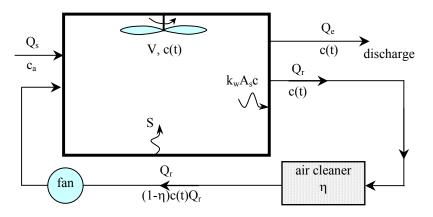
# **5** General Ventilation and the Well-Mixed Model

#### **5.7 Partially Mixed Conditions**

Sections 5.3 to 5.6 are analyses in which the concentration is uniform throughout the enclosed space, although it may vary in time, i.e. *spatial* uniformity but not *temporal* uniformity. If the ventilation volumetric flow rate (Q), source strength (S), and adsorption rate ( $k_w$ ) are constant, the mass conservation equations can be integrated in closed form. If these parameters vary with time, the equations can be integrated numerically. It must be emphasized that the notion of spatial uniformity is critical to the validity of the well-mixed model and the solutions that follow from it. Unfortunately in many situations, both spatial and temporal variations in concentration occur simultaneously, i.e. the enclosed space is not well mixed. Analysis of these situations is difficult since the equations of both mass and momentum transfer have to be solved simultaneously. Numerical computational procedures are available for this and are discussed in Chapter 10.

Over the years an alternative computational technique has arisen that many workers in indoor air pollution find useful. The technique employs using a scalar constant called a *mixing factor* (m) to modify the equations of the well-mixed model to account for non-uniform concentrations brought on by poor mixing. Consider the ventilated enclosed space with 100% recirculation shown in Figure 5.9. Other geometric configurations can be modeled in comparable fashion. Assuming well-mixed conditions and neglecting adsorption on the walls, the following expression for the contaminant can be written:



**Figure 5.9** Schematic diagram of a typical ventilation system with 100% recirculation and separate make-up air.

$$V\frac{dc}{dt} = S + Qc_a - Qc + (1-\eta)Q_rc - Q_rc$$

which reduces to

$$V\frac{dc}{dt} = S + Qc_a - Qc - \eta Q_r c$$
(5-36)

To account for non-uniform mixing, mixing factor (m) is adopted, and Eq. (5-36) can be rewritten as

$$V\frac{dc}{dt} = S + mQc_{a} - mQc - m\eta Q_{r}c$$
(5-37)

Eq. (5-37) can be written in the standard form of Eq. (5-7) as usual, with

$$A = \frac{m(Q + \eta Q_r)}{V} \qquad B = \frac{S + mQc_a}{V}$$

If m, S,  $c_a$ , Q, Q<sub>r</sub>, and  $\eta$  are constants, the ODE can be solved in closed analytical form using Eqs. (5-10) and (5-11),

$$\frac{c_{ss} - c(t)}{c_{ss} - c(0)} = \exp\left[-At\right] = \exp\left[-\frac{m(Q + \eta Q_r)}{V}t\right]$$
(5-1)

where

$$c_{ss} = \frac{B}{A} = \frac{S + mQc_a}{m(Q + \eta Q_r)}$$
(5-2)

Esmen (1978) states that values of m are normally 1/3 to 1/10 for small rooms and possibly less for large spaces. Table 5.1 contains values of m referenced by Repace and Lowery (1980). If m is less than unity, the concept of mixing factor suggests that a fraction of each flow, mQ and mQ<sub>r</sub>, is well mixed while another fraction,  $(1 - m)Q_{rr}$ , bypasses the enclosure. Consequently

-  $\underline{m=1}$  implies well-mixed model and concentration that is spatially uniform

 $\underline{m < 1}$  implies nonuniform mixing and spatial variations in concentration

The parameter "m" is a discount rate or handicap factor. It implies that the enclosed space is a wellmixed region in which the effective ventilation rate is a fraction m times the actual volumetric flow rate. Conversely, the reciprocal of m could be called a "safety factor," i.e. the actual flow rate is equal to the well-mixed value times the safety factor.

Table 5.1Mixing factors (m) for various enclosed spaces.

enclosed space	m
perforated ceiling	1/2
trunk system with anemostats	1/3
trunk system with diffusers	1/4
natural draft and ceiling exhaust fans	1/6
infiltration and natural draft	1/10

The difficulty in selecting the proper value of "m" can be seen in Figure 5.10 taken from Ishizu (1980). Six cigarettes were allowed to smolder in the center of a room of volume 70. m<sup>3</sup>. Ventilation consisted of 32. m<sup>3</sup>/min of ambient air and 8.0 m<sup>3</sup>/min of cleaned recirculated air. No information was given on the location of the inlet and outlet ducts. The concentration of smoke was measured in the center of the room before, during, and after the cigarettes were burned. During the burning phase, a steady-state concentration was not reached even though the well-mixed model predicted adequate time for one to occur. Figure 5.10 shows the sensitivity of the calculations of concentration on the choice of m. The maximum concentration exceeded the steady-state, well-mixed value (m = 1.0 in Figure 5.10) by a factor of about two, clearly indicating non-uniform conditions

within the enclosed space. During the smoldering period,  $m \approx 0.4$ , but after extinction, a single value of m could not explain the data; m appears to decrease with time from around 0.4 to less than 0.3.

Uniform mixing is synonymous with the well-mixed model. It is not possible to insert a constant, scalar multiplier into the equations for the well-mixed model and expect to acquire equations appropriate for non-uniform concentrations. There are several fundamental flaws in the concept of mixing factor:

- The principles of science governing the motion of air and contaminants do not justify the use of a scalar multiplier m.
- Experimental values of m are unique to the volumetric flow rates, geometry of the enclosed space, location of inlet and outlet duct openings, and location of the point where the contaminant is measured.
- The value of m cannot be predicted with any precision. Once it is found experimentally for a particular enclosure, it can't be generalized for other enclosed spaces.
- The range of values used for m is so large as to make it an ineffective parameter for design and economic analysis.

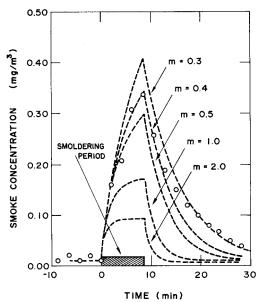


Figure 5.10 Comparison of measured smoke concentrations (circles) in a ventilated room (V = 71.  $m^3$ ) with analytical predictions (dashed lines) for different mixing factors (m); Q = 32.  $m^3$ /min (redrawn from Ishizu, 1980).

In the final analysis, modifying an equation based on the well-mixed model to account for non-uniform concentrations is a contradiction in terms. Either the concentration is uniform in space or it is not; and if it is not, no amount of fudging can yield meaningful answers. Nevertheless, arcane practices that have been used for a considerable time have a sizable following and are not going to be changed simply because they are illogical. The well-mixed model implies something concrete, i.e. c(x,y,z,t) = c(t). Non-uniform mixing and the concept of mixing factor mean that the equality does not hold, but the concept does not predict how, where, or in what way the concentration varies. The present authors recommend that the use of mixing factors be abandoned.

#### 5.8 Well-Mixed Model as an Experimental Tool

While general ventilation is of narrow and limited use to control contaminants in the workplace, the well-mixed model is ideally suited as a laboratory technique to measure the following (Whitby et al., 1983; Donovan et al., 1987):

- wall-loss coefficient (k<sub>w</sub>)
- contaminant emission rate, i.e. source strength (S)
- efficiency of room air cleaners (η<sub>room</sub>), defined as the contaminant mass removal rate divided by the contaminant mass flow rate entering the cleaner

Consider the test apparatus shown schematically in Figure 5.5. Air inside the chamber is sampled at rate  $Q_{s}$ , and the concentration (c) of the contaminant (particle or gas) is measured by a suitable analyzer. Fresh air at the same volumetric flow rate ( $Q_s$ ) is added to the chamber after passing through an "absolute filter" ( $\eta_m = 100\%$ ) or adsorber, etc. that removes all but a negligible amount of contaminant. Inside the chamber there is an internal room air-cleaning device with its own value of efficiency ( $\eta_{cleaner}$ ). It is assumed that no contaminant enters the chamber except via the source (S) in the room. It is also assumed that there is no extraneous air entering or leaving the chamber, i.e. air infiltration or exfiltration. Inside the chamber a mixing fan ensures well-mixed conditions. The mass concentration inside the chamber (c) satisfies the following conservation of mass equation:

$$V\frac{dc}{dt} = S - \left(A_s k_w + Q_s + \eta_{cleaner} Q_{cleaner}\right)c$$
(5-40)

The known, easily measurable quantities are chamber volume (V), elapsed time (t), internal surface area (A<sub>s</sub>), volumetric flow rate through the sampling instrument (Q<sub>s</sub>), and volumetric flow rate through the room air cleaner (Q<sub>cleaner</sub>). The remaining quantities in Eq. (5-40), i.e. wall-loss coefficient (k<sub>w</sub>), source strength (S), and efficiency of the room air-cleaning device ( $\eta_{cleaner}$ ) are to be obtained through the analysis discussed here. It is assumed that only the concentration varies with time, c = c(t); all the other parameters above have constant (but perhaps unknown) values.

### 5.8.1 Wall-Loss Coefficient

To use the test chamber to measure source characteristics or room air cleaner performance, the wall-loss coefficient ( $k_w$ ) must be known for each contaminant to be studied. Alternatively the researcher's explicit goal may be to study the adsorption characteristics of wall hangings, furniture, etc. Clean air is allowed to enter the chamber at a volumetric flow rate equal to the sampling rate  $Q_s$ . To measure  $k_w$ , the air-cleaning device is shut off ( $Q_{cleaner} = 0$ ) and the source is allowed to fill the chamber with contaminant. Once a satisfactory concentration is achieved (which need not be the steady-state value), the source is shut off (S = 0), and the decreasing contaminant concentration is measured over a period of time. Under these conditions Eq. (5-40) becomes

$$\frac{1}{c}\frac{dc}{dt} = \frac{d(\ln c)}{dt} = -\left[\frac{A_{s}k_{w} + Q_{s}}{V}\right]$$
(5-41)

Assuming the sampling rate  $(Q_s)$  is known and is constant, the slope of  $(\ln c)$  versus time enables one to determine the wall-loss coefficient  $(k_w)$ . Consider formaldehyde emissions from building materials and home products such as:

- urea-formaldehyde foam insulation
- fiberglass, sealants, and adhesives
- gypsum wallboard and pressed wood products, such as wood paneling and particle board
- carpeting, wall coverings, and upholstery

The net emission of formaldehyde depends on formaldehyde emitted by the material minus wall losses due to adsorption. Unfortunately adsorption depends on the temperature and the concentration of formaldehyde in the material (called *bulk concentration*,  $c_{bulk}$ ), the concentration of formaldehyde in air, temperature (T), and relative humidity ( $\Phi$ ) of the air.

Rather than deal with a separate source strength and wall loss, some researchers (Hawthorne and Matthews, 1987; Matthews et al., 1987; Tichenor and Mason, 1988) suggest using a *net source strength* (S'), defined as

$$S' = k_0(T, \Phi) [r_1(t) \cdot r_2(T) \cdot r_3(\Phi)] (c_{bulk} - c)$$
(5-42)

where  $k_0(T,\Phi)$  is the air transport property that reflects dependence on temperature and humidity. Hawthorne and Matthews (1987) suggest that the term can be expressed as

$$k_{0}(T,\Phi) = k_{0}(T_{0},\Phi_{0}) \Big[ 1 - a_{1} (T - T_{0}) \Big] \Big[ 1 - a_{2} (\Phi - \Phi_{0}) \Big]$$
(5-43)

where  $a_1$  and  $a_2$  are model constants unique to the application. The functions  $r_1$ ,  $r_2$ , and  $r_3$  are functional relationships that account for the fact that the rate of formaldehyde emission depends on the age of the material, the temperature, and the relative humidity respectively:

<u>age dependence:</u>

$$\mathbf{r}_{1}(t) = \exp\left[-\frac{t-t_{0}}{t'}\right]$$
(5-44)

where  $(t - t_0)$  is the age of the material since measurement of the emission rate, and t' is a characteristic time of the order of 1 to 5 years.

temperature dependence:

$$\mathbf{r}_{2}(\mathbf{T}) = \exp\left[-\mathbf{B}\left(\frac{1}{\mathbf{T}} - \frac{1}{\mathbf{T}_{0}}\right)\right]$$
(5-45)

where B is a coefficient to be determined and T<sub>0</sub> is a reference temperature.

- relative humidity dependence:

$$\mathbf{r}_{3}(\Phi) = \left(\frac{\Phi}{\Phi_{0}}\right)^{a_{3}}$$
(5-46)

where the exponent  $a_3$  in is a coefficient to be determined, and  $\Phi_0$  is a reference value.

Before one can use the above expressions, the model constants  $(a_1, a_2, a_3, and B)$  and reference values  $(k_0, T_0, \Phi_0, and t_0)$  have to be determined from data obtained either from the literature or from experiment. Silberstein et al. (1988) suggest alternative equations that include relative humidity, age, and temperature. But like the above equations, they also include a number of parameters and reference states that have to be determined experimentally. Kelly et al. (1999) describe the initial emission rate of formaldehyde (HCOH) from 55 diverse common-place materials and consumer products. The authors report experimental data for products in which HCOH is contained in a dry product, and products in which HCOH is applied to a surface as a wet coating.

#### 5.8.2 Source Strength

The well-mixed model in Figure 5.5 can also be used to determine the *source emission rate*, i.e. the source strength (S) (Matthews, Hawthorne, and Thompson,1987). The experiment is begun by running the air-cleaning device over a long period of time without the source (S = 0). When a steady minimum concentration is obtained, the air cleaner is turned off ( $Q_{cleaner} = 0$ ), the source is turned on, and the rising concentration is measured and recorded. The mass conservation equation, Eq. (5-40) becomes

$$V\frac{dc}{dt} = S - (A_s k_w + Q_s)c$$
(5-47)

Immediately after the source is activated, and while the concentration (c) is still small, the second term on the right-hand side is small with respect to S. Thus, initially

$$S \approx V \frac{dc}{dt}$$
 (5-48)

and the initial source strength can be found from the slope of concentration versus time. Obtaining S by Eq. (5-48) is inherently inaccurate owing to the difficulty of computing a derivative from a few concentration values obtained over a short period of time. If the concentration rises slowly, the accuracy improves. There are two other ways to measure a constant value of S: (a) S can be calculated from measured values of concentration obtained over a period of time. Specifically, S can be found by integrating Eq. (5-47) between elapsed times  $t_1$  and  $t_2$ , which yields

$$S = \frac{(A_{s}k_{w} + Q_{s})\left\{c_{2} - c_{1}\exp\left[-\frac{(A_{s}k_{w} + Q_{s})(t_{2} - t_{1})}{V}\right]\right\}}{1 - \exp\left[-\frac{(A_{s}k_{w} + Q_{s})(t_{2} - t_{1})}{V}\right]}$$
(5-49)

where  $c_1$  and  $c_2$  are the concentrations at times  $t_1$  and  $t_2$ , respectively. (b) One can wait until equilibrium (steady-state) conditions occur, so that the left-hand side of Eq. **Error! Reference source not found.** is zero and  $c = c_{ss}$ . Under these conditions the constant source strength and steady-state concentration  $c_{ss}$  are related by

$$\mathbf{S} = \left(\mathbf{A}_{s}\mathbf{k}_{w} + \mathbf{Q}_{s}\right)\mathbf{c}_{ss} \tag{5-50}$$

If steady state is achieved in a reasonable time, Eq. **Error! Reference source not found.** should be used, since it represents the most accurate (and simplest) solution. If achievement of steady-state conditions requires a large amount of time, Eq. (5-49) can be used instead. The reader can verify that as  $t_2 - t_1$  gets very large, and c approaches  $c_{ss}$ , the exponential terms in Eq. (5-49) become negligible, and Eq. (5-49) reduces to Eq. (5-50).

If the source strength S is not constant, Eq. (5-47) cannot be integrated in closed form. The instantaneous value of S(t) at some instant (t) can instead be found from a graph of mass concentration (c) versus time (t). From Eq. (5-47),

$$S(t) = V \frac{dc}{dt} + c \left( A_s k_w + Q_s \right)$$
(5-51)

where dc/dt is the slope of c(t) at the instant of time t. Since it is inherently difficult to measure slopes from experimental data, Eq. (5-51) may not yield highly accurate values of S(t).

## Example 5.9 - "New Car Smell": Emission Rate of a Hydrocarbon in a New Automobile

*Given*: Most people enjoy the "new car smell" produced by hydrocarbon emissions from the interior coverings inside a new car. An automobile manufacturer is concerned about how long the odor lasts, and needs to measure the decaying source strength, S(t), of a particular hydrocarbon inside the car. The interior volume of the car is  $V = 4.0 \text{ m}^3$ . An experiment is run in which the car is sealed tight, but a small amount of fresh air is added to its interior ( $Q_s = 200 \text{ cm}^3/\text{hr}$ ,  $c_a = 0$ ), and the same volumetric flow rate of air from inside the automobile is withdrawn. A small circulating fan is placed inside the automobile interior to ensure well-mixed conditions. The air in the car is purged just prior to the experiment so that the initial hydrocarbon concentration is small. The concentration is then measured and recorded twice per month for nine months. Shown below is the instantaneous hydrocarbon mass concentration (in units of mg/m<sup>3</sup>) as a function of elapsed time (in months).

time (mo)	c(mg/m <sup>3</sup> )	time (mo)	c(mg/m <sup>3</sup> )	time (mo)	c(mg/m <sup>3</sup> )
0	20.	3.5	96.	6.5	15.
0.5	238	4.0	80.	7.0	11.
1.0	235	4.5	61.	7.5	8.
1.5	215	5.0	42.	8.0	6.
2.0	162	5.5	31.	8.5	4.
2.5	135	6.0	21.	9.0	3.
3.0	108				

Adsorption of hydrocarbon vapors on interior coverings in the automobile is negligible, i.e.  $k_w = 0$ .

To do: From these data compute and plot the instantaneous source strength, S(t), over the elapsed time.

**Solution**: The authors used Mathcad (the file is available on the book's web site) to generate a cubic spline fit of c(t) from the empirical data, and to differentiate c(t) to obtain dc/dt. The source strength S(t) can then be found from Eq. (5-51), which simplifies to

$$S(t) = V \frac{dc}{dt} + Q_s c$$

Figures E5.9a and b show hydrocarbon mass concentration and source strength as functions of time.

**Discussion**: The computed source strength decreases as expected when hydrocarbons desorb from a surface; it decays to zero, but the curve is not smooth. The reason for this is inaccuracies in the measurement of concentration that become magnified when taking derivatives of experimental data. Smoother data can be generated by using a least-squares polynomial fit rather than a cubic spline fit.

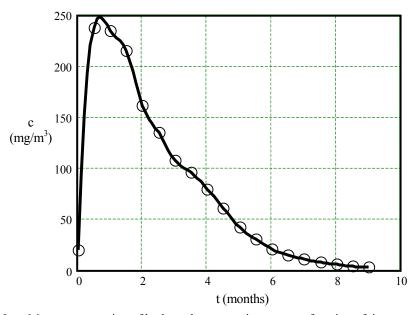


Figure E5.9a Mass concentration of hydrocarbon vapor in a car as a function of time.

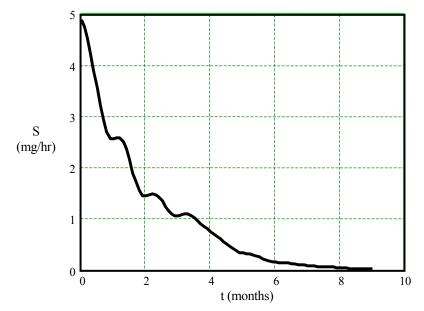


Figure E5.9b Source strength of hydrocarbon vapor in a car as a function of time.

### 5.8.3 Efficiency of an Air Cleaning Device

To find the efficiency ( $\eta_{cleaner}$ ) of a room air-cleaning device, the source and cleaning device are run at steady rates for a long period of time until a steady-state concentration ( $c_{ss}$ ) is obtained. Under these conditions Eq. (5-40) reduces to

$$\eta_{\text{cleaner}} = \frac{\frac{S}{c_{\text{ss}}} - Q_{\text{s}} - A_{\text{s}}k_{\text{w}}}{Q_{\text{cleaner}}}$$
(5-52)

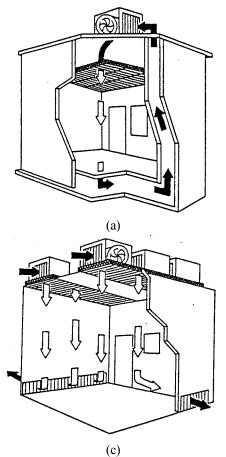
Alternatively, the source is allowed to produce a significant concentration (although not necessarily its steady-state value), the source is then removed or turned off (S = 0), and the air-cleaning device is turned on. The concentration begins to fall and the efficiency can be obtained from

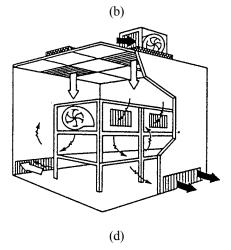
$$\eta_{\text{cleaner}} = \frac{-V \frac{d(\ln c)}{dt} - Q_s - A_s k_w}{Q_{\text{cleaner}}}$$
(5-53)

As discussed previously, if enough time is available for steady-state conditions to be reached, the method leading to Eq. (5-52) is recommended because it yields more accurate results. The time derivative term in Eq. (5-53) is inherently inaccurate.

### 5.9 Clean Rooms

*Clean rooms* (see Figure 1.17 and Figure 5.11) are enclosed spaces in which individuals work and in which the following atmospheric properties are controlled within stringent limits: temperature, humidity, concentration of particles, and concentration of contaminant gases and vapors. Fredrickson (1993) discusses the design criteria for clean rooms. The geometry and operation of clean rooms vary, but all are designed to provide an environment that protects a manufactured product from contamination. Unfortunately many materials used in clean rooms are toxic. In the manufacture of semiconductors, the principal concern is to remove small airborne particles that can short-circuit the minute integrated circuits on silicon wafers. Often overlooked however, are emissions of vapors of corrosive, reactive, and toxic materials used to fabricate the wafers. The amount of these materials is





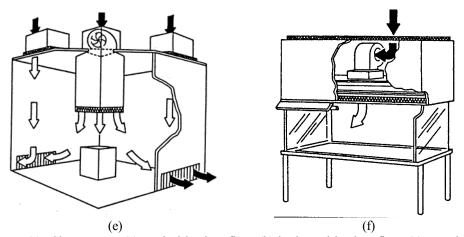


Figure 5.11 Clean rooms: (a) vertical laminar-flow, (b) horizontal laminar-flow, (c) tunnel laminar-flow, (d) tabletop tunnel laminar-flow, (e) island laminar-flow, and (f) unitary work station (miniature) (from Canon Communications, 1987).

small, but handling them can produce spills, splash, and airborne emissions. The fabrication process begins by applying photoresist to the wafer. *Photoresist* is an ultraviolet-sensitive, polymeric material mixed in a solvent carrier. Following curing in ovens, the wafer is exposed to ultraviolet light and placed in an alkaline developer. The exposed resist dissolves in the developer leaving the open surface for subsequent processing. A wet etching process using bases or corrosive acids such as hydrofluoric acid may be employed to remove unwanted material. Alternatively a *dry etching* process involving an RF plasma can remove unwanted material, but in so doing a variety of gaseous compounds may be formed that must be controlled. Thin films of material such as silicon nitride, silicon dioxide, etc. are then deposited on the wafer by liquid and gaseous processes involving silane, tetraethylorthosilicate, phosphine, diborane, ammonia, etc. Next, highly toxic or reactive materials called *dopants* (arsenic, phosphorous, arsine, phosphine, or boron trifluoride), which have unique electrical properties, are imbedded into the surface of the silicon wafer. Liquid solutions of dopants pass into high temperature furnaces by bubblers using inert gases whereupon the dopant atoms diffuse to the silicon surface. Because of the acute toxicity of dopant materials, safety procedures must be strictly adhered to, and sophisticated controls must be used. Layers of noble or common metals such as gold, aluminum, titanium, tantalum, or tungsten are next deposited as thin films by evaporative or sputtering processes. In between all steps in the process, wafers are cleaned by a variety of solvents such as carbon tetrachloride, methylene chloride, and trichloroethylene, which have long-term toxicity.

Clean rooms should not be confused with *laboratory fume hoods* (Figure 1.19), *biological cabinets*, or *glove-boxes*. The objective of clean rooms is to protect a product that is being manufactured, as distinct from protecting the worker. Standards for the purity of air in clean rooms are considerably more stringent than those to ensure the health and safety of workers. Air entering clean rooms is cleaned and conditioned continuously. Well-mixed conditions are achieved because of the unique ways air enters and leaves the clean room rather than because there is a vigorous mixing mechanism within the room.

The cleanliness of a clean room is classified by Federal Standard 209E according to its *class*, which is based on particle number concentration ( $c_{number}$ ). Specifically, *class limits* are based on the total number of particles 0.5 µm and larger permitted per cubic foot of air. For example,  $c_{number}$  for a class 10 clean room cannot exceed 10 particles/ft<sup>3</sup>. Other particle diameters can alternatively be used to determine the class of a clean room, as listed in Table 5.2. SI (metric) classes have also been defined based instead on the *exponent* of the total number of 0.5 µm or larger particles permitted per cubic

*meter* of air. For example,  $c_{number}$  for a class M2 clean room cannot exceed  $10^2 = 100$  particles/m<sup>3</sup>. Intermediate SI classes have also been defined to correspond to the older English classifications. For example, SI class M2.5 has been designated as the equivalent to class 10, even though more precise unit conversion would yield class M2.548. Similarly, class M3.5 is the same as class 100, etc. The data of Table 5.2 are plotted in Figure 5.12. Since the slope for each class is the same on a log-log plot of  $c_{number}$  versus  $D_{p_2}$  extrapolation to other particle sizes is also possible.

Workers in clean rooms are clothed in garments designed to prevent particles from being emitted into the room from clothing and the body. The humidity is set to values appropriate for the product being manufactured and equipment being used. The temperature is normally set at 68 °F. Floor, ceiling, and wall surfaces are designed so as not to generate particles. In addition, floor coverings and garments are designed so as not to generate static electricity.

As requirements for high performance filters have become more demanding, new international classifications have been developed. Two main classifications are the following (ASHRAE HVAC Applications Handbook, 1999):

- (a) A *high efficiency particulate air* (*HEPA*) *filter* is defined as a filter with an efficiency in excess of 99.97% for 0.3 μm particles
- (b) An *ultra low penetration air (ULPA) filter* is defined as a filter with a minimum efficiency of 99.999% for 0.12 μm particles

clas	class name D <sub>p</sub> ≥0.1 µm		$D_p \ge 0.2 \ \mu m$		$D_p \ge 0.5 \ \mu m$		$D_p \ge 5 \mu m$		
SI	English	$\#/m^3$	#/ft <sup>3</sup>	#/m <sup>3</sup>	#/ft <sup>3</sup>	#/m <sup>3</sup>	#/ft <sup>3</sup>	#/m <sup>3</sup>	#/ft <sup>3</sup>
M1		350	9.9	75.0	2.14	10 <sup>1</sup>	0.283	-	-
M1.5	1	1240	35	265	7.5	35.3	1	-	-
M2		3500	99.1	757	21.4	10 <sup>2</sup>	2.83	-	-
M2.5	10	12400	350	2650	75.0	353	10	-	-
M3		35000	991	7570	214	10 <sup>3</sup>	28.3	-	-
M3.5	100	-	-	26500	750	3530	100	-	-
M4		-	-	75700	2140	<b>10<sup>4</sup></b>	283	-	-
M4.5	1000	-	-	-	-	35300	1000	247	7.00
M5		-	-	-	-	10 <sup>5</sup>	2830	618	17.5
M5.5	10000	-	-	_	-	353000	10000	2470	70.0
M6		-	-	-	-	10 <sup>6</sup>	28300	6180	175
M6.5	100000	-	-	-	-	3530000	100000	24700	700
M7		-	-	-	-	<b>10</b> <sup>7</sup>	283000	61800	1750

Table 5.2	Clean room class limits; maximum permissible c <sub>number</sub> in English and SI units; bold
	c <sub>number</sub> indicates number concentration on which the corresponding <b>bold</b> class name is
	based (abstracted from ASHRAE HVAC Applications Handbook, 1999.)

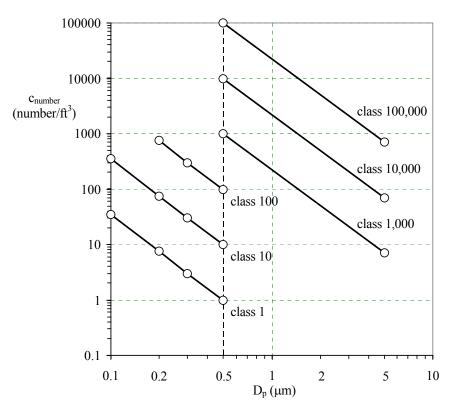


Figure 5.12 Class definitions for clean rooms in the US; class based on cubic feet – conversion: 1.00 particles/ $ft^3 = 35.3$  particles/ $m^3$ .

The efficiencies of HEPA and ULPA filters are based on 0.3 and 0.12 µm particles, respectively, because the *most penetrating particle size* (MPPS) of fibrous filters is typically between these two values. MPPS is discussed in more detail in Chapter 9. In vertical laminar flow clean rooms (Figure 5.11a), the entire ceiling is a high efficiency (HEPA or ULPA) filter and the floor is the receiving plenum. Typical air velocities entering a vertical laminar flow clean room are 60-100 FPM (ft/min). Temperature and humidity control are achieved by a separate air handling system. Class 100 conditions can be achieved by such designs. The performance of laminar-air flow rooms is hampered by wake regions downstream of equipment and personnel. Such wakes are recirculation regions that tend to accumulate airborne particles and prevent their removal.

It must be emphasized that while air may enter a laminar-flow room in a laminar fashion, the existence of wakes and recirculation regions produces limited degrees of turbulence that are unavoidable. In addition, Reynolds numbers for the rooms themselves or the obstacles around which the air passes can be considerably large (several thousand), and thus the assumption of laminar flow may be incorrect.

# **Example 5.10 - Time to Achieve Clean Room Conditions**

*Given*: Consider a vertical laminar-flow clean room similar to Figure 5.11, and assume that its schematic diagram is given by Figure E5.7. The clean room will be operated using existing equipment with the following specifications:

- $\eta_1 = 98.\%, \eta_2 = 98.\%$  (air cleaner efficiencies)
- f = 0.050 (fresh make-up air fraction)

- $c_a = 10^3$  particles/m<sup>3</sup> (particle concentration in the ambient make-up air)
- $D_p = 1.0 \,\mu m$  (particle size of concern)
- $Q_s = 20. \text{ m}^3/\text{min}$  (supply ventilation rate into the clean room)
- S = 300 particles/min (particle emission rate within the clean room)
- $V = 300 \text{ m}^3$  (volume of the clean room)
- $A_s = 320 \text{ m}^2$  (total surface area of the clean room)
- $k_w = 0.030$  m/min (wall loss coefficient)
- $c(0) = 10^5$  particles/m<sup>3</sup> (initial particle concentration within the clean room)

The goals of management are to achieve a class 1 clean room.

*To do*: Advise the company if a class 1 clean room can be achieved. Estimate how long it will take to achieve class 10,000, class 1,000, class 100, class 10, and class 1 conditions.

*Solution*: Using Figure 5.12, maximum permissible particle concentration at  $D_p = 1.0 \mu m$  can be tabulated as a function of class. Note that for classes 1, 10, and 100, extrapolation is required:

class	$c_{max}$ (particles/ft <sup>3</sup> ) for $D_p = 1.0 \ \mu m$	$c_{max}$ (particles/m <sup>3</sup> ) for $D_p = 1.0 \ \mu m$
10,000	2,100	74,000
1,000	210	7,400
100	21.	740
10	2.1	74.
1	0.21	7.4

Conservation of mass for the particles in Figure E5.7 can be written in standard form, as in Eq. (5-7):

$$\frac{\mathrm{dc}}{\mathrm{dt}} = \mathrm{B} - \mathrm{Ac}$$

where

$$A = \frac{Q_{s} + k_{w}A_{s} + Q_{s}(1-f)(1-\eta_{1})}{V} \qquad B = \frac{S + Q_{s}c_{a}f(1-\eta_{2})}{V}$$

The solution of the differential equation is given by Eq. (5-10), with steady-state concentration ( $c_{ss}$ ) given by Eq. (5-11). For the conditions given above,

$$A = 0.0999 \frac{1}{\min} \qquad B = 1.07 \frac{\text{particles}}{\min \cdot \text{m}^3}$$

The steady-state particle concentration within the room will thus be

$$c_{ss} = \frac{B}{A} = \frac{1.07 \frac{\text{particles}}{\text{min} \cdot \text{m}^3}}{0.0999 \frac{1}{\text{min}}} = 10.7 \frac{\text{particles}}{\text{m}^3}$$

Thus, the minimum possible particle concentration is about 11. particles/m<sup>3</sup>, where two significant digits of precision is the most that can be expected from these calculations. Therefore, the company can achieve a class 10 clean room, which allows a maximum of 74. particles/m<sup>3</sup>, but cannot achieve a class 1 clean room with the existing equipment, although it can come close. Any increase in the particle emission rate (S) or reduction in the volumetric flow rate (Q<sub>s</sub>) will worsen the situation.

If the initial particle concentration, c(0), is  $10^5$  particles/m<sup>3</sup>, Eq. (5-12) can be used to calculate the time to achieve the various classes of clean rooms:

class	time (min)
10,000	3.0
1000	26.
100	49.
10	74.
1	$\infty$

**Discussion**: The only way to achieve a class 1 clean room with the existing equipment is to operate the manufacturing process in **batch process** mode, i.e. intermittently (operate for some time period, during which the particle concentration in the room rises to nearly the class 1 limit of 7.4 particles/m<sup>3</sup>, and then shut down the process (S = 0) for a while to allow the concentration to drop.) Alternatively, minor improvements to one or more of the components may be just enough to achieve a class 1 clean room, e.g. if  $\eta_2$  can be increased from 98.% to 99.%.

#### 5.10 Infiltration and Exfiltration

The transfer of air into and out of an enclosed space is equal to deliberate input and removal of air (forced ventilation) plus uncontrolled air leakage through cracks, holes, etc. Uncontrolled flow of air into a building is called *infiltration*, and uncontrolled removal of air is called *exfiltration* (Perera et al., 1986). Infiltration and exfiltration are produced primarily by pressure differences between the building interior and the atmosphere resulting from the aerodynamic flow of air around and over the building. To a lesser extent they are also due to temperature differences between the building interior and the atmosphere, and to diffusion processes. To a first approximation one may assume that the volumetric flow rates of infiltration and exfiltration are equal. The relative air leakage of a typical building is distributed as in Table 5.3. Infiltration can be expressed in three ways:

- empirical estimates of air changes per hour
- equations based on construction details
- empirical equations

source of leakage	relative leakage (%)
walls (top and bottom joints, plumbing and electrical penetrations)	18 to 50, avg. 35
ceiling	3 to 30, avg. 18
heating system	3 to 28, avg. 18
windows and doors	6 to 22, avg. 15
fireplaces	0 to 30, avg. 12
vents in conditioned spaces	2 to 12, avg. 5
diffusion (conduction) through walls	<1

Table 5.3	Sources of air l	eakage in a	typical building	(from ASHRAE, 1997).

Table 5.4	Infiltration and exfiltration; air changes per hour occurring under average conditions in
	residences exclusive of air provided for ventilation (abstracted from ASHRAE, 1981).

room description	single glass, no weather-stripping	storm sash or weather stripping
no windows or exterior doors	0.5	0.3
windows or exterior doors on one side	1.0	0.7
windows or exterior doors on two sides	1.5	1.0
windows or exterior doors on three sides	2.0	1.3
entrance halls	2.0	1.3

Table 5.4 is a condensation of ASHRAE's 1981 estimates of infiltration of air into a room in terms of number of air changes per hour for average buildings under average conditions. In the newer editions of the ASHRAE Fundamentals Handbook (e.g. ASHRAE, 2001), infiltration is estimated as a function of building construction details such as wall, ceiling, and floor construction, window and door specifications, etc., along with even finer details such as number of recessed ceiling lights, electrical outlets, etc. Each component source of infiltration is assigned an *effective leakage area*,  $A_L$  (typically in units of cm<sup>2</sup>); these components can be summed to obtain the total effective air leakage area of the building. Infiltration volumetric flow rate (Q<sub>infiltration</sub>) is then calculated according to

$$Q_{\text{infiltration}} = A_{\text{L}} \sqrt{C_{\text{s}} \Delta T + C_{\text{w}} V^2}$$
(5-3)

where the symbols and their typical units are:

- $Q_{infiltration}$  = infiltration volumetric flow rate (L/s)
- $A_L$  = total building effective leakage area (cm<sup>2</sup>)

- Cs Cw = stack coefficient ( $L^2$ cm<sup>-4</sup>s<sup>-2</sup>K<sup>-1</sup>); varies with number of stories
- = wind coefficient ( $L^2$ cm<sup>-4</sup>m<sup>-2</sup>); varies with number of stories and amount of shielding (trees, shrubbery, sheds, other buildings, etc.)
- $\Delta T$ = average absolute value of indoor-outdoor temperature difference (K or  $^{\circ}$ C)
- V = average wind speed (m/s) \_

Tables for calculating these parameters, along with examples, are provided in the ASHRAE Fundamentals Handbook (ASHRAE, 2001), and are too lengthy to duplicate here. A typical modern two-story single-family home, for example, has a total volume of 340. m<sup>3</sup>, with a total effective air leakage area of about 500 cm<sup>2</sup>. Consider the following winter design conditions for Lincoln, Nebraska: wind speed = 6.7 m/s,  $\Delta T = 39$ . °C,  $C_s = 0.000290 \text{ L}^2 \text{cm}^{-4} \text{s}^{-2} \text{K}^{-1}$ , and  $C_w =$  $0.000231L^{2}cm^{-4}m^{-2}$ . Equation (5-54) yields

$$Q_{\text{infiltration}} = (500 \text{ cm}^2) \sqrt{0.000290 \frac{L^2}{s^2 \text{ cm}^4 \text{K}} (39. \text{ K}) + 0.000231 \frac{L^2}{\text{ cm}^4 \text{m}^4} (6.7 \frac{\text{m}}{\text{s}})^2} = 73.6 \frac{L}{\text{s}}$$

Eq. (5-14) can be used to convert the infiltration rate to number of air changes per hour (N),

N = 
$$\frac{Q}{V} = \frac{73.6 \frac{L}{s}}{340. m^3} \left(\frac{m^3}{1000 L}\right) \left(\frac{3600 s^2}{hr}\right) = 0.78 \frac{1}{hr}$$

Building infiltration rates have improved (decreased) significantly over the past several decades, prompted largely by the increasing cost of energy. The infiltration rate calculated above for a typical modern home is less than one air change per hour, even in severe winter design conditions. It would be even lower in less severe weather. While this is good for the family budget, it is not so good in terms of indoor air quality, the spread of airborne contaminants and diseases, etc., as discussed in Chapter 2.

For quick estimates, Wadden and Scheff (1983) report the following empirical equation for the number of air changes per hour (N):

$$N = \frac{Q}{V} = 0.315 + 0.0273U + 0.0105 |T_{outside} - T_{inside}|$$
(5-55)

where the units of N are hr<sup>-1</sup>, U is the wind speed in miles per hour, and T<sub>outside</sub> and T<sub>inside</sub> are the outside and inside temperatures in degrees Fahrenheit. The absolute value signs in Eq. (5-55) ensure a component of N due to any temperature difference between T<sub>outside</sub> and T<sub>inside</sub>, regardless of which temperature is greater.

# Example 5.11 – Did the Professor Suffer Mercury Poisoning?

Given: The sons and daughters of a deceased faculty member have sued his university because they believe their father died from complications related to failure of his central nervous system caused by hazardous airborne concentrations of mercury vapor in his university office. Unknown to everyone at the time, liquid mercury lay under the floor boards of his office. In 1900 the university's chemistry laboratory was built containing a small storeroom for chemical supplies. The room was supported by 8-inch floor joists separating the storeroom from the ceiling of the room one floor below. The floor of the room was constructed of un-joined boards. Over time, narrow spaces developed between the boards. Stored in the room were 5-pound bottles of mercury, mercury thermometers, glass barometers; and U-tube manometers containing mercury used by students in their experiments. From time to time the barometers and manometers broke and mercury was spilled on the floor. Mercury was also spilled by students trying to fill glass manometers. Some of the liquid mercury fell through the spaces between the floor boards, and remained there. No record was ever kept of the mercury that was spilled or swept up afterwards. In 1940, all the mercury was removed from the storeroom and the room was used to store laboratory glassware. In 1945 the storeroom was remodeled into an office for a new faculty

member, and he used the room for the next 35 years until he retired in 1980. When he retired he displayed symptoms indicating failure of his central nervous system. The symptoms became progressively worse and contributed to his death in 1985. A ventilation system, including air conditioning, was installed in 1982, but there are no records about how the office had been ventilated before 1982. Discussions with some of the older employees revealed that there was no forced air ventilation system at all prior to 1982. An exterior window was added to the office sometime in the 1950s after the professor received tenure, but there is some dispute as to the date. In 1991 the building was again remodeled. The old floor was removed, and approximately 40. kg of liquid mercury was found lying at the bottom of the dead-air space beneath the floor. The clean-up crew reported that the mercury was dispersed in puddles of various sizes, but most of it was in the form of small nearly spherical balls; they estimated the average size of the mercury balls to be around a half centimeter.

Upon hearing of the discovery of mercury, the professor's family filed suit against the university, claiming that his death was caused by exposure to mercury vapor during the 35 years he occupied his office. The university claimed that the failure of his central nervous system was a genetic predisposition, unrelated to mercury. Toxicologists were called to testify about the health issues (see Chapter 2 for a discussion of mercury poisoning), but their testimony depends on information about the concentration of mercury vapor in the office during the period between 1945 and 1980. Since no mercury vapor concentration measurements were ever made, you have been called as an expert witness on indoor air quality.

To do: Prepare three analyses:

- <u>Analysis 1 Compute the maximum possible mercury vapor concentration</u>: Estimate the maximum airborne concentration of mercury vapor that could possibly occur in the office, and determine if the concentration exceeds safe levels.
- 2. <u>Analysis 2 Estimate the amount of mercury in the room between 1945 and 1991</u>: Since liquid mercury was found beneath the floor in 1991, even *more* liquid mercury would have been there in earlier years, since some of it would have evaporated during the period. The evaporation rate must be determined, and the mass of liquid mercury must be extrapolated back in time. As a worst-case scenario, assume the maximum possible evaporation rate.
- 3. <u>Analysis 3 Estimate realistic mercury vapor concentrations for different ventilation</u> <u>rates for the period 1945-1980</u>: The vapor concentration depends on the evaporation rate, how the room was ventilated, and how much mercury remained below the floor. Estimate the mercury vapor concentration for three types of ventilation:
  - (a) infiltration if the room had no exterior windows (conditions prior to sometime in the 1950s), which gives an upper bound for the vapor concentration
  - (b) infiltration if the room had one exterior window containing single-plane glass without weather stripping (conditions since sometime in the 1950s), which gives a lower bound for the vapor concentration
  - (c) forced ventilation assuming 62-1989 standards of 20 SCFM/person in addition to the infiltration rate of case (a); this condition did not exist until 1982, but is calculated for educational purposes

**Solution**: The room dimensions are measured: floor area  $(A_{floor}) = 20 \text{ m}^2$  (4m by 5m), height (h) = 3.5m, volume (V) = 50 m<sup>3</sup>, and height of the dead-air space under the floor  $(z_2 - z_1) = 8$  inches (0.203 m). Note that V is less than the total room volume because the room was partially filled with furniture, books, etc. The appropriate properties of mercury (Hg) are tabulated:

 $PEL = 0.1 \text{ mg/m}^3 (1.2 \text{ x } 10^{-2} \text{ PPM})$   $P_{v,Hg} = vapor \text{ pressure at } 300 \text{ K} = 0.0012 \text{ mm Hg}$ 

 $\rho_{Hg}$  = liquid density = 13,530 kg/m<sup>3</sup> M<sub>Hg</sub> = molecular weight = 200.6 kg/kmol

<u>Analysis 1</u> – As an *upper limit* of mercury concentration, consider the room to be totally isolated, receiving *no* fresh air ventilation whatsoever. The evaporation of mercury is a slow process, so one can assume there is sufficient time to achieve well-mixed conditions in the room. Mercury evaporates until its partial pressure is equal to its vapor pressure, whereupon evaporation ceases. Under these conditions, the steady-state mercury vapor mol fraction is given by Eq. (5-4),

$$y_{ss} = \frac{P_{v,Hg}}{P} = \frac{0.0012 \text{ mm Hg}}{760. \text{ mm Hg}} = 1.579 \times 10^{-6} \approx 1.6 \text{ PPM}$$

The concentration of mercury vapor corresponding to this mol fraction can be obtained from Eq. (1-30),

$$c = \frac{[PPM]M_{Hg}}{24.5} \left(\frac{mg}{m^3}\right) = \frac{(1.6)(200.6)}{24.5} \frac{mg}{m^3} = 13.\frac{mg}{m^3}$$

which is well in excess of the PEL. Since the office was *not* totally sealed off, the actual concentrations would have been much lower than this; therefore, further analysis is warranted. (Note that if this upper limit turned out to be less than the PEL, no further analysis would be necessary – it is unlikely that the university would be liable.)

<u>Analysis 2</u> – The air in the space under the floor boards is stagnant; the discussion in Chapter 4 about evaporation in stagnant air is therefore relevant here. It is assumed that evaporation progresses at its maximum possible rate. This occurs when the far-field mercury vapor mol fraction (just above the floor boards) is zero; i.e. following the notation in Chapter 4,  $y_{Hg,2} = 0$ . This is a reasonable approximation if the room was adequately ventilated with fresh air, which is highly unlikely for a storeroom. Nonetheless assuming  $y_{Hg,2} = 0$  yields the maximum evaporation. It is also assumed that the spilled liquid mercury is in the form of spheres approximately 5.0 mm in diameter, uniformly dispersed in the dead space. A differential equation of mass balance for the liquid mercury beneath the floor between 1940 and 1991 can be written:

$$\frac{dm_{\text{liquid Hg}}}{dt} = S_{\text{liquid Hg}} - \dot{m}_{\text{evap Hg}} = S_{\text{liquid Hg}} - A_{\text{drop}} n_{\text{drops}} M_{\text{Hg}} N_{\text{Hg}}$$

where

- t = elapsed time (yr)
- m<sub>liuqid Hg</sub> = mass of accumulated liquid mercury (kg)
- $S_{\text{liquid Hg}}$  = source of liquid mercury into the room due to breakage and spillage = 0 beyond 1940
- $A_{drop}$  = surface area of a 5.0-mm spherical drop of liquid mercury = 7.854 x 10<sup>-5</sup> m<sup>2</sup>
- $\dot{m}_{evap Hg}$  = rate of evaporation of liquid mercury (kg/yr)
- $M_{Hg}$  = molecular weight of mercury = 200.6 kg/kmol
- $n_{drops}$  = number of spherical drops of mercury in the room
- $N_{Hg}$  = molar evaporation rate of liquid mercury into mercury vapor [kmol/(m<sup>2</sup> yr)]

Since the number of drops of liquid mercury is

$$n_{drops} = \frac{m_{liquid Hg}}{m_{drop}}$$

the mass balance can be written as

$$\frac{dm_{\text{liquid Hg}}}{dt} = -\frac{A_{\text{drop}}M_{\text{Hg}}N_{\text{Hg}}}{m_{\text{drop}}}m_{\text{liquid Hg}}$$

where the mass of a 5.0-mm spherical drop of mercury is

$$m_{drop} = \rho_{Hg} \frac{\pi D_{drop}^{3}}{6} = 13530 \frac{kg}{m^{3}} \frac{\pi (0.005 \text{ m})^{3}}{6} = 8.855 \times 10^{-4} \text{ kg}$$

Since the space below the floor boards is quiescent, the molar evaporation rate can be estimated from Eq. (4-57),

$$N_{Hg} = P \frac{D_{Hg,a}}{R_{u}T(z_{2} - z_{1})y_{am}} (y_{Hg,1} - y_{Hg,2})$$

where  $(z_2 - z_1) = 0.203$  m. The diffusion coefficient of mercury in air  $(D_{Hg,a})$  can be estimated from Eq. (4-32),

$$D_{\mathrm{Hg,a}} = D_{\mathrm{water,a}} \sqrt{\frac{\mathrm{M}_{\mathrm{water}}}{\mathrm{M}_{\mathrm{Hg}}}}$$

where  $M_{water}$  is the molecular weight of water (18.0 kg/kmol), and  $D_{water,a}$  is the diffusion coefficient of water in air (2.2 x 10<sup>-5</sup> m<sup>2</sup>/s).

$$D_{\text{Hg,a}} = 2.2 \times 10^{-5} \,\frac{\text{m}^2}{\text{s}} \sqrt{\frac{18.0}{200.6}} \left(\frac{3600 \text{ s}}{\text{hr}}\right) = 2.372 \times 10^{-2} \,\frac{\text{m}^2}{\text{hr}}$$

The maximum evaporation rate occurs when the far-field mercury vapor mol fraction  $(y_{Hg,2})$  is zero, i.e.  $y_{a,2} = 1$ . From Eq. (4-53),

$$y_{am} = \frac{y_{a,2} - y_{a,1}}{\ln\left(\frac{y_{a,2}}{y_{a,1}}\right)} = \frac{1 - (1 - 1.579 \times 10^{-6})}{\ln\left[\frac{1}{(1 - 1.579 \times 10^{-6})}\right]} = 0.9999999 \cong 1$$

The partial pressure of mercury vapor at the interface between liquid mercury and air is equal to the vapor pressure of mercury. Thus, the mol fraction of mercury vapor at the surface of each drop is

$$y_{Hg,1} = y_{Hg,i} = \frac{P_{v,Hg}}{P} = \frac{0.0012 \text{ mm Hg}}{760. \text{ mm Hg}} = 1.579 \times 10^{-6}$$

Thus, the molar evaporation rate is

$$N_{Hg} = (101.3 \text{ kPa}) \frac{2.372 \times 10^{-2} \frac{\text{m}^2}{\text{hr}}}{8.3143 \frac{\text{kJ}}{\text{kmol K}} (300 \text{ K}) (0.203 \text{ m}) (1)} (1.579 \times 10^{-6} - 0) \left(\frac{\text{kJ}}{\text{m}^3 \text{kPa}}\right)$$
$$= 7.49 \times 10^{-9} \frac{\text{kmol}}{\text{m}^2 \text{hr}} \left(\frac{8766 \text{ hr}}{\text{yr}}\right) = 6.57 \times 10^{-5} \frac{\text{kmol}}{\text{m}^2 \text{yr}}$$

After substitution of  $N_{\rm Hg}$  and the other parameters into the mass balance,

$$\frac{dm_{_{liquid Hg}}}{dt} = -\frac{\left(7.854 \times 10^{-5} \ m^2\right) \left(200.6 \frac{kg}{kmol}\right) 6.57 \times 10^{-5} \frac{kmol}{m^2 yr}}{8.855 \times 10^{-4} \ kg} m_{_{liquid Hg}}$$

which reduces to

$$\frac{dm_{\text{liquid Hg}}}{dt} = -1.169 \times 10^{-3} \frac{1}{\text{yr}} m_{\text{liquid Hg}}$$

The above ODE is of the same form as Eq. (5-7), but with mass concentration (c) replaced by mass  $(m_{\text{liquid Hg}})$ ,

$$\frac{\mathrm{d}m_{\mathrm{liquid Hg}}}{\mathrm{d}t} = \mathbf{B} - \mathbf{A}m_{\mathrm{liquid Hg}}$$

with coefficients

$$A = -1.169 \times 10^{-3} \frac{1}{yr}$$
  $B = 0$ 

Thus, the solution is given by an equation similar to Eq. (5-10) with the steady-state mass equal to zero, but with the "initial" mass of liquid mercury set to the mass discovered in 1991, considering time relative to the year 1991. The mass of mercury under the floorboards during the period from 1940 to 1991 is thus

$$m_{\text{liquid Hg}}(t_{\text{years}}) = m_{\text{liquid Hg}}(1991)\exp\left(-A\left(t_{\text{years}}-1991\right)\right)$$

where  $t_{years}$  is the year number (1945, 1946, etc.). Thus in 1945, when the professor moved into the office,

$$m_{\text{liquid Hg}}(1945) = (40. \text{ kg}) \exp\left(-1.169 \times 10^{-3} \frac{1}{\text{yr}}(1945 - 1991)\right) = 42.2 \text{ kg}$$

When he retired in 1980, the mass of liquid mercury remaining below the floorboards was

$$m_{\text{liquid Hg}}(1980) = (40. \text{ kg}) \exp\left(-1.169 \times 10^{-3} \frac{1}{\text{yr}}(1980 - 1991)\right) = 40.5 \text{ kg}$$

Mercury does not evaporate rapidly; even if one assumes the maximum possible evaporation rate, the amount of liquid mercury under the floor was fairly constant during the entire period (35 years) in which the professor occupied his office. It must be kept in mind that several assumptions were made in the above analysis. For example, as the spheres of liquid mercury evaporate, their diameter decreases; this was not taken into account. In addition, the evaporation rate would be somewhat less than its maximum value and less mercury would have therefore existed beneath the floor in 1945. However, since the evaporation rate is so small, these assumptions are reasonable.

<u>Analysis 3</u> – An accurate estimate of the mercury vapor concentration in the professor's office since the year 1945 can be made only if:

- (a) the ventilation rate is known
- (b) account is taken of the fact that the amount of liquid mercury decreases as it evaporates
- (c) the far-field vapor mol fraction  $(y_{Hg,2})$  is not zero, but varies with time; thus the driving potential for evaporation  $(y_{Hg,1} y_{Hg,2})$  is not constant

Each of these points is examined: (a) Unfortunately, the ventilation rate between 1945 and 1980 is *not* known; two possible values, with and without an exterior window, are used in the calculations to determine the upper and lower bounds of vapor concentration respectively. A third ventilation rate is also used to see the effect of forced ventilation, even though it did not exist until 1982. (b) The amount of liquid mercury during the period has already been calculated in Analysis 2 above. (c) An equation needs to be solved describing how the vapor mol fraction varies with time. This is accomplished by writing a mass balance for mercury vapor in the ventilated room,

$$V\frac{dc}{dt} = Qc_a + S - Qc$$

where Q is the ventilation rate, assumed to be constant, c<sub>a</sub> is the mass concentration of mercury vapor in the ambient air, assumed to be zero, and S is the source of mercury vapor, which is equal to the evaporation rate previously calculated,

$$S = \dot{m}_{evap Hg} = \frac{A_{drop}M_{Hg}N_{Hg}}{m_{drop}} m_{liquid Hg}$$

Since the far-field concentration varies slowly (months and years), it is realistic to assume that at any instant the mass concentration, c (mg/m<sup>3</sup>), can be expressed as the quasi-steady-state value given by Eq. (5-11), with coefficients B = S/V and A = Q/V. Thus at any time between 1945 and 1980 (t<sub>years</sub>),

$$c_{ss}(t_{years}) = \frac{\dot{m}_{evap Hg}}{Q} = \frac{A_{drop}M_{Hg}N_{Hg}}{m_{drop}Q}m_{liquid Hg}(t_{years})$$

Converting steady-state mass concentration  $(c_{ss})$  to steady-state mol fraction  $(y_{ss})$ ,

$$y_{ss}(t_{years}) = \frac{R_u T c_{ss}(t_{years})}{M_{Hg} P} = \frac{A_{drop} N_{Hg} R_u T}{m_{drop} Q P} m_{liquid Hg}(t_{years})$$

where  $y_{ss} = y_{Hg,2}$ . Substitution of the equation for  $N_{Hg}$  from Analysis 2 above yields

$$\mathbf{y}_{ss}(\mathbf{t}_{years}) = \frac{\mathbf{A}_{drop}}{\mathbf{m}_{drop}\mathbf{Q}} \frac{D_{Hg,a}}{(\mathbf{z}_2 - \mathbf{z}_1)\mathbf{y}_{am}} (\mathbf{y}_{Hg,1} - \mathbf{y}_{ss}) \mathbf{m}_{liquid Hg}(\mathbf{t}_{years})$$

For simplicity, the mass of liquid mercury under the floorboards ( $m_{liquid Hg}$ ) at any year ( $t_{years}$ ) between 1945 and 1980 is assumed to decrease according to the rate calculated in Analysis 2 above. Simplifying and rearranging the above, and solving for  $y_{ss}$  gives

$$\mathbf{y}_{ss}(\mathbf{t}_{years}) = \frac{\mathbf{C}_{1}(\mathbf{t}_{years})\mathbf{y}_{Hg,1}}{1 + \mathbf{C}_{1}(\mathbf{t}_{years})}$$

where  $C_1(t_{vears})$  is a collection of parameters from the above equation,

$$C_{1}(t_{years}) = \frac{A_{drop}}{m_{drop}Q} \frac{D_{Hg,a}}{(z_{2} - z_{1})y_{am}} m_{liquid Hg}(t_{years})$$

The above equation can be solved for the three different ventilation conditions given in the problem statement. From Table 5.4 and the ASHRAE handbook, the rates are as follows:

- (a) infiltration when there are no exterior windows or doors; number of room air changes N =  $Q/V = 0.50 \text{ hr}^{-1}$ ,  $Q = NV = (0.50 \text{ hr}^{-1}) (50 \text{ m}^3) = 25 \text{ m}^3/\text{hr}$
- (b) infiltration when there is one exterior window containing a single-plane glass and no weather stripping; number or room air changes  $N = Q/V = 1.0 \text{ hr}^{-1}$ ,  $Q = 50 \text{ m}^3/\text{hr}$
- (c) ASHRAE Standard 62-1989 ventilation rate, i.e. Q = 20. SCFM (34. m<sup>3</sup>/hr) in addition to the infiltration rate of case (a) above; total Q = 34. + 25. = 59. m<sup>3</sup>/hr

As a sample calculation, consider the mercury vapor mol fraction in the year 1945, when the professor first moved into his office. For ventilation case (a),

$$C_{1}(1945) = \frac{7.854 \times 10^{-5} \text{ m}^{2}}{8.855 \times 10^{-4} \text{ kg}\left(25.\frac{\text{m}^{3}}{\text{hr}}\right)} \frac{2.372 \times 10^{-2} \frac{\text{m}^{2}}{\text{hr}}}{(0.203 \text{ m})0.9999999} 42.2 \text{ kg} = 1.75 \times 10^{-2} \text{ kg}$$

and

$$y_{ss}(1945) = \frac{1.75 \times 10^{-2} \left(1.579 \times 10^{-6}\right)}{1 + 1.75 \times 10^{-2}} = 2.72 \times 10^{-8} \approx 0.027 \text{ PPM}$$

This value is well above the PEL (0.012 PPM). Similar calculations must be performed for each year and for each of the three ventilation rates. A plot of  $y_{ss}$  (in PPM) versus time (in years) is

shown in Figure E5.11. The authors used Excel to generate this plot; a copy of the Excel spreadsheet is available on the book's web site. The reader is encouraged to experiment with different values of flow rates to see the effect on mercury vapor concentration in the room. Recall that case (a) is an upper limit and case (b) is a lower limit, reflecting conditions of the office without and with an exterior window, respectively. The actual concentration should lie somewhere between these two limits, depending on when the window was added. From the figure,

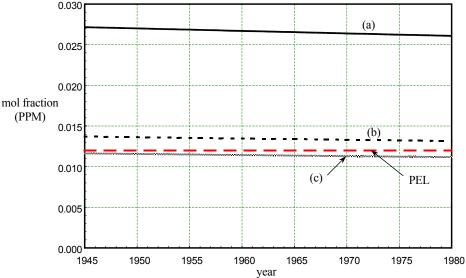


Figure E5.11 Mercury vapor mol fraction in the professor's office versus year since 1945, for three values of ventilation flow rate: (a) 25. m<sup>3</sup>/hr, (b) 50. m<sup>3</sup>/hr, and (c) 59. m<sup>3</sup>/hr.

it is seen that the mercury vapor concentration decreased very slowly between 1945 and 1980, but the concentration was always above the PEL for either ventilation rate (a) or (b). The case with forced room ventilation, case (c), would have reduced the mercury vapor concentration below its PEL, but unfortunately forced ventilation was not added until after the professor retired. In conclusion, the professor was exposed to mercury vapor of hazardous concentration for 35 years. Since mercury is a cumulative toxin that accumulates in the body, it can be concluded that the dose associated with this exposure constitutes a hazardous condition.

**Discussion**: This example illustrates why stringent precautions are taken concerning liquid mercury. Certainly the air in rooms or buildings that formerly contained liquid mercury should be sampled at a variety of points to determine if hazardous mercury vapor concentrations are below the PEL (or whatever other standard is used) before the space is used for human occupancy. The example also illustrates why one's intuition about mercury can be misleading. Since evaporation is very slow, hazardous mercury vapor concentrations persist for a much longer time than most people would suspect. Finally, ventilation conditions (b) existed for the majority of time, and the predicted concentrations are only about 20% higher than the PEL. One may argue that since PELs are rather conservative, the professor may not have been in hazardous conditions after all. Is the university to blame for the professor's illness and death? The final answer to this question is left to the attorneys.