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# ESTIMATING INTERROOM CONTAMINANT MOVEMENTS

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Development of infiltration and interroom airflow calculation methods, driven by a concern for indoor air quality have led to a computer simulation of interroom contaminant movement. The model, which assumes fully mixed room air, shows that open doorways provide rapid mixing between rooms in buildings using forced air heating. It also confirms that it is most energy efficient to remove the contaminant nearest its source. Detailed modeling of the variations in contaminant concentration within a room is not presently feasible for long term energy analysis simulations. The need for computer modeling is demonstrated by the subtle behavior of a very simple system which removes contaminants by forced ventilation.

## INTRODUCTION

The removal of odors and contaminants and the provision of adequate amounts of fresh air is a requirement for any occupied space. Buildings without mechanical ventilation systems do this by natural infiltration, but uncontrolled infiltration leads to many hours with excessive infiltration which results in a large energy cost. Therefore, it is usually recommended that infiltration be minimized and ventilation be done mechanically as required. However, even mechanical ventilation systems may not be performing well. A recent study Persily and Grot (1) found that most of the buildings studied operated at near or below the recommended ventilation rate. These low ventilation rates occured during periods of extreme weather when ventilation was reduced to conserve energy. Further gains in energy efficiency without sacrificing comfort or endangering health will require analysis of the migration of contaminants in buildings. This paper will look at some of the modeling requirements for estimating contaminant movements within the context of a building energy analysis computer program.

## CONTAMINANTS

There are many contaminants potentially present as gasses and particulates in rooms. Among the contaminants of interest (McNall (2)) are:

- radon - a radioactive gas from the earth and some masonry products,
- formaldehyde - principally from pressed wood products,
- carbon monoxide (CO), carbon dioxide ($CO_2$), and nitrous oxides (NO, $NO_2$) - from combustion processes,
- tobacco smoke - both gases and particulates,
- particulates - including biomaterials and allergens, and
- volatile organic compounds - such as cleaning materials.

The important common characteristic of these different contaminants is that they mix well with air and are transported through a building primarily by air movement (rather than difusion).

Moisture can also be considered a contaminant. Except in dry climates, accurate analysis of night ventilation must account for the storage and release of moisture from the building and its furnishings. The behavior of some contaminants may be influenced by humidity. Only the most preliminary work has been done on determining appropriate absorption coefficients for common building materials and furnishings (Kusuda (3)).

The time dependent behavior of a contaminant which is perfectly mixed with the air in a single room is described by a simple ordinary differential equation. By perfect mixing it is meant that any gasses or pollutants entering the room mix instantaneously and uniformly. If the contaminant generation and loss rates are known, there is a simple solution to the equation. Real world complexities limit the accuracy of such a simple solution. The contaminant may not be well mixed with the room air. Concentrations are highest at the source and contaminants may preferrentially drift to certain areas of the room. Generation and absorption rates may be complex functions of conditions such as temperature and humidity in the room. The outdoor air ventilation rate can be difficult to determine, especially for natural ventilation, and the outdoor air may not mix well with the room air. Buildings contain many rooms with all processes occuring simultaneously. Such factors make detailed analysis very difficult.

## MULTIPLE ROOM, SINGLE ZONE MODEL

Prediction of the time-varying concentration of a contaminant in each room of a building begins with a mass balance on the airflows into and out of the room under assumed quai-steady conditions:

$$\Sigma F_i + F_s = \Sigma F_o + F_e \quad \dots\dots\dots\dots \quad (1)$$

where
$F_i$ = air flow rates into room n (kg/s),
$F_s$ = air handling system supply air flow rate (kg/s),
$F_o$ = air flow rates out of room n (kg/s),
$F_e$ = air handling system exhaust air flow rate (kg/s).

There is also a mass balance for each contaminant species: the rate of change of the total mass of a contaminant in a room is equal to the total gains into the room minus the losses from the room. The contaminant gains may be due to flows through doors or cracks from other rooms, from air introduced by the air handling system, and from generation of the contaminant within the room. The contaminant is removed from the room air by airflows out of the room including HVAC return air. It may also be removed by various mechanical or natural absorption and chemical conversion processes. These latter removal mechanisms may be mathematically combined with the generation mechanism into a single term in the contaminant mass balance equation -- the net generation rate. Assuming that (1) the contaminant mixes well with the room air (one zone per room), (2) the contaminant follows the airflows through the building and (3) the mass of contaminant is very small compared to the mass of room air leads to the following contaminant mass balance equation:

$$\rho_n V_n \frac{dC_n}{dt} = \Sigma F_i C_i + F_s C_s + G_n - C_n(\Sigma F_o + F_e) \quad \dots\dots\dots\dots \quad (2)$$

where
$\rho n$ = room air density (kg/m$^3$),
$V_n$ = volume of room n (m$^3$),
$C_n$ = contaminant concentration in room n (kg/kg),
$C_i$ = contaminant concentration of incoming air (kg/kg),
$C_s$ = contaminant concentration in the system supply air (kg/kg),
$G_n$ = contaminant net generation rate (kg/s),

There is one contaminant equation per room per contaminant species. The equations for each species tend to be independent of each other (unless one contaminant strongly influences the net generation rate of another, e.g., humidity and formaldehyde). The equations for multiple rooms for a single species tend to be simultaneous (unless there is no airflow between rooms). It is relatively easy to add this calculation to a building simulation program if the program computes the interroom air flow rates. The TARP computer program by Walton (4) computes the interroom airflows by considering the openings in the walls between rooms and the pressure differences across those openings. The mass flows through the openings are computed by a modified Newton's method which solves a simultaneous mass balance in all rooms of the building (Walton (5)).

Equation (2) is an ordinary differential equation which can be solved by many methods. The Euler (standard explicit), improved Euler, and fourth-order Runge-Kutta methods Kreyszig (6) were tested. For a single room interacting with the outside air, the improved Euler method required the least amount of computation to achieve a given level of accuracy. However, for multiple rooms interacting with each other, the simple Euler method proved best because any method which normally allows a longer time step between function evaluations is using values of $C_n$ which have been updated less recently than if a short timestep were used. The accuracy was evaluated by considering step changes in the contaminant generation rate or in the supply air flow rate while other parameters were held constant. These conditions lead to simple exponential increases or decreases in the contaminant concentration to some new level. The new level and the exponential rates can be determined analytically. Time steps considerably shorter than one hour are required to model rapidly changing conditions. Time steps of one minute gave concentrations accurate to within 0.1 percent of the analytic values but required about 40 percent of the total simulation time. Five minute timesteps used only about 10 percent of the simulation time with an accuracy of four percent in the transient solution. The long timestep gives essentially the same result as the short timestep at the end of one hour. Therefore, programs which are primarily concerned with houly variations for computing long term average concentrations can use timesteps of about five minutes.

## SAMPLE CALCULATION

The following sample calculation was made to test and demonstrate the multiroom contaminant calculation combined with the airflow and heat balance calculations in TARP. A typical ranch style house by Hastings (7) was chosen for the study. Figure 1 shows the floor plan of the house which consisted of six rooms and an attic. The six rooms are the dining room, living room and hallway (D/L), the kitchen (K), the bath (B), the master bedroom (MB), the second bedroom (B2), and the third bedroom (B3). Doorways between rooms were simulated by pairs of openings which allow mixing of air between the rooms. The dining/living room is heated to 72F. The other rooms are heated only by natural convection through the doorways. This was done because TARP does not yet have an air handler model which would distribute air through ducts when the furnace is on. If the rooms were all controlled to the same temperature, there would be no mixing between the rooms. The model is therefore conservative in comparison to an actual forced air system with a central return in the hallway because the forced air system would have higher flow rates and more even temperature and contaminant distribution through the house. Three different combinations of openings in the envelope of the house were simulated to represent leaky, average, and tight construction (cases 1, 2, and 3, respectively).

Two weather patterns were used. One consisted of values measured on February 22, 1982 at Gaithersburg, Md. The average outdoor air temperature was 37.3F, the wind speed 5.2 mph, and the wind direction was from the northwest. The other pattern used constant values (the above averages) of temperature, wind speed, and wind direction in order to give nearly constant infiltration. The infiltration causes a drift of air through the house from the northwest to the southeast. This drift is combined with the interroom mixing by the mass balance algorithm.

In the sample calculation a contaminant is released into the kitchen three times per day at hours 6, 12, and 18. Infiltration is the only contaminant removal mechanism. Figure 2 shows the relative hourly contaminant concentrations in the kitchen for the three envelope leakage areas. The house with the highest infiltration has the lowest average contaminant concentration and vice versa as expected. The units of contaminant concentration require some explanation. Concentration is computed in (kg contaminant/kg air) for simple implementation in equation (2) and easy conversion to English units. In the simulation the contaminant is released at a rate of one pound per hour for one hour. (English units were used in the TARP input because the sample house is described (7) in English units). Therefore, an average concentration of 0.001 in figure 2 really means a concentration of that value times the contaminant generation rate, whatever its value.

Figure 3 shows the contaminant concentration in more detail for case 3 for two hours. The highest concentrations occur in the kitchen -- the source room. The kitchen air mixes primarily with the dining/living room air because of the arrangement of the doorways. The other rooms then mix with the dining/living room. They all have very similar concentrations. The concentrations start out nearly identical and the contaminant is released during the hour between 18 and 19. As contaminant generation begins, the concentration in the kitchen increases very rapidly. The D/L concentration increases slowly. The MB concentration increases even more slowly as the contaminant must mix from the kitchen through the dining/living room before mixing with the bedroom. When contaminant generation stops at hour 19, the kitchen concentration decreases very rapidly as the contaminant mixes throughout the house. After a few minutes all zones are at essentially the same contaminant concentration. This concentration decays exponentially as infiltration slowly clears the air in all rooms. The rapid mixing is caused by a temperature difference of about 5F between the dining/living room and the other rooms. On a mild day, when the rooms and outside air are all at about the same temperature and heating or cooling is not needed, there would be very little airflow between rooms causing contaminant concentrations to be much higher, especially in the kitchen.

The results of the simulations are summarized in Table 1. As the infiltration decreases, the heating load decreases, but the average contaminant concentrations increase. From case 2 to case 3 the infiltration decreases 48%; the heating load decreases 22% and the average contaminant concentration increases 87%. Further reductions in infiltration will produce less reduction in the heating load while greatly increasing the average concentration. The heating load would be 10.5 kBtu/h even if there were no infiltration. The differences between the constant weather and the variable weather are not significant. A fourth case is presented where a fan is on in the kitchen during the hours when the contaminant is produced. This fan removed air from the kitchen at a rate of four kitchen volumes per hour (64 cfm). Otherwise, the house is identical to case 3. The heating load is reduced 18% relative to case 2 while the average contaminant concentration is increased only 37%. This sample calculation shows that it is energy efficient to remove the contaminant nearest its source. In fact, this predicted contaminant concentration is a very conservative value because the contaminant fully mixes with the kitchen air before the mixture is removed. In actual practice the fan should be located near the contaminant before it mixes throughout the room.

TABLE 1: Sample Calculation for Contaminant Migration. One Pound of 'Contaminant' Released During Hours 6, 12, and 18.

| Constant weather T=37.3F W-5.2mph | | Case 1 | Case 2 | Case 3 | Case 3+fan |
|---|---|---|---|---|---|
| Infiltration ($h^{-1}$) | | .572 | .305 | .160 | .184 |
| Average load (kBtu/h) | | 26.3 | 18.4 | 14.4 | 15.1 |
| Daily Average Contaminant Concentrations x1000 | K | 3.47 | 6.16 | 11.51 | 8.46 |
| | D/L | 3.05 | 5.56 | 10.92 | 7.92 |
| | B3 | 3.02 | 5.61 | 10.86 | 7.87 |
| | B2 | 2.90 | 5.48 | 10.73 | 7.76 |
| | MB | 2.83 | 5.41 | 10.65 | 7.72 |
| | B | 3.05 | 6.65 | 10.92 | 7.92 |
| Variable weather | | | | | |
| Infiltration ($h^{-1}$) | | .609 | .314 | .160 | .181 |
| Average load (kBtu/h) | | 26.0 | 18.1 | 14.2 | 14.9 |
| Daily Average Contaminant Concentrations x1000 | K | 3.30 | 6.04 | 11.52 | 8.45 |
| | D/L | 2.87 | 5.52 | 10.92 | 7.92 |
| | B3 | 2.84 | 5.49 | 10.88 | 7.88 |
| | B2 | 2.73 | 5.36 | 10.73 | 7.76 |
| | MB | 2.65 | 5.27 | 10.64 | 7.70 |
| | B | 2.87 | 5.52 | 10.92 | 7.92 |

## TWO ZONE INTRA-ROOM MODEL

The discussion on the use of an exhaust fan indicates that the fully mixed room model is too simple for evaluating ventilation performance. However, a detailed model of the motion of air within a room requires numerical solution of the turbulent Navier-Stokes equation together with the energy and mass diffusion equations such as demonstrated by Ishizu and Kaneki (8). This is a very time consuming calculation. The concept of ventilation efficiency has been developed as a simple model for the simulation of room air flow (Sandberg (9), Skaret and Mathison (10)). In these references it is shown that ventilation for cooling is much more effective when outdoor air is introduced at low velocity near the floor and removed near the ceiling. This ventilation strategy is more effective than if the room and ventilation air are uniformly mixed. Both cases are much more effective than situations in which the ventilation air travels directly from inlet to exhaust leaving stagnant air in much of the room. Experimental studies (9, 10) have confirmed that air movement within a room can often be modeled as two fully mixed zones, upper and lower, when given appropriate values for inflow, outflow, and a mixing coefficient between the zones. Study is needed for recommending appropriate mixing values.

Equation (2) can be used with the two zone problem by applying it to each zone. The subscripts which referred to rooms will now refer to the upper and lower zones in each room. The flows between zones in the same room will usually be much greater than the flows between rooms. It is therefore best that the pair of equations for the two zones in a single room be solved simultaneously (i.e. an algebraic solution rather than iterative) at each timestep as part of the Euler solution for all rooms of the building. This calculation was tested and found to have no numerical problems such as convergence, and it gave correct results for the limiting cases of very high and very low mixing between the two zones of one room.

The calculation of the room air temperature should also be modified to compute the temperatures of both zones. This is one method of simplified stratification modeling. Again the temperatures of the upper and lower zones of one room should be calculated simultaneously. There are significant questions as to how the zones interact convectively with the room surfaces. It is not as simple as having convective heat and mass transfer between the zone and the surface. For example, there is a strong tendency in still air for the air that is near a warm vertical surface to rise in a boundary layer along the surface and mix only with the air in the upper zone. Convective gains from warm objects in the room may behave similarly with plumes of warm air carrying heat (and contaminants) predominantly into the upper zone. There is not yet enough information on the coefficients which would describe such processes to justify the major modifications that would be required to incorporate these effects into TARP.

## SYSTEM INTERACTIONS

The operation of the air distribution system will normally be the primary influence on the distribution of contaminants. The following two studies indicate that the requirement for system simulation will have a significant impact on the overall building/contaminant simulation program.

Most building energy analysis programs do not perform the detailed mass balance to estimate infiltration. They use simple correlations involving temperatures and wind speed such as developed by Coblenz and Achenbach (11). How should forced ventilation flows be combined with the naturally occurring infiltration? The requirement of a mass balance in each room and in the whole building must be used in developing a simplified correlation. Based on a study of combustion systems which draw air from the conditioned space, chapter 22 of the ASHRAE Handbook (12) indicates that 70% of the exhaust flow is from increased infiltration with the remaining 30% from decreased exfiltration. Another study by Levins (13), which considered the effects of electric clothes dryers vented to the outside, recommended the following correlation.

$$Iv = In + Fv\ e^{(In/Fv)} \quad \ldots\ldots (3)$$

where

Iv = the infiltration rate with forced ventilation,
In = the infiltration rate with no forced ventilation,
Fv = the forced ventilation rate.

The rather low regression coefficient (0.65) for this correlation and the great difference from the first correlation raise the question of the appropriateness of either. The detailed mass balance technique allows a theoretical/numerical study of the effect of forced ventilation on house infiltration as presented below.

Again consider the empirical equation for flow through a small opening:

$$F_i = K_i(P_i - P_h)^{x_i} \quad \text{.......} \quad (4)$$

where
$F_i$ = the flow rate (m@U3/s) through opening i (positive = into house; negative = out of house),
$K_i$ = airflow conductance,
$P_i$ = the total pressure (Pa) due to wind and stack effects at the outside of the opening,
$P_h$ = the total pressure at the inside of the opening--the house pressure,
$x_i$ = flow exponent, between 0.5 and 1, usually near 0.65 for leakage openings.

First consider a house where:
all cracks are consolidated into two openings, the first on the upwind side of the house and the second on the downwind side,
all air flows in at the upwind side $F_1 = K_1(P_1-P_h)$ ,
all air flows out at the downwind side $F_2 = K_2(P_2-P_h)$ ,
the openings are at the same height (no net stack effect),
and let $x_1 = x_2 = 1$ and $K_1 = K_2 = K$ for ease of analytical solution.

A mass balance on the house, which is treated as a single room, requires that the inward flow through the first opening equal the outward flow through the second when there is no forced ventilation. Therefore, the house pressure is given by

$$P_h = (P_1 + P_2)/2 \quad \text{.......} \quad (5)$$

Next consider a forced exhaust ventilation rate, Fv. A mass balance leads to a new house pressure during ventilation, $P_H$, given by

$$P_H = (P_1 + P_2 - Fv/K)/2 \quad \text{.......} \quad (6)$$

which reduces to

$$P_H = P_h - Fv/(2K) \quad \text{.......} \quad (7)$$

The natural infiltration rate is

$$In = K(P_1 - P_h) \quad \text{.......} \quad (8)$$

The total infiltration with ventilation is

$$Iv = K(P_1 - P_H) \quad \text{.......} \quad (9)$$

Therefore, the increase in infiltration is given by

$$Iv - In = Fv/2 \quad \text{.......} \quad (10)$$

This simply means that the airflow into the zone (the infiltration) has been increased by one half the forced ventilation rate while the airflow out of the zone (the natural exfiltration) has been increased (made less negative) by the same amount. This is true as long as $P_1 > P_H > P_2$. If the ventilation rate is large enough, then $P_1 > P_2 > P_H$ and there is infiltration at the downwind side of the house also. The total infiltration is then equal to the forced ventilation rate.

These ideas were tested numerically in a small computer program (5) which uses equation (4) and the mass balance requirement to compute the airflows through all openings in the bulding envelope. Figure 4 shows the results for the house with only two identical openings. The figure relates the relative increase in infiltration, (Iv-In)/Fv, to the relative infiltration rate, In/Fv. Three values of the flow exponent, x, are considered: 1.0, 0.65, and 0.5. Results discussed above (x=1) correspond to a diagonal line where Iv = Fv and a horizontal line where Iv - In = Fv/2. For x=.65 and .5, the relative increase in infiltration still approaches 0.5 at large In/Fv. These exponents are more characteristic of actual openings, but an exact solution is difficult. Levins′ correlation (13) is shown for comparison.

One may then consider a house with openings on four sides. Theoretical considerations similar to those above indicate that the flow through each opening in the house will increase by Fv/4 if the openings are identical and x=1. A test case is considered with identical openings on walls facing north, east, south, and west. A wind is assumed to blow from the north. A simplified model of the wind effects predicts pressures of 8.47 Pa on the north side, -3.39 Pa on the east and west sides, and -1.69 Pa on the south side. Figure 5 shows the relative increase of infiltration for three flow exponents. For x=1, the relative increase is equal to Fv/4 when In/Fv > 1.25, that is, when there is an inward flow on only the north surface. When In/Fv is less than 0.61, air flows in through all four surfaces, and between 0.61 and 1.25, it flows in through the north and south walls and out through the east and west walls. For x=0.65, there is inward flow through only one wall when In/Fv > 2.36, with a relative infiltration increase of about 0.14. For x=0.5, inward flow through only one wall is not achieved until In/Fv > 5 (beyond the range of figure 5) with a relative infiltration increase of about 0.07.

Now consider the effects of wind direction on the sample four-sided building. The pressure effects of a wind blowing from due north and 15, 30, and 45 degrees east of north were simulated with the simple model and the results are summarized in figure 6. For the wind at 45 degrees there are two surfaces upwind with identical positive pressures and two surfaces downwind with identical negative pressures effectively recreating the two surface case shown in figure 4. For the due north wind, the conditions are the same as in figure 5. The response for the wind at 15 degrees resembles the north wind, and the response for 30 degrees resembles the northeast wind.

This simple analysis could be conducted for more complex building configurations, but the complex nature of the effect of forced ventilation on infiltration is already apparent. It is dependent on the relative areas for inward and outward airflow and the degree to which forced ventilation reverses the outward flows. For simplified analysis, the performance shown in figure 6 may be approximately represented by

for In/Fv < 0.7, Iv = Fv .................................................. (11a)

for In/Fv > 0.7, Iv = In + 0.3 Fv .................................... (11b)

This correlation also is a reasonable representation of the data presented in reference (13) and could be used in energy analysis programs which cannot compute the detailed mass balance. However, the great variability in total infiltration indicates that the detailed mass balance is the preferred simulation approach.

The development of a simultaneous simulation of equipment performance and room heat transfer ran into convergence problems which are still unresolved in TARP. A mechanical ventilation model was developed to move a specified volume of air from one room to another based on relative temperatures in the two rooms. One of the "rooms" could be the outside. This model worked whenever one of the two control temperatures was the outside temperature which is constant during the timestep. This allowed simulation of common arrangements such as an exhaust fan or a whole house fan which exhausts from the house into the attic. However, when the fan was arranged to mix the air between two rooms (by blowing between them and having a large opening for a return air flow as might be used with a sunspace room), there were times when the heat balance iterations would not converge. This problem appears to be inherent in the long timestep (one hour), implicit heat balance method used in TARP. The method implements the implicit solution by iteration: (1) compute the outside surface temperatures using a heat balance based on the most recent estimate of inside temperatures; (2) compute the inside surface temperatures using the outside temperatures and most recent estimate of the room air temperatures; (3) compute the airflows based on room air temperatures; (4) compute new room air temperatures and heating or cooling loads based on the new inside surface temperatures and airflows; (5) if successive values of room temperature or load have not converged, return to (1); (6) after convergence, use the airflows to computer contaminant concentrations.

There are occasions when successive room temperatures during the iterations causes the fan to switch on and off repeatedly. Each such cycle often takes several iterations. Two potential solutions to this problem are (1) use of a direct, rather than iterative, solution of the simultaneous equations or (2) use of an explicit solution. An explicit solution would be easiest to implement, but could be very time consuming because it would require a much shorter timestep -- probably similar to the timestep used in solving the contaminant concentration equations. The short timestep would have the advantages of allowing contaminant concentration to control the operation of the ventilation system and easily simulating system devices which operate for only part of the hour. This would be very useful for modeling the typical residential forced air furnace which operates by cycling on and off and whose fan also cycles, but on a delayed basis. The nature of interroom contaminant migration is completely different during different parts of the hour depending on whether the fan is on or off.

## SUMMARY AND CONCLUSIONS

Development of infiltration and interroom airflow calculation methods and concern for indoor air quality have led to a computer simulation of interroom contaminant movements. Calculation of interroom contaminant migration is mathematically quite simple if it can be assumed that the air in each room is well mixed. It can be expressed by an ordinary differential equation describing the contaminant mass balance. However, computer implementation of the contaminant mass balance equations can be rather time consuming compared to the rest of the building thermal simulation. Detailed modeling of the concentration variations within a room is too time consuming to be considered for long term transient analysis of multiple room buildings. Employing the concept of ventilation effectiveness may provide a solution with sufficient accuracy and speed. It could be added to some existing energy analysis programs. The simple fully mixed room model showed that open doorways provide rapid mixing between rooms in buildings using forced air heating. It also confirmed that it is most energy efficient to remove the contaminant nearest its source.

The HVAC system can dominate contaminant migration and needs to be considered in modeling. Current simulation codes with long (one hour) timesteps tend to run into convergence problems when solving the system performance and interroom airflows simultaneously. It may be necessary to model with smaller timesteps with the conseqeunt increase in computation time. Calculation of the increase of outside air brought into a house by a fan showed than even simple systems can have subtle behavior. Until such interactions are well understood, there is no substitute for detailed modeling.

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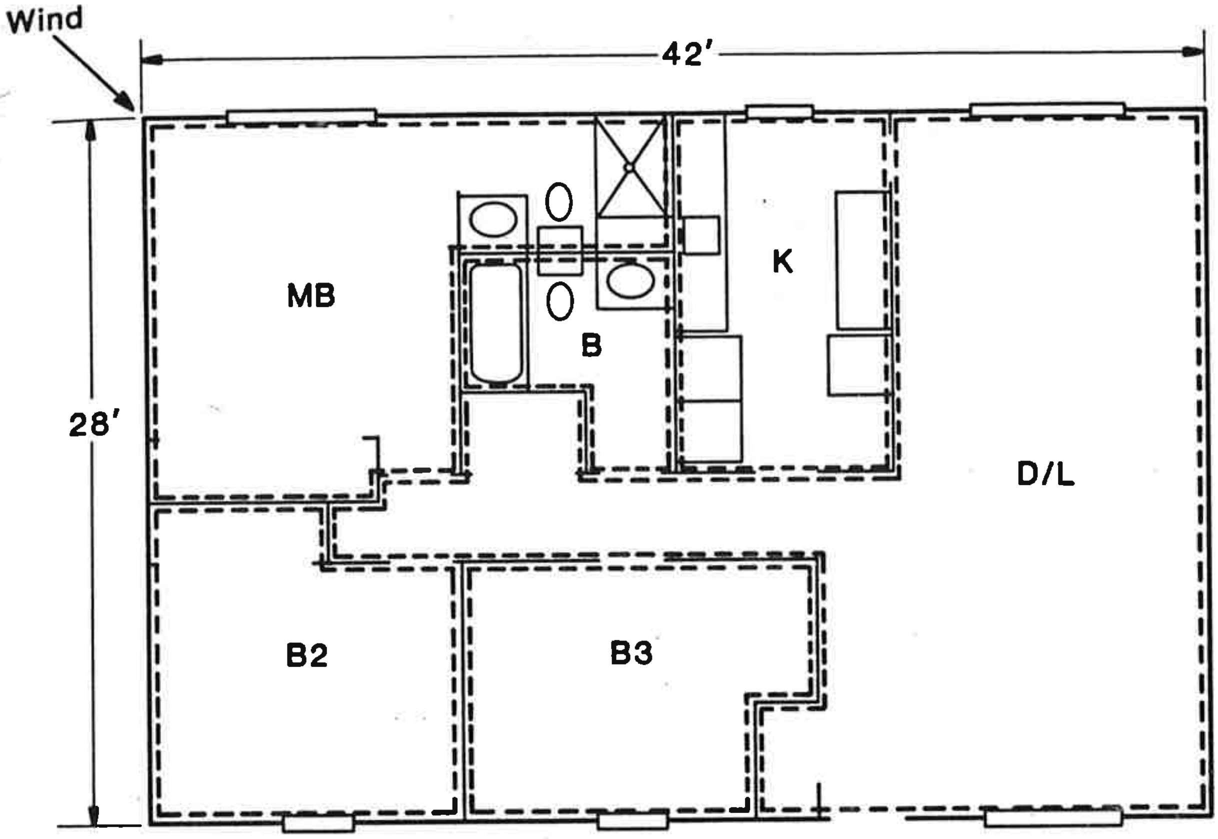

Figure 1. Floor plan of example house

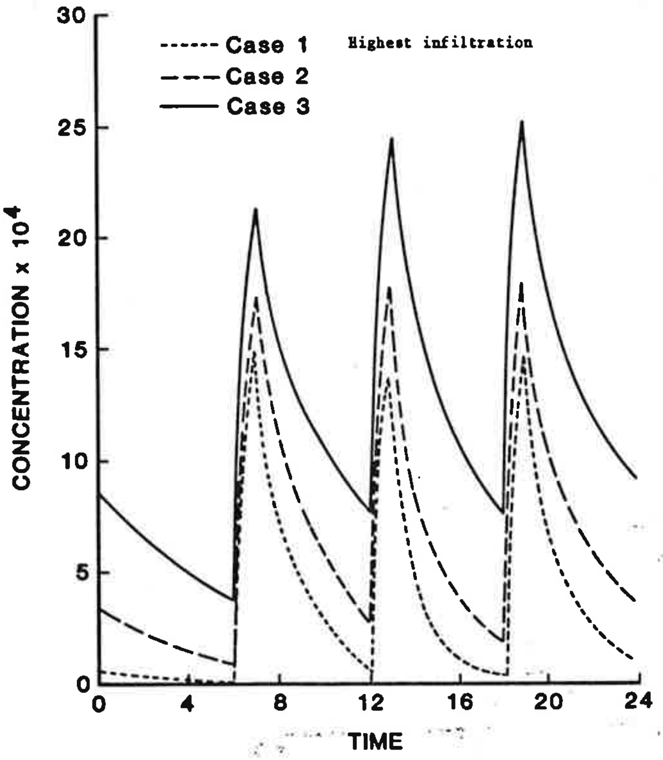

Figure 2. Contaminant concentrations for three levels of house leakiness

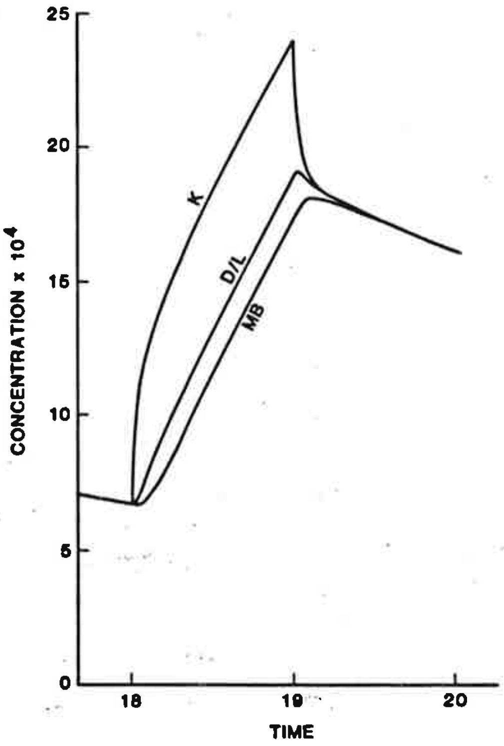

Figure 3. Contaminant concentrations in three rooms of one house (case 3)

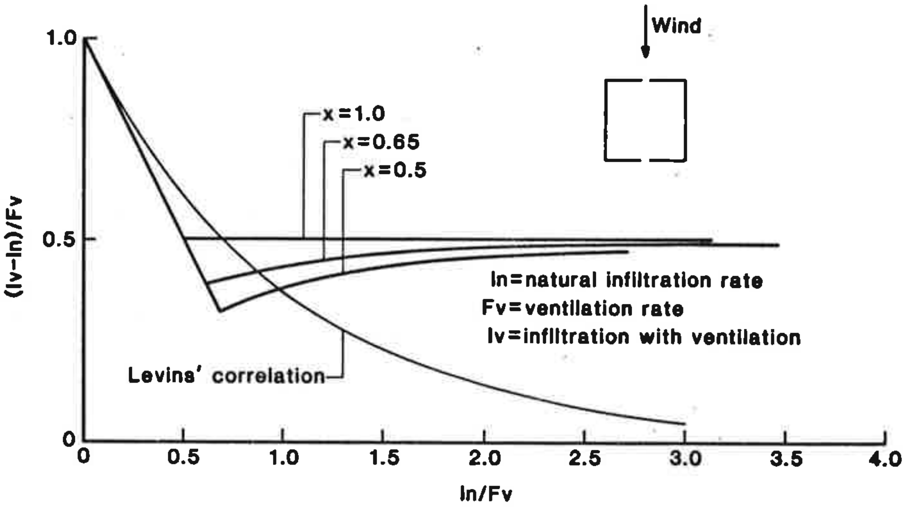

Figure 4. Infiltration response for a building with only upwind and downwind openings

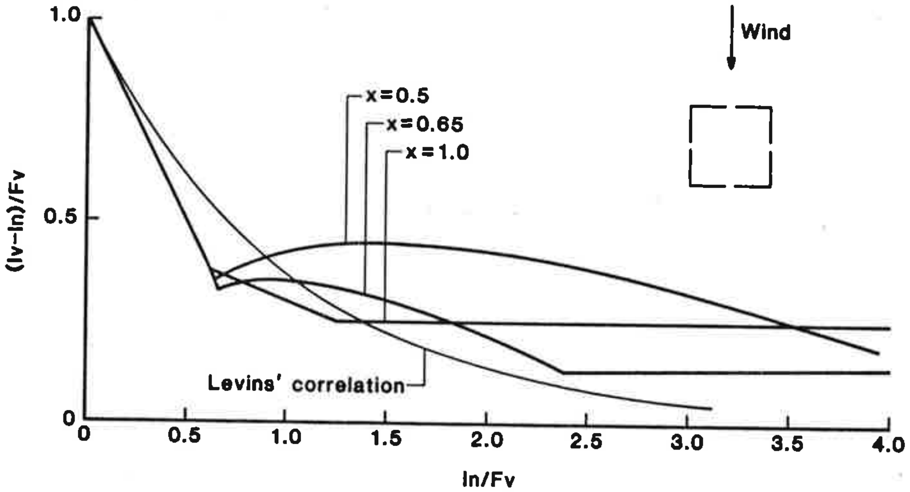

Figure 5. Infiltration response for a building with openings on four sides

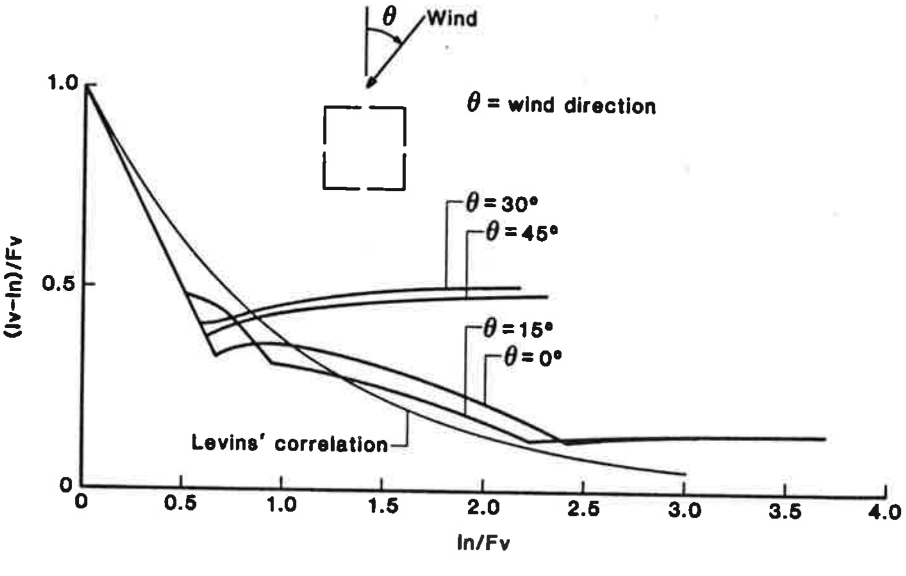

Figure 6. Infiltration response for various wind directions