way to analyze all the interactions, to integrate results from a variety of experiments, and to extend chamber studies to the "real world." Modeling can also be extended to develop realistic exposure scenarios by considering individual activity patterns.

THE MODEL

The interactions between sources, sinks, and buildings can best be analyzed by an appropriate model. Although there are several IAQ models,[1] the rest of the discussion in this paper will be based on the IAQ model EXPOSURE.[2] EXPOSURE is an enhancement of the model INDOOR.[3] EXPOSURE was developed to provide an easty-to-use, generally available IAQ model that allowed rapid analysis of the effects of a wide range of sources, sinks, air cleaners, and ventilation on indoor pollutant concentrations and exposure. EXPOSURE is a multizone mass balance model similar to many of the available IAQ models.

EXPOSURE treats a building as a collection of well-mixed rooms. A mass balance for room i and N rooms gives

$$V_i \frac{dC_i}{dt} = C_a Q_{a,i} + \sum_{j=1, j \neq i}^{j=N} C_j Q_{j,i} - C_i Q_{i,a} - \sum_{j=1, j \neq i}^{j=N} C_i Q_{i,j} + S_i - R_i \qquad (1)$$

where C_i is the concentration in room i, C_a is the concentration outdoors, $Q_{a,i}$ is the air flow from the outdoors into room i, C_j is the concentration in room j, $Q_{j,i}$ is the air flow from room j into room i, $Q_{i,a}$ is the air flow from room i to the outdoors, $Q_{i,j}$ is the air flow from room i into room j, S_i is the source term for pollutants produced in room i, and R_i is the removal term for pollutants removed in room i, including those removed by sinks and air cleaners.

Equation **1** is one of a set of identical equations that must be solved simultaneously in a multiple room model. If the source, sink, and air flow terms in equation 1 are constant, the equation can be solved analytically to give

$$C_i = C_i(t_0)e^{-L_i t} + \frac{P_i}{L_i}(1 - e^{-L_i t}) \tag{2}$$

where $C_i(t_0)$ is the concentration in room i at time t_0, t is some time greater than t_0, L_i is

$$L_i = \frac{Q_{i,\mathrm{a}} + Q_{i,h} + \sum_{j=1, j\neq i}^{N} Q_{i,j}}{V_i} \tag{3}$$

and P_i is given by

$$P_i = \frac{1}{V_i}\left[\sum_{j=1, j\neq i}^{n} Q_{j,i}C_j(t) + S_i - R_i + Q_{\mathrm{a},i}C_\mathrm{a} + Q_{\mathrm{h},i}C_\mathrm{h}\right] \tag{4}$$

where $Q_{i,j}$ is the air flow from room i into room j, $Q_{j,i}$ is the air flow from room j into room i, $Q_{i,\mathrm{a}}$ is the air flow from room i to the outdoors, $Q_{\mathrm{a},i}$ is the air flow from the outdoors into room i, $Q_{i,\mathrm{h}}$ is the air flow from room i into the heating, ventilating, and air conditioning (HVAC) system, $Q_{\mathrm{h},i}$ is the air flow from the HVAC into room i, $C_j(t)$ is the concentration in room j at time t, C_a is the outdoor concentration, and C_h is the concentration in the HVAC system.

As is discussed in the previous sections, the sources, sinks, and air movement terms in real buildings are not constants. An IAQ model must, therefore, solve the system of equations resulting from the mass balance numerically. Yamamoto *et al.*[4] have shown that an algorithm based on the exact solution can be used to solve the series of equations. The algorithm is based on the assumption that, for sufficiently small time steps, dt, the source and sink terms and all neighboring concentrations are constant. The algorithm has the advantage that it is stable for all time steps, and it is accurate for sufficiently small time steps. (The size of the time step depends on how rapidly concentrations are changing. In most situations a time step between 0.05 and 0.20 hr provides good results.)

SOURCES

Sources are the dominant factor in determining IAQ. The chemical composition of the source determines the chemical composition of the indoor air. More importantly, the behavior of the sources as a function of time plays a major role in determining the time concentration history of indoor air.
Sources can be divided into a few idealized classes:

—long-term, steady state sources such as moth crystals and air fresheners
—ON/OFF sources such as heaters
—decaying or wet sources such as paints, waxes, and stains
—burst sources such as aerosol products.

The time history of these ideal sources is shown in FIGURE 1.

The decaying or wet sources are difficult to simulate both because the emission rates change with time and because there are usually emissions, called application phase emissions, associated with applying the source. For example, there are emissions due to the act of painting a wall and emissions due to the paint on the wall. In many case the application emissions are much smaller than the long-term decaying emissions. Wet sources with and without application phase emissions are shown in FIGURE 1.

Sources are represented by a first-order decay equation of the form

$$ER = R_0\exp(-kt) + R_A \text{ for } t \leq t_A \qquad (5)$$
$$R_0\exp(-kt) \text{ for } t > t_A$$

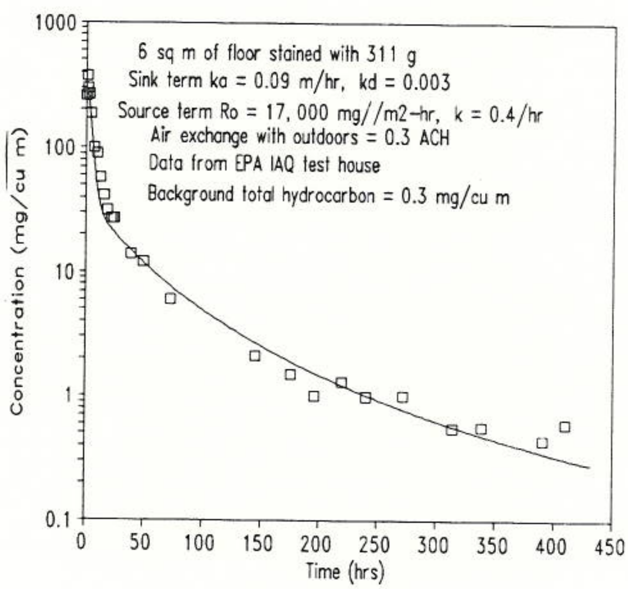

FIGURE 1. Comparison of model predictions and IAQ test house data for total VOCs from a wood stain source.

where ER is the emission rate, R_0 is the initial emission rate, k is a decay constant, R_A is the application emission rate, and t_A is the application time. This source model treats the application phase as a steady state source of limited duration. This type of source term allows simulation of a wide range of source types. If the source is a steady state source, k is equal to zero. R_0 and k can be determined from chamber studies.[5,6] In many cases all of the emissions are accounted for by R_0 and k as determined by chamber studies. The value of R_A can be estimated or at least bounded from large chamber studies, test house studies, mass balance analysis of small chamber studies, or other experiments.

SINK TERMS

Research in the Environmental Protection Agency test house and in the small chamber laboratory[3,7–9] has shown that sinks (that is, surfaces that act to remove pollutants from the indoor air) play a major role in determining indoor pollutant concentrations. These sinks may be reversible or irreversible. A reversible sink reemits the material collected in it and an irreversible sink does not. The sink behavior depends on the pollutant and the nature of the sink. A sink may appear to be irreversible when the pollutant concentration is high and then become reversible when the pollutant concentration is low.

A reasonable sink model is based on the research described by Tichenor *et al.*[9]

$$R_s = k_a C A_{\text{sink}} - k_d M_s^n A_{\text{sink}} \tag{6}$$

where R_s is the rate to the sink (mass per unit time), k_a is the sink rate constant (length per time), C is the in-room pollutant concentration (mass per length cubed), A_{sink} is the area of the sink (length squared), k_d is the reemission or desorption rate constant, M_s is the mass collected in the sink per unit area (mass per length square), and n is an exponent. This model is described by Tichenor *et al.* as the best fit model. When $n = 1$, the model becomes the Langmuir model presented by Tichenor *et al.*

The sink rate constant, k_a, is limited by the rate that pollutant molecules arrive at the surface of the sink. If we assume that transport of pollutant to the surface of the sink is due to diffusion (a reasonable assumption for the low turbulence situations common in indoor spaces where the large eddies keep the pollutants well mixed in the room but do not disturb the boundary layer), k_a is the deposition velocity of pollutant molecules hitting the sink surface. Fuchs[10] shows that the value of k_a can be calculated from gas kinetic theory as

$$k_a = \sqrt{\frac{D}{\pi(1h)}} \tag{7}$$

where D is the diffusivity of the pollutant. Typical values of D for volatile organic compounds (VOCs) are between 0.02 and 0.10 m^2/hr resulting in typical values of k_a between 0.08 and 0.20 m/hr. Small chamber data reported by Tichenor *et al.*[9] give k_a values from about 0.08 to 0.45 m/hr.

Although k_a can be estimated from properties of the pollutant, k_d and n must be determined experimentally. Tichenor *et al.* discuss the problems of determining k_d and n from small chamber data and indicate that the small chamber data for k_d for some pollutant/sink systems do not agree with values estimated from test house experiments.

The two rate constants, k_a and k_d, determine the behavior and the capacity of the sink. The capacity of a sink, that is, the amount of pollutant it can store, is related to k_a/k_d. The larger this ratio, the greater the capacity of the sink and the longer the time required to reach steady state concentrations. In short, the larger the ratio the greater the sink's impact on IAQ. Based on the limited research on sinks for VOCs, a typical value of k_a is 0.1 and a typical value of k_d is 0.008. All the sink calculations later in this paper are based on these values of k_a and k_d.

The nature of the source determines the importance of the sink. If the source is a steady state source and if k_d is greater than zero, the final steady state pollutant concentration is the same with or without the sink. If k_d is zero, the final steady state concentration with a sink will be less than the final steady state concentration without a sink. When the source strength is a function of time, the relative importance of the source and sinks is difficult to assess without modeling or experiment.

EXPOSURE

Individual exposure is determined by the time spent at a given pollutant concentration. Therefore, it is a function of both the building concentration time curve and the individual activity pattern—that is, where the individual is located when. Different activity patterns, for example, entering and leaving a building at different times, result in different exposures to the same building pollutant concentration time history.

Exposure analysis requires first prediction of the building concentration time history. Then individual activity patterns are imposed on the building time history to develop individual exposure. Two classes of exposure are of interest—instantaneous or peak exposure and cumulative exposure. Which of these two classes of exposure is appropriate for a given situation depends on the nature of the pollutant and on the nature of the effect.

Because the most common route for exposure to indoor air pollutants is via inhalation, it is convenient to define inhalation exposure, E_i, as

$$E_i = C(t)bv \tag{8}$$

where C is the pollutant concentration, b is the breathing rate, and v is the volume per breath. The exposure defined by equation **6** is instantaneous; that is, the exposure at any instant in time, t. The peak exposure is the maximum of the instantaneous exposure versus time curve. The cumulative inhalation exposure, E_{ic}, is given by

$$E_{ic} = \int_{t1}^{t2} C(t)bvdt \tag{9}$$

The advantage of defining inhalation exposure is that the exposures calculated by the computer can be used without requiring the user to manually calculate the amount breathed. For exposure by mechanisms other than inhalation, the instantaneous exposure, E, to a pollutant at time t is the concentration, $C(t)$, the person being exposed at time t

$$E = C(t) \tag{10}$$

The cumulative exposure from $t1$ to $t2$ is given by

$$E_c = \int_{t1}^{t2} C(t)dt \tag{11}$$

Calculation of exposure requires the pollutant concentration, the time exposed to the concentration, and (for inhalation exposure) the breathing rate and the volume per breath. The time exposed to the concentration depends on the individual activity pattern.

MODEL VERIFICATION

The model predictions of concentration versus time have been compared to experimental data from the Environmental Protection Agency IAQ test house.[7,8] In all cases the agreement between predictions and experiment has been excellent. An example from a recent experiment is shown in FIGURE 1.

EXAMPLES OF INTERACTIONS BETWEEN BUILDING, SOURCES, AND SINKS

Concentration Predictions

The model can be used to analyze the effects of building factors, sources, and sinks on indoor pollutant concentrations. The model analysis covers two different

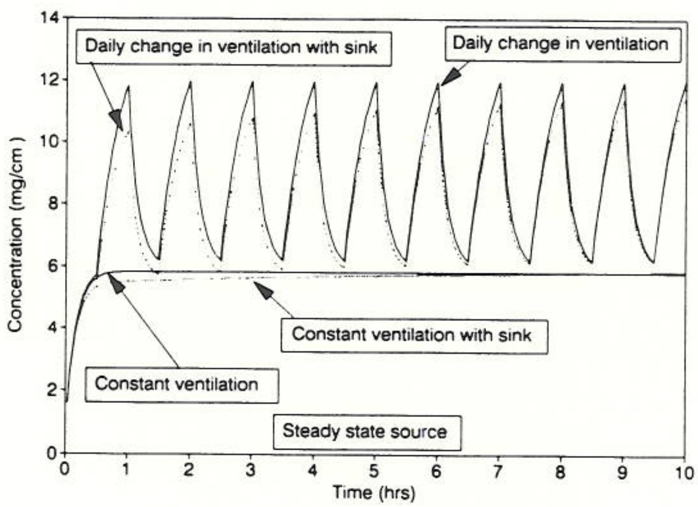

FIGURE 2. Effects of ventilation and sinks on concentration from a steady state source.

source types—steady state and decaying. In each case following situations are analyzed:

1. Constant ventilation of 0.5 ACH without a sink, labeled constant ventilation.
2. Constant ventilation of 0.5 ACH with a sink, labeled constant ventilation with sink.
3. A daily change in ventilation from 0.5 ACH to 0.2 ACH without a sink, labeled daily change in ventilation.
4. A daily change in ventilation from 0.5 to 0.2 ACH with a sink, labeled daily change in ventilation with sink.

The results for the steady state source are shown in FIGURE 2. Note that as expected the with and without sink curves are essentially the same after about 7 days for the constant ventilation case and after about 9 days for the daily change in ventilation case. Also note the effect of reducing ventilation. The concentration increases when the ventilation rate is reduced and then drops when the ventilation rate increases. The concentration, however, does not return to the high ventilation base.

The results for the decaying source are shown in FIGURE 3. The most obvious features of FIGURE 3 is the effect of the reemitting sinks. The sinks maintain a nearly constant pollutant concentration long after the concentration due to the source has dropped to zero.

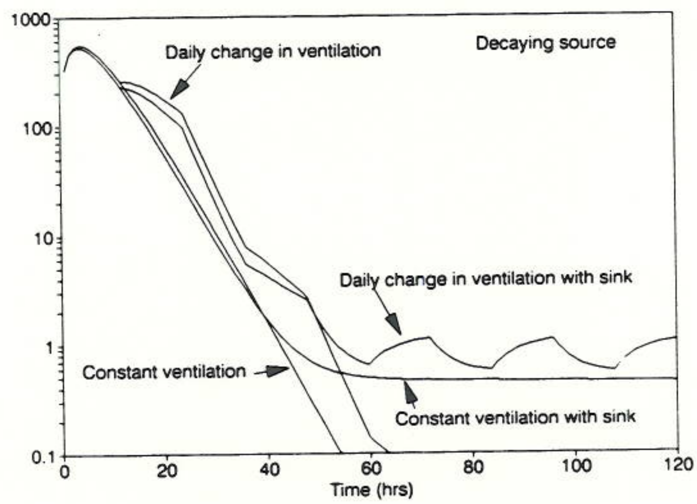

FIGURE 3. Effects of ventilation and sinks on concentration from a decaying source.

Exposure Predictions

The analysis of the impact of sources on individual exposure must include all the factors discussed above and the individual activity pattern. Failure to consider activity patterns can result in unrealistic analysis. The importance of activity patterns can be illustrated by two examples. These examples are based on experiments conducted in the Environmental Protection Agency test house. All model input is based on the conditions in the test house at the time of the experiments. The model predictions of concentration versus time for both cases are in excellent agreement with the test house data.

The first example is calculation of the exposure to an aerosol spray product. The activity patterns are for a person who uses the product, remains in a bathroom for 10 min, moves to the living room, and then leaves the building after 1 hr; and for a person who stays in the building for 24 hr. The instantaneous and cumulative inhalation exposures for the two individuals are given in FIGURES 4 & 5. Note that, although the initial instantaneous exposure for the person using the product is

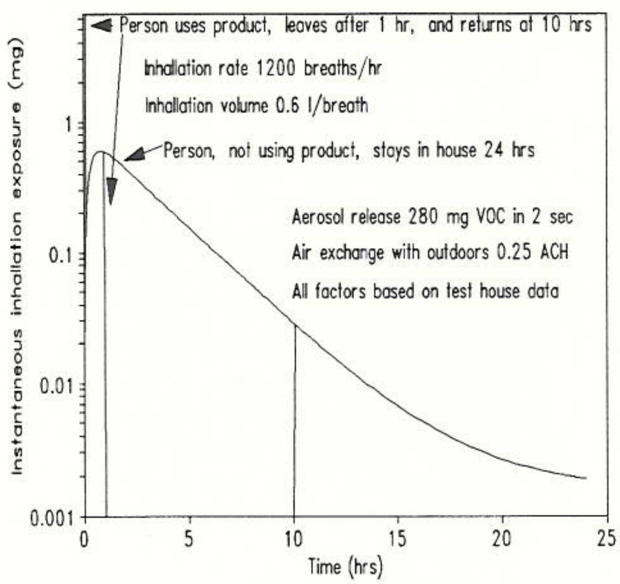

FIGURE 4. Instantaneous inhalation exposure from use of an aerosol product.

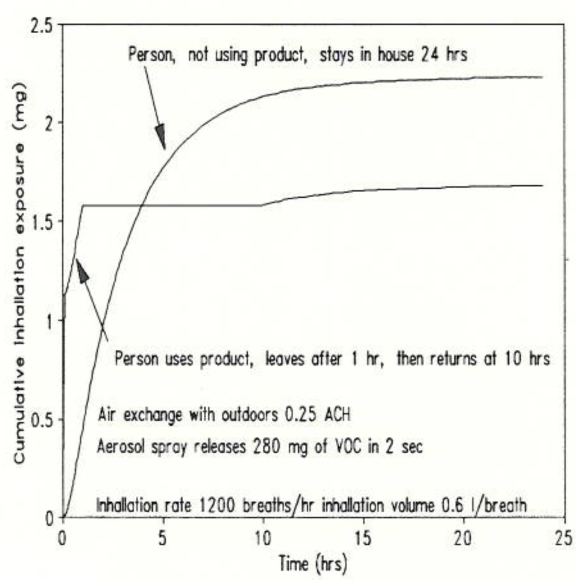

FIGURE 5. Cumulative inhalation exposure from use of an aerosol product.

much higher than for the other person, the cumulative exposure for the person using the product is less. The exposure for the person using the product, however, is probably underestimated in this example. The local concentration near the person is somewhat higher for several minutes than the average room concentration. EXPOSURE can deal with this situation if a pseudo room with a volume of about 5 m^3 and an air exchange of 30 m^3/hr with the rest of the room is defined. For the case shown in FIGURE 4, the difference in exposures is not great because the volume of the bathroom is relatively small (20 m^3).

The second example shows the exposure due to wood stain, a "typical wet source." Because of adsorption and reemission from sinks, the exposure lasts for a considerable time. The cumulative exposures for a person spending 24 hr in the

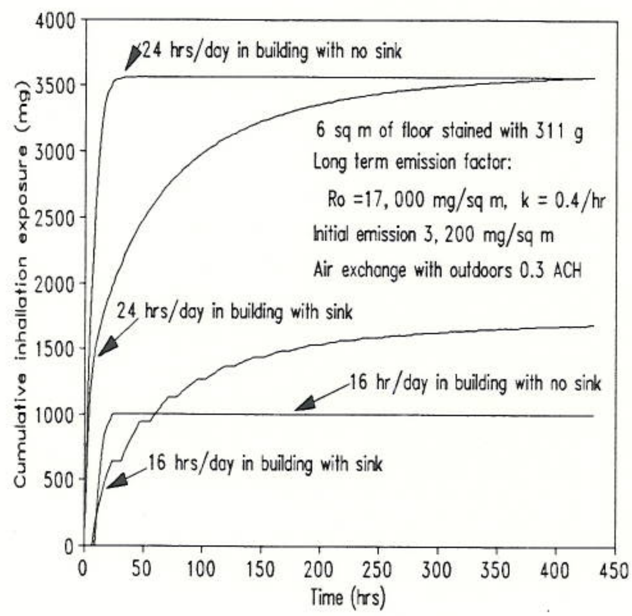

FIGURE 6. Cumulative inhalation exposure from use of a wood stain.

building and for a person spending 16 hr in the building (starting 8 hr after the stain is applied) are shown in FIGURE 6 both with and without a sink. Note the major effect of the sink on the exposure of the person spending part of the time in the building.

CONCLUSIONS

All of the building, sources, sinks, and activity pattern factors discussed above must be considered in a realistic assessment of the impact of sources on IAQ and pollutant exposure. Such treatment is especially important in analysis of effects of exposure to indoor pollutants. Modeling provides a powerful tool for conducing the required analysis and for developing realistic scenarios.

MODEL AVAILABILITY

The documentation for EXPOSURE is being written. The documentation and MS-DOS-readable disk will be available from the NTIS as soon as they have been cleared for publication by the Environmental Protection Agency.

SUMMARY

The effects of indoor air pollutants depend on the concentrations of the pollutants and the exposure of individuals to the pollutants. The air pollutant concentrations are determined by the complex interactions of sources, sinks, in-building air movement, and air exchange between the indoors and the outdoors. Individual exposure to indoor pollutants is determined by the indoor pollutant concentrations and individual activity patterns. An assessment of the effects of indoor pollutants must include analysis of these complex interactions to ensure that the analysis is done under realistic conditions. The use of an IAQ model, EXPOSURE, to predict pollutant concentrations and exposures is presented.

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