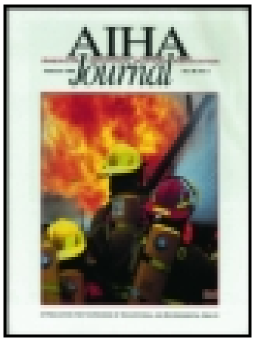

AIHAJ - American Industrial Hygiene Association

ISSN: 1529-8663 (Print) (Online) Journal homepage: https://www.tandfonline.com/loi/uaah20

Modeling Turbulent Diffusion and Advection of Indoor Air Contaminants by Markov Chains

Mark Nicas

Modeling Turbulent Diffusion and Advection of Indoor Air Contaminants by Markov Chains

AUTHOR
Mark Nicas

Center for Occupational and Environmental Health, School of Public Health, University of California, Berkeley, CA 94720

Turbulent eddy diffusion models are used to describe a continuous concentration gradient with distance from an in-room contaminant emission source. A refined diffusion model termed the Drivas model also accounts for contaminant reflection by wall surfaces and partially accounts for removal by exhaust air. This article develops two models based on Markov chains to describe indoor air contaminant dispersion by turbulent diffusion and advection, and removal by the exhaust airflow. Markov model I is equivalent to the Drivas model and is computationally simple. Markov model II can provide more realism by accounting for the locations of air inlets and outlets, advective flow patterns, in-room reflective surfaces, and contaminant removal mechanisms at specific room positions. The price paid for this greater realism is greater computational complexity. Both Markov models are explicitly probabilistic and estimate the expected concentration values at given room positions.

Keywords: diffusion models, indoor air quality, Markov chains, mathematical exposure, modeling

This work was funded by NIOSH/CDC award no. K01-OH00155. Additional support was provided by the Division of Occupational Safety and Health, California Department of Industrial Relations. The ideas expressed are solely the author's and do not necessarily represent the official views of the funding agencies.

When monitoring for indoor air contaminants is not feasible, mathematical modeling permits estimates of exposure intensity.[1] In general, a model should account for the pollutant's emission rate and pattern of dispersion through room air. The dispersion pattern usually assumed is instantaneous perfect mixing, which would create a spatially uniform concentration at all times (i.e., a well-mixed room). However, this construct can lead to substantially underestimating exposure intensity for persons near the source.[2] In the alternative, a multicompartment model can account for a nonuniform pollutant concentration. For a fixed emission source, the simplest construct is the near-field/far-field (NF/FF) model.[2,3] The source is located within a conceptual NF zone, and the remainder of the room comprises the FF zone. The air in each zone is perfectly mixed, but there is a limited air exchange between the two zones. The predicted exposure intensity is higher in the NF zone than in the FF zone. One drawback of this model is that it yields an unrealistic spatial discontinuity in concentration. For example, if the predicted NF concentration is 50 mg/m³, then 1 cm away across the zonal boundary the predicted FF concentration might be 5 mg/m³.

Finer detail in terms of describing a continuous concentration gradient with distance from the source is provided by a turbulent eddy diffusion model.[4] For an emission point source in space, the simplest construct is spherical diffusion due to turbulent air motion (zero velocity on average) with no reflecting boundaries. Without loss of generality, pollutants will be referred to hereafter as particulate in form. For a pulse release of M (number) particles, the spherical diffusion model predicts the concentration (number/m³) at time t (sec) and radial distance r (m) from the source to be:[5]

$$C(r,\,t) = \frac{M}{(4\cdot\pi\cdot D\cdot t)^{1.5}}\exp\left[-\frac{1}{2}\left(\frac{r^2}{2\cdot D\cdot t}\right)\right] \quad \textbf{(1)}$$

where D (m²/sec) is the turbulent eddy diffusion coefficient, which is assumed to be constant over time and space. D is distinct from, and far greater in magnitude than, molecular diffusivity. Molecular diffusion coefficients in air are on the order of 10^{-5} m²/sec, whereas reported D values for turbulent diffusion in indoor industrial environments range from .0014 to 0.19 m²/sec.[6] The eddy diffusion coefficient is an empirical parameter that can be experimentally estimated for a given room setting.[7] There is also a published algorithm for predicting D based on several factors including the supply air discharge speed, the room height, and the ceiling-to-floor temperature difference.[8]

Some limitations of Equation 1 are that it fails to account for dispersion by advective flow, for reflection of contaminant by room walls, and for removal of contaminant via the exhaust air flow. The equation can be modified to incorporate advection along a room axis,[7] and Drivas et al. further refined the model to account for wall reflection, and to partially account for removal by exhaust air, as follows:[8]

$$C(x, y, z, t) = \frac{M_{x_0,y_0,z_0}}{(4\cdot\pi\cdot D\cdot t)^{1.5}}\cdot R_x\cdot R_y\cdot R_z\cdot e^{-[(Q/V)\cdot t]} \quad (2)$$

where M_{x_0,y_0,z_0} is the number of particles released at room position (x_0, y_0, z_0); Q is the room exhaust air rate (m^3/sec); V is the room volume (m^3); and R_x, R_y, and R_z are wall reflection terms along the x-, y- and z-axis, respectively, and represent infinite but convergent sums of exponential terms.

A shortcoming of Equation 2, hereafter termed the Drivas model, is that at a given instance in time removal by exhaust air applies to particles at all room positions, whereas only those particles near an exhaust outlet would be subject to removal. The same problem exists in compartmental models. For example, in the NF/FF model, all particles in the FF zone are subject to exhaust removal at a given instance in time, whereas it is plausible that only those particles near an outlet could be exhausted.

The first aim of this article is to cast the Drivas model in terms of a three-dimensional random walk using Markov chain techniques. The corresponding construct, termed Markov model I, is equivalent to Equation 2 and is computationally simple. The second aim is to extend the Markov modeling approach to account for the positions of air inlets and outlets, for reflection by walls and other in-room surfaces, and for advective flow as well as diffusion. The latter construct, termed Markov model II, is more complex than model I but is still tractable. Both models yield concentration values with an explicit probabilistic interpretation.

DIFFUSION AS A RANDOM WALK

Consider a continuous-time diffusion process without drift operating along the x-axis, where X(t) denotes the position of a diffusing particle at time t (sec). The term "no drift" means that the particle has no greater tendency to move in one direction than the other. For simplicity, let $X(0) = 0$, the origin. At a future time, the particle position is normally distributed with expected value $E[X(t)] = 0$, and with a variance given by:[9]

$$Var[X(t)] = 2\cdot D\cdot t \quad (3)$$

where D is the diffusion coefficient. Next, assume the particle can simultaneously diffuse along the y-axis and z-axis in an independent and identically distributed manner, such that $E[Y(t)] = E[Z(t)] = 0$, and $Var[Y(t)] = Var[Z(t)] = 2\cdot D\cdot t$. Given that the particle position is (0,0,0) at time zero (at the origin on all three axes), the probability that the particle position is (x,y,z) at time t is described by the joint distribution of the three independent normal variables X(t), Y(t), and Z(t), which is implicit in Equation 1, where $r = \sqrt{x^2 + y^2 + z^2}$.

Now, discretize the diffusion process as a random walk. First consider the walk on the x-axis. In one time step of duration Δt (sec), the particle can move length Δx (m) to the right with probability p, or Δx to the left with probability p, such that there is no drift. A step to the right is assigned a positive value $+\Delta x$; a step to the left is assigned a negative value $-\Delta x$. Let h denote the probability that the particle holds its position (does not move), where: $h = 1-2p$. The probabilities that the particle holds its position or moves to the right or left must sum to 1. After one time step, the expected value and variance of the particle position are, respectively:

$$E[X(\Delta t)] = -\Delta x\cdot p + \Delta x\cdot p + 0\cdot h = 0$$

$$\begin{aligned} Var[X(\Delta t)] &= E[(X(\Delta t) - E[X(\Delta t)])^2] \\ &= (-\Delta x - 0)^2\cdot p + (\Delta x - 0)^2\cdot p = 2\cdot(\Delta x)^2\cdot p \end{aligned}$$

After $n = t/\Delta t$ time steps, the particle position is the sum of the positive increments to the right and the negative increments to the left. The expected position is: $E[X(t)] = n\cdot E[X(\Delta t)] = 0$. Due to mutual independence among particle movements at different time steps, the variance of the position is: $Var[X(t)] = n\cdot Var[X(\Delta t)]$, and can be written as:

$$Var[X(t)] = 2\cdot p\cdot\frac{(\Delta x)^2}{\Delta t}\cdot t \quad (4)$$

The probability law of the random walk particle position X(t) is related to the binomial distribution, but with parameters $\mu = 0$ and $\sigma^2 = 2\cdot p\cdot[(\Delta x)^2/\Delta t]\cdot t$. For large t, the probability distribution tends toward the same normal distribution used to describe the continuous-time diffusion process. In turn, inspection of Equations 3 and 4 shows that

$$D = p\cdot\frac{(\Delta x)^2}{\Delta t} \quad (5)$$

The diffusion coefficient reflects the tendency of the particle to move, as measured by the single-step probability p and the rate $\Delta x/\Delta t$. In the limit as $\Delta t \rightarrow 0$, D remains constant in value if Δt decreases by $1/f$ as Δx decreases by $1/\sqrt{f}$.[10] Next, assume that in each time step the particle can move along the x-, y-, and z-axes in an independent and identically distributed manner. This idea is akin to performing three identical but independent experiments at each time step, where the outcome of a given experiment determines how the particle moves along a given axis. If the particle position is (0,0,0) at time zero, the probability that the particle position is (x,y,z) at time t is well approximated by the same joint distribution implicit in Equation 1, where $r = \sqrt{x^2 + y^2 + z^2}$.

THE RANDOM WALK AND MARKOV MODEL I

The random walk of a particle in one or more dimensions is a Markov process, because the particle's next move depends only on its current position (state).[10,11] In turn, a particle's random walk in a room can be modeled as the simultaneous movement along three orthogonal room axes, each described by an independent Markov chain. To explain, let **PX** denote the single-step transition probability matrix for the particle's x-axis position. If one uses a 0.1-m length increment, a length of 10 m, say, along the room's x-axis corresponds to a 100 × 100 matrix **PX**, where each state represents a room cell of length 0.1 m. The matrix **PX** is defined in Figure 1. The entry in the i^{th} row and j^{th} column of **PX** is the probability that a particle currently in position i on the x-axis will make a transition (move) to position j on the x-axis in the next time step.

$$
\mathbf{PX} = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ . \\ 97 \\ 98 \\ 99 \\ 100 \end{array}
\begin{array}{c}
\begin{array}{cccccccccccc} 1 & 2 & 3 & 4 & 5 & . & 96 & 97 & 98 & 99 & 100 \end{array} \\
\left[\begin{array}{ccccccccccc}
h+p & p & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\
p & h & p & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\
0 & p & h & p & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & p & h & p & \ldots & 0 & 0 & 0 & 0 & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 & 0 & 0 & 0 & 0 & \ldots & p & h & p & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \ldots & 0 & p & h & p & 0 \\
0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & p & h & p \\
0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & p & h+p
\end{array}\right]
\end{array}
$$

FIGURE 1. The single-step transition probability matrix PX for the particle position along a 10-m room axis divided into one hundred 0.1-m segments.

The numbers outside the Figure 1 matrix index the state numbers. States 1 and 100 border the room walls, and states 2–99 are interior room positions. For the moment, it is assumed that the particle never leaves room air. For a particle in an interior state, in the next time step it can hold with probability h, or move to the adjacent higher or lower state with probability p. For a particle in a wall border state, in the next time step it can hold with probability $h + p$, or move to the adjacent state with probability p. This set of transition probabilities yields a uniform probability distribution at equilibrium; that is, a particle has the same chance of being in any given state. The value of p that corresponds to a particular value of D is determined by Equation 5 after specifying Δt (as well as Δx). In turn, $h = 1 - 2p$. Given that a particle is currently in state i, the probability that the particle is in state j after $n = t/\Delta t$ time steps is denoted $PX_{i,j}^{t/\Delta t}$, which corresponds to the i^{th} row and j^{th} column entry in the matrix $\mathbf{PX^{(n)}}$, or **PX** multiplied by itself n times. $\mathbf{PX^{(n)}}$ specifies the probability distribution of the particle's position along the room's x-axis after n time steps.

Similarly, let **PY** and **PZ** denote the single-step transition probability matrices for the particle's y-axis and z-axis positions, respectively. The number of states in **PY** and **PZ** correspond to the respective room width and height divided by the 0.1-m length increment, with the assumption that the quotients are integer values. Given that a particle starts in room position (x_0,y_0,z_0), where the three values denote the initial state numbers in the matrices **PX**, **PY**, and **PZ**, respectively, the probability that the particle is at room position (x,y,z) at time t is the product of the three independent probabilities: $(PX_{x_0,x}^{t/\Delta t})$ $(PY_{y_0,y}^{t/\Delta t})$ $(PZ_{z_0,z}^{t/\Delta t})$.

Next, let $V_{(x,y,z)}$ denote a volume element (m^3) at room position (x,y,z); for the 0.1-m length increment, $V_{(x,y,z)} = .001\ m^3$. Again, let M_{x_0,y_0,z_0} denote the number of particles released as a pulse at room position (x_0,y_0,z_0). Given that no particles leave room air because $Q = 0$, the expected particle concentration at room position (x,y,z) at time t after the release is given by:

$$E[C(x, y, z, t)]_{Q=0} = \frac{M_{(x_0,y_0,z_0)}}{V_{(x,y,z)}} \cdot PX_{x_0,x}^{t/\Delta t} \cdot PY_{y_0,y}^{t/\Delta t} \cdot PZ_{z_0,z}^{t/\Delta t}$$

The above expression is equivalent to the Drivas model, Equation 2, except for the dilution ventilation factor $e^{-(Q/V)\cdot t}$. By multiplying the right-hand side of the expression by $e^{-(Q/V)\cdot t}$, Markov model I is obtained:

$$E[C(x, y, z, t)] = \frac{M_{(x_0,y_0,z_0)}}{V_{(x,y,z)}} \cdot PX_{x_0,x}^{t/\Delta t} \cdot PY_{y_0,y}^{t/\Delta t} \cdot PZ_{z_0,z}^{t/\Delta t} \cdot e^{-[(Q/V)t]} \quad \textbf{(6)}$$

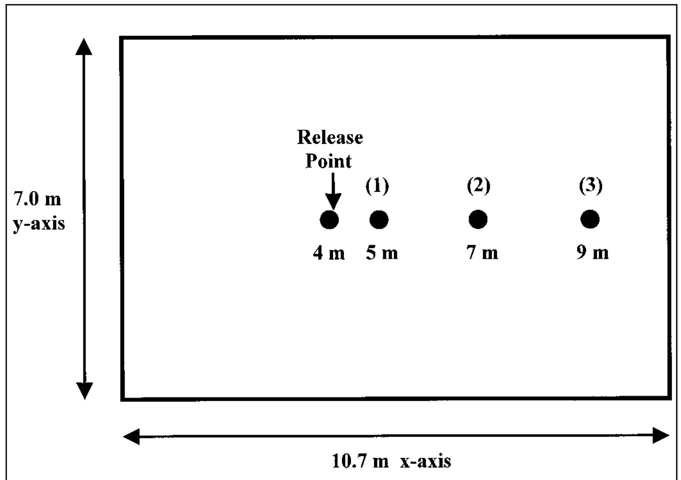

FIGURE 2. The x,y-plane view of a 10.7 × 7 × 2.6 m room. At time zero, 1000 particles are released at a position 4 m from the left-hand wall, 3.5 m along the y axis, and 1 m above the floor (along the z axis). Three receptor positions are located 5, 7, and 9 m, respectively, from the left-hand wall; all receptor positions are 3.5 m along the y axis and 1 m above the floor.

Note that the published form of the Drivas model also incorporates a pollutant surface deposition factor, $e^{-(w_d \cdot A/V)\cdot t}$, where w_d is the deposition rate on surfaces (m/sec), and A is the surface area (m^2) available for deposition. Markov model I can be made equivalent by multiplying the right-hand side of Equation 6 by $e^{-(w_d \cdot A/V)\cdot t}$.

An Illustrative Scenario

Consider a room with length, width, and height dimensions of 10.7 × 7 × 2.6 m. The room receives 15 nominal air changes per hour, and the diffusion coefficient is $D = .04\ m^2/sec$. These parameters correspond to a test room described in the Drivas et al. article.[8]

Based on $\Delta x = 0.1$ m, the **PX**, **PY**, and **PZ** matrices are, respectively, 107 × 107, 70 × 70, and 26 × 26 in dimension. Based on $\Delta x = 0.1$ m and $\Delta t = 1/60$ sec, $p = .0667$ and $h = 0.8666$ by Equation 5. Appendix 1 provides a MATLAB® code that assigns the matrix entries and performs the matrix multiplications over a 30-min interval, or 1.08×10^5 time steps.

Next, assume that 1000 particles are released at a point 4 m from the left-hand wall, 3.5 m or midway along the width axis, and 1 m in height from the floor. In the context of the states in **PX**, **PY**, and **PZ**, this release position corresponds to $x_0 = 40$, $y_0 = 35$, $z_0 = 10$. Figure 2 depicts the x,y plane of the room and the release position at 4 m from the left-hand wall. Figure 3 depicts the particle concentration predicted by Markov model I over the first 5 min at three room positions also shown in Figure 2: (1) x = 5 m, y = 3.5 m, z = 1 m; (2) x = 7 m, y =3.5 m, z = 1 m; and (3) x = 9 m, y = 3.5 m, z = 1 m. The same scenario was presented in reference 8. Figure 3 shows a rapid increase and decline in the particle concentration at Position 1, which is 1 m from the release point, and a more gradual increase and decline at Positions 2 and 3, which are, respectively, 3 m and 5 m away. The Figure 3 curves are similar to those generated by the Drivas model, as presented in Reference 8.

A more quantitative comparison is made by considering the integrated particle concentrations at each position over four intervals following the pulse release: (i) 0 to 30 min; (ii) 0 to 1 min;

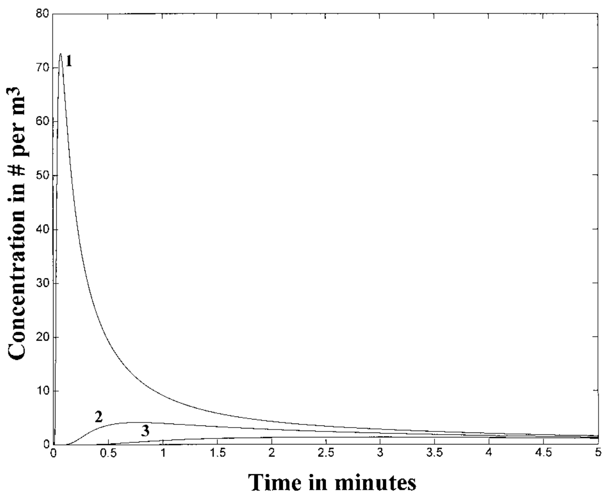

FIGURE 3. The expected particle concentrations at three room positions predicted by Markov model I following the pulse release of 1000 particles at source position (x = 4 m, y = 3.5 m, z = 1 m). The receptor positions are (1) x = 5 m, y = 3.5 m, z = 1 m; (2) x = 7 m, y = 3.5 m, z = 1 m; and (3) x = 9 m, y = 3.5 m, z = 1 m. The room receives 15 nominal air changes per hour and is partially depicted in Figure 2.

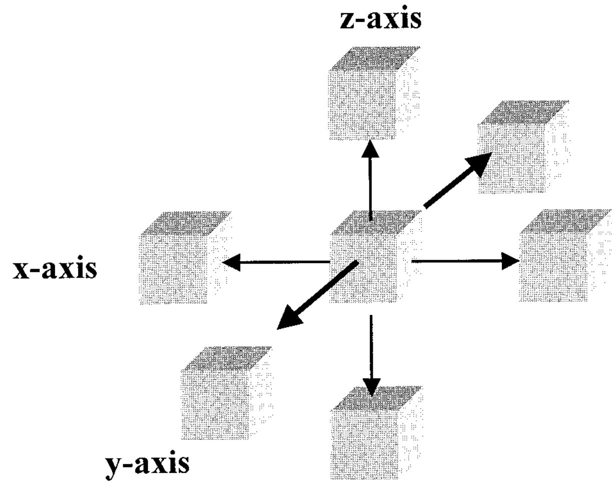

FIGURE 4. An interior room cell with its six nearest neighbors—two along the x axis, two along the y axis, and two along the z axis. Although the cubic cells are spaced apart in the diagram, the interior cell is considered physically contiguous with each neighbor and shares a planar surface. The arrows indicate that in one time step a particle in the interior cell can move to one of its nearest neighbors; the particle can also hold its position in the interior cell.

(iii) 1 to 5 min; and (iv) 5 to 15 min. These periods correspond to measurement intervals also described in reference 8. Table I presents the integrated concentrations predicted by Markov model I, where each value has been normalized by dividing by the 0-to-30 min integrated concentration at Position 1 and multiplying by 100%. The Table I entries are within several percent of respective normalized values predicted by the Drivas model and presented in reference 8. In summary, Markov model I is equivalent to the Drivas model and can be implemented by a code similar to that presented in Appendix I.

THE RANDOM WALK AND MARKOV MODEL II

Markov model I uses the simple approach of applying the ventilation removal term $e^{-(Q/V)\cdot t}$, and if applicable the surface deposition removal term $e^{-(Q/V)\cdot t}$, to particles at all room positions. Further, the model cannot account for reflective barriers (physical objects) inside the room, which in some circumstances may be important to consider. A more detailed approach would account for three-dimensional advective flows, for particle removal by ventilation only at exhaust air outlets and exfiltration points, for particle removal by deposition only near room surfaces, and for reflection by in-room surfaces. A construct termed Markov model II that can incorporate these factors is now developed.

The room is divided into cubic cells with length aspect Δx, and the positions of air inlets and outlets are specified. Given m cells in the room, the single-step transition probability matrix **P** has dimensions $(m + 1) \times (m + 1)$. **P** has one state for each cell in the room plus an additional absorbing state that represents particle removal from room air. For simplicity, it is assumed that the only particle loss mechanism is removal by exhaust air, and that once exhausted from the room, a particle cannot reenter. However, other particle loss mechanisms can be accommodated, as well as absorbing states corresponding to these removal pathways.

In one time step, a particle in a given room cell can hold its position or move to a physically contiguous "nearest neighbor" cell with which it shares a planar surface. Figure 4 depicts an interior room cell with its six nearest neighbors—two on the x-axis, two on the y-axis, and two on the z-axis; the arrows indicate the alternative directions in which an interior cell particle can move in one time step. A cell that borders one wall (or surface) has five nearest neighbors. A cell that borders two walls (or surfaces) has four nearest neighbors, and a room corner cell has three nearest neighbors. A cell bordering the exhaust air outlet can be considered to have six nearest neighbors if one counts the absorbing state as a neighbor, although a particle that enters the absorbing state can never leave that state.

The reason for limiting a particle's movement in a given time step to a neighboring cell sharing a planar surface is to model advective flow in a simple manner, and to maintain an analogy to Markov model I such that model II exhibits the same diffusion rate for a specified D value. To explain, again consider a particle's position along the x-axis, where the starting position is the interior midpoint of an infinitely large room. Let the initial x-axis position be $X(0)=0$. Assume for the moment that turbulent diffusion is the only mechanism of particle movement. In the next time step of the nearest neighbor random walk, the particle can hold its position with probability $h_{I,D}$ (where the subscript I designates an interior room cell, and D signifies that only diffusive flow is considered), or the particle can move to one of six nearest neighbors,

TABLE I. Normalized Integrated Concentrations Predicted by Markov Model I at Three Room Positions over Four Different Intervals

	Time Intervals			
Position (m)	0–30 Min (%)	0–1 Min (%)	1–5 Min (%)	5–15 Min (%)
(1) x = 5, y = 3.5, z = 1	100	56	30	12
(2) x = 7, y = 3.5, z = 1	38	6.1	20	11
(3) x = 9, y = 3.5, z = 1	23	0.52	11	10

with probability $1/6 \cdot (1-h_{I,D})$ for each neighbor. The expected value and variance of the particle position along the x-axis are, respectively:

$$E[X(\Delta t)] = -\Delta x \cdot \frac{1}{6} \cdot (1 - h_{I,D}) + \Delta x \cdot \frac{1}{6} \cdot (1 - h_{I,D}) = 0$$

$$\begin{aligned} Var[X(\Delta t)] &= (-\Delta x - 0)^2 \cdot \frac{1}{6} \cdot (1 - h_{I,D}) + (\Delta x - 0)^2 \cdot \frac{1}{6} \cdot (1 - h_{I,D}) \\ &= \frac{1}{3} \cdot (1 - h_{I,D}) \cdot (\Delta x)^2 \end{aligned}$$

After $n = t/\Delta t$ time steps, the x-axis position is the sum of the positive increments to the right and the negative increments to the left. The expected position is $E[X(t)] = n \cdot E[X(\Delta t)] = 0$. Due to mutual independence among particle movements at different time steps, the variance of the position is $Var[X(t)] = n \cdot Var[X(\Delta t)]$, and can be written as

$$Var[X(t)] = \frac{1}{3} \cdot (1 - h_{I,D}) \cdot \frac{(\Delta x)^2}{\Delta t} \cdot t \quad \textbf{(7)}$$

Inspection of Equations 3 and 7 shows that for the nearest neighbor random walk:

$$D = \frac{1}{6} \cdot (1 - h_{I,D}) \cdot \frac{(\Delta x)^2}{\Delta t} \quad \textbf{(8)}$$

The value of $h_{I,D}$ that corresponds to a particular value of D is determined by Equation 8, after specifying Δx and Δt. In turn, the probability that an interior room cell particle moves to a given neighboring cell due to diffusion, denoted $p_{I,D}$. is

$$p_{I,D} = \frac{1}{6} \cdot (1 - h_{I,D}) \quad \textbf{(9)}$$

For a given set of values $\{D, \Delta x, \Delta t\}$, the single-step transition probability $p_{I,D}$ in Markov model II equals the model I single-step transition probability p, which ensures that the expected diffusion rate along a given room axis is the same in both models. For $p < .02$, it happens that $h_{I,D} \cong (1 - 2p)^3 = h^3$. The complete set of equations specifying the single-step transition probabilities that account for wall reflection is presented in Appendix II.

Transition Probabilities Incorporating Advection

Assume that a particle in an interior room cell can move by advection as well as diffusion. Let s_A denote the advective air speed (m/sec). For simplicity, consider that advective flow is perpendicular to only one cell face, in which case a cell with face area $(\Delta x)^2$ receives an advective air supply in (m^3/sec) equal to $s_A \cdot (\Delta x)^2$. Because a cell has volume $(\Delta x)^3$, this advective air supply divided by the cell volume corresponds to $s_A/\Delta x$ air changes per second. If air in a cell is assumed to be well-mixed, the advective air supply can be treated as a "dilution" air supply, and the time that a particle resides in the cell before removal by the advective airflow can be modeled as a type of exponential probability density function with rate parameter $s_A/\Delta x$. The probability that a particle is not removed due to advection in time step Δt is denoted $h_{I,A}$ (where the subscript A signifies that only advective flow is considered), and is specified by

$$h_{I,A} = e^{-(s_A/\Delta x) \cdot \Delta t} \quad \textbf{(10)}$$

Equation 10 is analogous to the idea that in a well-mixed room with volume V and dilution supply air rate Q, the probability that an airborne particle will not be removed by the exhaust airflow in time interval Δt is $e^{-(Q/V) \cdot \Delta t}$. If particle removal from the cell by diffusive flow and by advective flow are treated as independent mechanisms, the probability that the particle holds its position in time step Δt is the product $(h_{I,D})(h_{I,A})$.

If only diffusive flow applies, the probability that a particle moves to a given neighboring cell is specified by $p_{I,D}$ in Equation 9. However, where both diffusive and advective flows apply, the probabilities that a particle moves to the "downstream" neighboring cell (in the direction of advective flow), denoted $p_{I,down}$, or to one of the five other neighboring cell, denoted $p_{I,other}$, are respectively given by

$$p_{I,down} = \frac{(1/6) \cdot \alpha + (s_A/\Delta x) \cdot \Delta t}{\alpha + (s_A/\Delta x) \cdot \Delta t} \cdot (1 - h_{I,D} \cdot h_{I,A}) \quad \textbf{(11)}$$

$$p_{I,other} = \frac{(1/6) \cdot \alpha}{\alpha + (s_A/\Delta x) \cdot \Delta t} \cdot (1 - h_{I,D} \cdot h_{I,A}) \quad \textbf{(12)}$$

where $\alpha = -\ln (h_{I,D})$. The derivation of Equations 11 and 12 is provided in Appendix II. For a particle in a cell bordering the exhaust air outlet, $p_{I,down}$ is also the probability that the particle is exhausted from the room, that is, enters the absorbing state. This general construct represents a three-dimensional random walk with drift along the room axis in the direction of the advective flow.

Given a specified matrix **P**, and given the release of M particles at time zero in state *i* corresponding to room position (x_0,y_0,z_0), the expected concentration in state *j* corresponding to room position (x,y,z) after $t/\Delta t$ time steps is

$$E[C(x, y, z, t)] = \frac{M_{(x_0,y_0,z_0)}}{(\Delta x)^3} \cdot P_{i,j}^{t/\Delta t} \quad \textbf{(13)}$$

An Illustrative Scenario

Consider a hypothetical room, 3 × 3 × 3 m. The room is isothermal and receives six nominal air changes per hour. Based on Δx=0.2 m, the room is divided into 3375 cubic cells, and the P matrix is 3376 × 3376. Air enters through a 3-m wide by 0.6-m high register running the length of the left-hand wall at height position 1.4 to 2 m. Air is exhausted through a register of the same dimensions at the same height position on the right-hand wall. The supply air discharge velocity is .025 m/sec. Figure 5 depicts the x,y plane of the room. The inward arrows along the left-hand wall indicate the entering flow of supply air; the outward arrows along the right-hand wall indicate the exiting flow of exhaust air.

An algorithm presented in reference 8 predicts the turbulent diffusion coefficient for this room to be .0189 m^2/sec. For Δx = 0.2 m, Δt = 1/30 sec, and D = .0189 m^2/sec, the transition probabilities for interior cell particles not subject to advective flow are $h_{I,D} = 0.9055$ and $p_{I,D} = .0158$. For simplicity, it is assumed that all advective flow goes uniformly from left to right in the 1.4- to 2-m height zone, in which case s_A =.025 m/sec and $h_{I,A} = 0.9958$. For interior cell particles in the 1.4- to 2-m height zone, the transition probabilities are: $(h_{I,D})(h_{I,A}) = 0.9017$, $p_{I,down} = .0197$, $p_{I,other} = .0157$. The transition probabilities for particles in cells bordering wall surfaces can be found by the formulae in Appendix II.

Figure 5 also depicts four positions along the room's x axis. At time zero, 2700 particles are released at position x_0=1.1 m, y_0=1.5 m, z_0=1.5 m. The three receptor positions shown in Figure 5 are as follows: (1) x = 0.1 m, y = 1.5 m, z = 1.5 m, which is 1 m upstream from the release point and next to the supply air register; (2) x = 2.1 m, y = 1.5 m, z = 1.5 m, which is 1 m

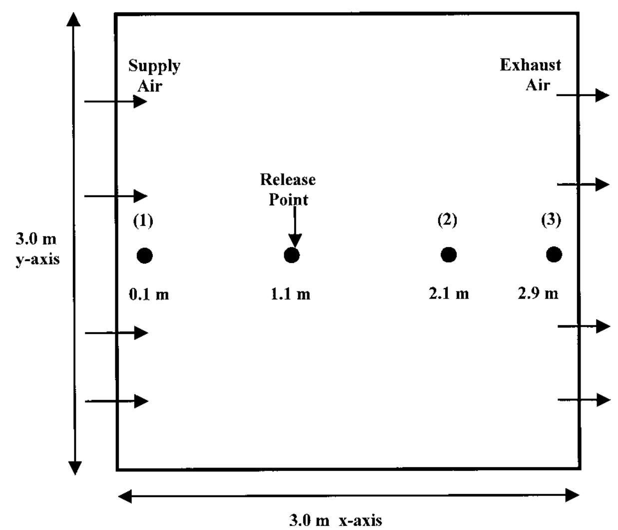

FIGURE 5. The x,y plane view of a hypothetical 3 × 3 × 3 m room. Supply air enters the room along the entire length of the left-hand wall between 1.4 and 2 m above the floor (along the z axis). Exhaust air exits the room along the entire length of the right-hand wall between 1.4 and 2 m above the floor. At time zero, 2700 particles are released at a position 1.1 m from the left-hand wall, 1.5 m along the y axis, and 1.5 m above the floor. Three receptor positions are located 0.1, 2.1, and 2.9 m, respectively, from the left-hand wall; all receptor positions are 1.5 m along the y axis, and 1.5 m above the floor.

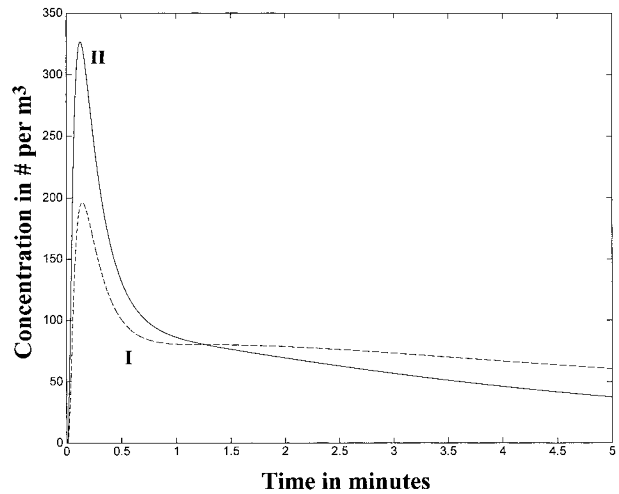

FIGURE 7. The expected particle concentrations at receptor midpoint position (x = 2.1 m, y = 1.5 m, z = 1.5 m) predicted by Markov model I (the dashed-line curve labeled I) and Markov model II (the solid-line curve labeled II) following the pulse release of 2700 particles at source midpoint position (x = 1.1 m, y = 1.5 m, z = 1.5 m). The room receives six nominal air changes per hour (Q = .045 m^3/sec) and is partially depicted in Figure 4. The receptor position is in the room interior and 1 m downstream from the release position.

downstream from the release point; and (3) x = 2.9 m, y = 1.5 m, z = 1.5 m, which is 1.8 m downstream from the release point and next to the exhaust outlet. Note that these (x,y,z) tuples are the midpoint coordinates of the 0.2-m cubic cells. Figures 6–8 compare the expected concentrations at the same respective room positions predicted by Markov model II (the solid-line curves) and by Markov model I (the dashed-line curves) per Equation 6. For the latter model, the matrices **PX**, **PY**, and **PZ** are each 15 × 15 in dimension, and the parameters $\Delta x = 0.2$ m, $\Delta t = 1/30$ sec, and D = .0189 m^2/sec correspond to h=0.9685 and p=.0158.

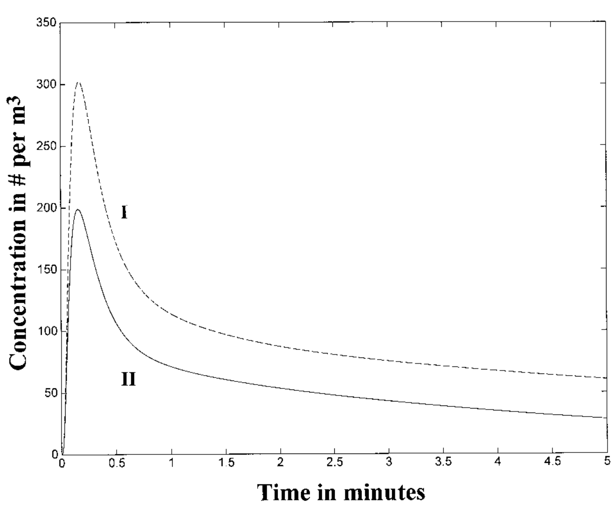

FIGURE 6. The expected particle concentrations at receptor midpoint position (x = 0.1 m, y = 1.5 m, z = 1.5 m) predicted by Markov model I (the dashed-line curve labeled I) and Markov model II (the solid-line curve labeled II) following the pulse release of 2700 particles at source midpoint position (x = 1.1 m, y = 1.5 m, z = 1.5 m). The room receives six nominal air changes per hour (Q = .045 m^3/sec) and is partially depicted in Figure 4. The receptor position adjoins the air inlet and is 1 m upstream from the release position.

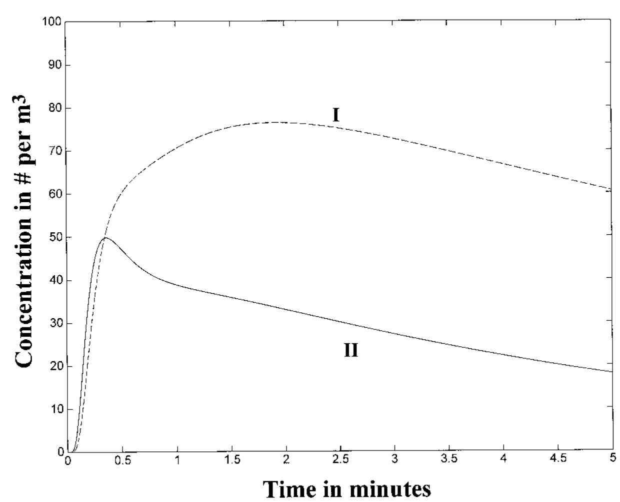

FIGURE 8. The expected particle concentrations at receptor midpoint position (x = 2.9 m, y = 1.5 m, z = 1.5 m) predicted by Markov model I (the dashed-line curve labeled I) and Markov model II (the solid-line curve labeled II) following the pulse release of 2700 particles at source midpoint position (x = 1.1 m, y = 1.5 m, z = 1.5 m). The room receives six nominal air changes per hour (Q = .045 m^3/sec) and is partially depicted in Figure 4. The receptor position adjoins the air outlet and is 1.8 m downstream from the release position.

Further, the posited advective air speed s_A=.025 m/sec combined with a supply register surface area of 1.8 m^2 (0.6 × 3 m) corresponds to Q = .045 m^3/sec, or six nominal air changes per hour given room volume V = 27 m^3.

Figure 6 shows the concentrations at Location 1, which is 1 m upstream from the release point and next to the air inlet. Model II describes a lower concentration than does model I; for example, the peak level in the former model (200 per m^3) is 33% lower than the peak value in the latter (300 per m^3). This result is intuitively reasonable. There is less tendency for particles to move against the advective flow toward the air inlet, and the discharge of clean air at the inlet exerts a greater local dilution effect than if clean air were somehow uniformly discharged at all room positions, as assumed in model I.

Figure 7 shows the expected concentrations at Location 2, which is 1 m downstream from the release point. Model II describes a higher concentration than does model I in the first 1.25 min, and a lower concentration thereafter; for example, the peak level in the former model (330 per m^3) is 70% higher than the peak value in the latter (195 per m^3). This result is also intuitively reasonable, because there is a greater initial tendency for particles to migrate toward Location 2 due to the advective flow. The impact of advection is also seen by comparing $p_{I,down}$=.0197 (the transition probability to the right-hand neighboring cell due to both advection and diffusion) and $p_{I,D}$ = .0158 (the transition probability to the right-hand neighboring cell due to diffusion alone). Note that advection has a substantial effect even though the advective air speed is only .025 m/sec (5 ft/min).

Figure 8 shows the expected concentrations at Location 3, which is 1.8 m downstream from the release point and next to the exhaust outlet. After the first half minute, model II describes a lower concentration than does model I. This result is somewhat counterintuitive. Given that all particles are eventually exhausted at the outlet, it might be expected that the particle level would be higher near the outlet than if particles were somehow uniformly exhausted from all room positions, as assumed in model I. However, the room has a relatively large 1.8 m^2 (19 ft^2) exhaust outlet area, which decreases the exiting particle concentration in cells adjacent to the outlet. A smaller exhaust area would funnel a greater number of particles through a smaller volume adjacent to the outlet and increase the local particle concentration.

Although not shown, if Q and s_A were zero and the room were sealed such that no particles could escape, the expected concentration curves predicted by Markov models I and II would be coincident, and a particle concentration of 100 per m^3 would eventually develop at all room positions. The latter value is expected because 2700 particles would be uniformly distributed in a 27 m^3 volume. The coincidence of the concentration curves indicates that the models produce the same turbulent diffusion rate in three dimensions and are equivalent under the special conditions of no particle removal and no advective flow.

The Effect of an In-Room Barrier

Consider a pulse release of particles immediately in front of an individual. If the person's back faces the advective flow stream, the particle concentration in the breathing zone will likely be higher than if the individual's body somehow presented no barrier to the advective flow. One reason is that the body decreases or eliminates advective flow immediately in front of the person (on the downstream side). A second reason is that the body reflects particles diffusing in the upstream direction. The net effect is that particles tend to remain relatively longer in front of the person before migrating away.

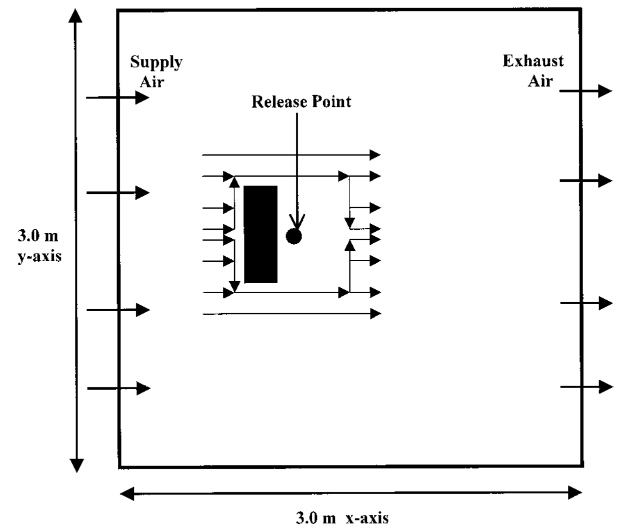

FIGURE 9. The x,y-plane view of the posited airflow pattern around a barrier (the solid rectangle) positioned at 0.8 to 1 m along the x axis, at 1.2 to 1.8 m along the y axis, and at 0 to 1.8 m along the z axis. That portion of the advective flow striking the upstream barrier face evenly distributes around the barrier ends. The advective flow returns to a uniform pattern 0.4 downstream from the barrier. The particle release position is x_0 = 1.1 m, y_0 = 1.5 m, z_0 = 1.5 m.

To approximate this scenario, previous model II for the hypothetical 3-m cubic room was modified as partially depicted in Figure 9, which shows the room's x,y plane. A barrier representing a person was placed along the x axis at 0.8 to 1 m from the left-hand wall, midway along the y axis from 1.2 to 1.8 m, and along the z axis at 0 to 1.8 m from the floor. Therefore, the barrier's depth, width, and height were, respectively, 0.2, 0.6, and 1.8 m. That portion of the advective airflow hitting the left-hand face of the barrier (at height 1.4 to 1.8 m) was evenly split around the ends of the barrier in the same height zone, but made to return to a uniform flow pattern 0.4 m downstream from the right-hand face of the barrier at x = 1.4 m. In effect, a wake zone free of advective flow was created in front of the barrier on the downstream side (on the x axis from 1 to 1.4 m, on the y axis from 1.2 to 1.8 m, and on the z axis from 1.4 to 1.8 m). For simplicity, the turbulent diffusion coefficient was kept the same in the wake zone as elsewhere in the room. As before, assume that 2700 particles are released at room position x_0=1.1 m, y_0=1.5 m, z_0=1.5 m, which is intended to represent a person's breathing zone position.

Figure 10 shows the particle concentration (on a logarithmic scale) at the release position over the first minute. The solid-line curve is the concentration profile with the barrier present, and the dashed-line curve is the concentration without the barrier. The particle concentration at the time of release is the same in both scenarios (3.38 × 10^5 per m^3), but the concentration initially decreases less rapidly with the barrier present. The 5-min TWA values with and without the barrier are 800 per m^3 versus 630 per m^3, respectively. The barrier increased the 5-min TWA value by 27%.

DISCUSSION

This article presented two models based on Markov chains that describe contaminant dispersion and removal from room air.

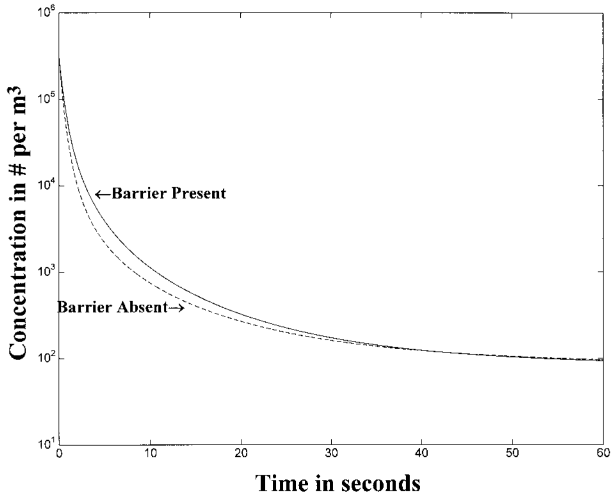

FIGURE 10. The expected particle concentrations at source midpoint position (x = 1.1 m, y = 1.5 m, z = 1.5 m) following the pulse release of 2700 particles predicted by Markov model II with a barrier immediately upstream of the source position (the solid-line curve) or with no barrier (the dashed-line curve). The room receives six nominal air changes per hour (Q = .045 m^3/sec) and is partially depicted in Figure 9.

Model I is equivalent to the previously published Drivas model and is computationally simple. Model II can provide more realism by accounting for the locations of air inlets and outlets, for advective flow patterns, for in-room reflective surfaces, and for local particle loss mechanisms such as surface deposition (although such mechanisms were not illustrated in this analysis). The price paid for this greater realism is greater computational complexity.

Both models yield contaminant concentrations with an explicit probabilistic interpretation, that is, E[C(x, y, z, t)] is the expected concentration value at the given room position. As explained elsewhere, the particle concentration is a random variable, because the number of particles at a given location is a binomial random variable if mutual independence between particles pertains.[12] The stochastic nature of the particle concentration in an individual's breathing zone is important to consider when small numbers of particles are involved, but where these small numbers still pose a threat to health, as applies to pathogens with a low infectious dose, for example, *Mycobacterium tuberculosis* bacilli.

Although model I provides less realism than does model II, the former can be an adequate descriptor of TWA contaminant levels at interior room positions not influenced by strong advective flows or in-room barriers. As reported in reference 8, the equivalent Drivas model predicted the measured TWA particle concentrations in a test room experiment with reasonable accuracy. In the context of Figure 4, which compared models I and II with respect to the influence of advection 1 m downstream from the particle release position, model I underestimated the peak concentration by 41% relative to model II (195 per m^3 versus 300 per m^3, respectively), yet the 5-min TWAs were within 4% in value (80 per m^3 for model I versus 77 per m^3 for model II). Of course, if the peak concentration value is toxicologically important, or if contaminant emission occurs throughout a work shift (for example, a series of many pulse releases), model II is the better descriptor.

The greatest uncertainties in this Markov modeling approach are the value of the turbulent diffusion coefficient D, and for model II, the pattern and values of the advective flow. Clearly, it is necessary to develop tractable methods for predicting both D and the room airflow patterns, and this analysis has not contributed to such methods. In this regard, computational fluid dynamics (CFD) might be considered the preferred approach for dispersion modeling, because CFD predicts the room air velocity field.[13,14] However, the CFD approach is still being adapted to indoor air work, and the cost of a CFD software license remains substantial for an individual hygienist. In the alternative, a simple approximation of the advective flows in model II, as posed for the in-room barrier scenario for example, may provide reasonable predictive value.

A useful property of both Markov models is the ability to account for multiple in-room sources of contaminant. In model II, by specifying the cell location of each source and the number of particles released at time zero, the particle concentration at a given receptor cell at time t due to all sources is easily computed from the matrix $\mathbf{P}^{(t/\Delta t)}$ as follows:

$$E[C(x, y, z, t)] = \frac{1}{(\Delta x)^3} \sum_{i=1}^{k} M_i \cdot P_{i,j}^{t/\Delta t} \qquad \textbf{(14)}$$

where i indexes the source cell, i = 1,2,. . . , k; M_i is the number of particles released in the ith source cell; and j indexes the receptor cell (x,y,z).

Moreover, one can account for ongoing contaminant emission by multiple in-room sources, where the emission rate (number of particles per second) at a given source need not be constant. For example, one might model the emission rate at one source as exponentially decreasing, the rate at a second source as sinusoidal, and the rate at a third source as constant. The particle concentration at a given receptor cell j = (x,y,z) at time t is

$$E[C(x, y, z, t)] = \frac{1}{(\Delta x)^3} \sum_{i=1}^{k} \left[\sum_{q=0}^{t/\Delta t} (M_i)_q \cdot P_{i,j}^{t/\Delta t - q} \right] \qquad \textbf{(15)}$$

where i again indexes the source cell; $(M_i)_q$ is the number of particles released in the ith source cell at time q; and $P_{i,j}^{0} = 0$ and $P_{i,i}^{0} = 1$. If desired, the times of emission events and the number of particles emitted per event can also be modeled as probabilistic entities.[12] Consideration of how these latter distributions might be specified is beyond the scope of the present analysis.

CONCLUSIONS

Markov chain techniques can be used to model dispersion of indoor air contaminants by turbulent diffusion and advection, and removal by exhaust airflows and other mechanisms such as particle settling. The Markov models are explicitly probabilistic and provide expected concentration values at different room positions. A current limitation is that the models do not independently predict the turbulent diffusion coefficient or the room airflow patterns and are conceptual rather than physics-based constructs. It is anticipated that these Markov models can eventually be combined with deterministic physics-based approaches to predict contaminant concentrations more realistically at room locations of interest.

ACKNOWLEDGMENT

The author thanks Dr. Jim Pitman for his illuminating discussions of diffusion processes.

REFERENCES

1. **Jayjock, M.:** Assessment of inhalation exposure potential from vapors in the workplace. *Am. Ind. Hyg. Assoc. J. 49*:380–385 (1988).
2. **Nicas, M.:** Estimating exposure intensity in an imperfectly mixed room. *Am Ind. Hyg. Assoc. J. 57*:542–550 (1996).
3. **Furtaw, E.J., M.D. Panadian, D.R. Nelson and J.V. Behar:** Modeling indoor air concentrations near emission sources in imperfectly mixed rooms. *J. Air Waste Manage. Assoc. 46*:861–868 (1996).
4. **Roach, S.A.:** On the role of turbulent in ventilation. *Ann. Occup. Hyg. 24*:105–132 (1981).
5. **Banks, R.B.:** *Growth and Diffusion Phenomena: Mathematical Frameworks and Applications.* New York: Springer-Verlag, 1994. p. 331.
6. **Keil, C.B., and D.R. Krupinski:** Eddy diffusivity measurements for exposure modeling. [Abstract 182] American Industrial Hygiene Conference and Exposition, Dallas, Texas, May 1997.
7. **Scheff, P.A., R.L. Friedman, J.E. Franke, L.M. Conroy, and R.A. Wadden:** Source activity modeling of Freon® emissions from open-top vapor degreasers. *Appl. Occup. Environ. Hyg. 7*:127–134 (1992).
8. **Drivas, P.J., P.A. Valberg, B.L. Murphy, and R. Wilson:** Modeling indoor air exposure from short-term point source releases. *Indoor Air 6*:271–277 (1996).
9. **Doucet, P., and P.B. Sloep:** *Mathematical Modeling in the Life Sciences.* London: Ellis Horwood, 1992. pp. 224–230.
10. **Taylor, H.M., and S. Karlin:** *An Introduction to Stochastic Modeling*, 3rd ed. San Diego: Academic Press, 1998.
11. **Ross, S.M.:** *Introduction to Probability Models*, 5th ed. San Diego: Academic Press, 1993.
12. **Nicas, M.:** Markov modeling of contaminant concentrations in indoor air. *Am. Ind. Hyg. Assoc. J. 61:* 484–491 (2000).
13. **Andersson, I.M., and S. Alenius:** A comparison between measured and numerically calculated styrene concentrations in hand lay-up moulding. *Occup. Hyg. 3*:399–415 (1996).
14. **Buchanan, C.R., and D. Dunn-Rankin:** Transport of surgically produced aerosols in an operating room. *Am. Ind. Hyg. Assoc. J. 59*:393–402 (1998).

APPENDIX I

A MATLAB Script for Generating Figure 3

```
% figure3.m
% The cells are cubic with Δx = 0.1 m. The time step is Δt =
   1/60 sec. The room volume V = 194.74 m³. Q corre-
   sponds to 15 air changes per hour. The diffusion coefficient
   is D = .04 m²/sec. At time zero, M0 = 1000 particles are
   released at position x0 = 40, y0 = 35, z0 = 10.

PX = zeros(107,107); PY = zeros(70,70); PZ = zeros(26,26);
deltaX = 0.1; deltaT = 1/60; D = .04;
p = (D*deltaT)/(deltaX^2);
h = 1 − (2*p);
M0 = 1000;
VROOM = 194.74;
ACH = 15;
Q = (ACH*VROOM*deltaT)/3600;
F1 = M0/(deltaX^3);
F2 = −(Q/VROOM);

PX(1,1) = h + p; PX(107,107) = h + p; PX(1,2) = p;
   PX(107,106) = p;
for i = 2:106
PX(i,i) = h;
PX(i,i-1) = p;
PX(i,i+1) = p;
end

PY(1,1) = h + p; PY(70,70) = h + p; PY(1,2) = p; PY(70,69)
   = p;
for i = 2:69
PY(i,i) = h;
PY(i,i-1) = p;
PY(i,i+1) = p;
end

PZ(1,1) = h + p; PZ(26,26) = h + p; PZ(1,2) = p;
   PZ(26,25) = p;
for i = 2:25
PZ(i,i) = h;
PZ(i,i-1) = p;
PZ(i,i+1) = p;
end

TEMPX = PX; TEMPY = PY; TEMPZ = PZ;
x0 = 40; y0 = 35; z0 = 10;
OUTPUT = zeros(108001,3);
TIME = zeros(108001,1);
for t = 1:108000
TIME(t + 1,1) = t;
OUTPUT(t + 1,1) = TEMPX(x0,50)*TEMPY(y0,35)*TEMPZ
   (z0,10)*F1*exp(F2*t);
OUTPUT(t + 1,2) = TEMPX(x0,70)*TEMPY(y0,35)*TEMPZ
   (z0,10)*F1*exp(F2*t);
OUTPUT(t + 1,3) = TEMPX(x0,90)*TEMPY(y0,35)*TEMPZ
   (z0,10)*F1*exp(F2*t);
TEMPX = TEMPX*PX;
TEMPY = TEMPY*PY;
TEMPZ = TEMPZ*PZ;
end
TIME = (1/3600)*TIME;

plot(TIME,OUTPUT(:,1),'-',TIME,OUPUT(:,2),'–',
   TIME,OUTPUT(:,3),'-.')
xlabel('Time in minutes')
ylabel('Concentration in # per m^{3}')
```

APPENDIX II

Single-State Transition Probabilities for Markov Model II

For reference, Equation 8 of the main text is rearranged here to express the hold probability for a particle in an interior room cell, $h_{I,D}$, as a function of D, Δx, and Δt

$$h_{I,D} = 1 - 6 \cdot D \cdot \frac{\Delta t}{(\Delta x)^2} \quad \textbf{(B1)}$$

Equation B1 pertains to particle movement by turbulent diffusion with no involvement of advective flow. The corresponding probability that the interior cell particle moves (jumps) to a given nearest neighbor cell (of which there are six) due to turbulent diffusion, $p_{I,D}$, is

$$p_{I,D} = \frac{1}{6} \cdot (1 - h_{I,D}) \quad \textbf{(B2)}$$

A particle in a cell that borders one room wall surface will be reflected back into the cell (not leave the cell) if it moves toward the wall. Therefore, the hold probability for this particle, denoted $h_{one\text{-}wall,D}$, is

$$h_{\text{one-wall,D}} = h_{I,D} + p_{I,D} \tag{B3}$$

The corresponding probability that a particle in a cell bordering one wall moves (jumps) due to turbulent diffusion to one of the five nearest neighbor cells, denoted $p_{\text{one-wall,D}}$, is

$$p_{\text{one-wall,D}} = \frac{1}{5}\cdot(1 - h_{\text{one-wall,D}}) = p_{I,D} \tag{B4}$$

By similar arguments, the respective hold and jump probabilities for a particle that borders two wall surfaces or three wall surfaces can be derived:

$$h_{\text{two-walls,D}} = h_{I,D} + 2\cdot p_{I,D} \tag{B5}$$

$$p_{\text{two-walls,D}} = \frac{1}{4}\cdot(1 - h_{\text{two-walls,D}}) = p_{I,D} \tag{B6}$$

$$h_{\text{three-walls,D}} = h_{I,D} + 3\cdot p_{I,D} \tag{B7}$$

$$p_{\text{three-walls,D}} = \frac{1}{3}\cdot(1 - h_{\text{three-walls,D}}) = p_{I,D} \tag{B8}$$

Next, assume that a particle can move by advective flow as well as diffusion, where s_A is the advective air speed. For simplicity, advective flow is treated as perpendicular to only one cell face with area $(\Delta x)^2$. The advective air supply, $s_A \bullet (\Delta x)^2$, divided by the cell volume, $(\Delta x)^3$, corresponds to $s_A/\Delta x$ air changes per second and is treated as dilution air. Consider any cell that is subject to advective flow. The probability that a particle in the cell is not removed by advection in interval Δt is denoted $h_{..,A}$ (where the dot subscript signifies that the cell's position need not be specified), and is given by

$$h_{..,A} = e^{-(s_A/\Delta x)\cdot \Delta t} \tag{B9}$$

If particle removal from the cell by diffusive flow and by advective flow are treated as independent mechanisms, the probability that the particle holds its position is the product of the hold probability based on diffusion alone and the hold probability based on advection alone. Therefore:

Hold Probability for an Interior Cell Particle

$$= h_{I,D}\cdot h_{..,A} \tag{B10}$$

Hold Probability for a One-Wall Border Particle

$$= h_{\text{one-wall,D}}\cdot h_{..,A} \tag{B11}$$

Hold Probability for a Two-Wall Border Particle

$$= h_{\text{two-wall,D}}\cdot h_{..,A} \tag{B12}$$

Hold Probability for a Three-Wall Border Particle

$$= h_{\text{three-wall,D}}\cdot h_{..,A} \tag{B13}$$

If $s_A = 0$, these expressions simplify to the hold probabilities due to turbulent diffusion alone. The derivation of the jump probabilities where both diffusion and advection apply is presented for an interior cell particle. The hold probability can be written as

$$h_{I,D}\cdot h_{..,A} = e^{\ln(h_{I,D})}\cdot e^{-(s_A/\Delta x)\cdot\Delta t} = e^{-[-\ln(h_{I,D})+(s_A/\Delta x)\cdot\Delta t]}$$

For notational simplicity, let $\alpha = -\ln(h_{I,D})$, in which case:

$$e^{-[-\ln(h_{I,D})+(s_A/\Delta x)\cdot\Delta t]} = e^{-[\alpha+(s_A/\Delta x)\cdot\Delta t]}$$

The power term $\alpha + (s_A/\Delta x)$ is a type of exponential rate and can be treated as the sum of six independent rates. The quantity $(1/6) \bullet \alpha + (s_A/\Delta x) \bullet \Delta t$ is the rate at which a particle moves to the downstream neighboring cell (by turbulent diffusion or advection), where it is assumed for simplicity that advective flow from a cell is in just one direction. The quantity $(1/6) \bullet \alpha$ is the respective rate at which the particle moves to each of the other five nearest neighbor cells (due to turbulent diffusion). Given that the particle moves, the probability that it moves to a specific neighboring cell is the rate of movement to that cell divided by the total rate of movement. Because the probability that the particle moves is $1 - h_{I,D} \bullet h_{..,A}$, it follows that

$$p_{I,\text{down}} = \frac{(1/6)\cdot\alpha + (s_A/\Delta x)\cdot\Delta t}{\alpha + (s_A/\Delta x)\cdot\Delta t}\cdot(1 - h_{I,D}\cdot h_{I,A}) \tag{B14}$$

$$p_{I,\text{other}} = \frac{(1/6)\cdot\alpha}{\alpha + (s_A/\Delta x)\cdot\Delta t}\cdot(1 - h_{I,D}\cdot h_{I,A}) \tag{B15}$$

By similar arguments, the jump probabilities for a particle in the other cells can be derived:

$$p_{\text{one-wall,down}} = \frac{(1/5)\cdot[-\ln(h_{\text{one-wall,D}})] + (s_A/\Delta x)\cdot\Delta t}{[-\ln(h_{\text{one-wall,D}})] + (s_A/\Delta x)\cdot\Delta x} \times (1 - h_{\text{one-wall,D}}\cdot h_{..,A}) \tag{B16}$$

$$p_{\text{one-wall,other}} = \frac{(1/5)\cdot[-\ln(h_{\text{one-wall,D}})]}{[-\ln(h_{\text{one-wall,D}})] + (s_A/\Delta x)\cdot\Delta t} \times (1 - h_{\text{one-wall,D}}\cdot h_{..,A}) \tag{B17}$$

$$p_{\text{two-wall,down}} = \frac{(1/4)\cdot[-\ln(h_{\text{two-wall,D}})] + (s_A/\Delta x)\cdot\Delta t}{[-\ln(h_{\text{two-wall,D}})] + (s_A/\Delta x)\cdot\Delta t} \times (1 - h_{\text{two-wall,D}}\cdot h_{..,A}) \tag{B18}$$

$$p_{\text{two-wall,other}} = \frac{(1/4)\cdot[-\ln(h_{\text{two-wall,D}})]}{[-\ln(h_{\text{two-wall,D}})] + (s_A/\Delta x)\cdot\Delta t} \times (1 - h_{\text{two-wall,D}}\cdot h_{..,A}) \tag{B19}$$

$$p_{\text{three-wall,down}} = \frac{(1/3)\cdot[-\ln(h_{\text{three-wall,D}})] + (s_A/\Delta x)\cdot\Delta t}{[-\ln(h_{\text{three-wall,D}})] + (s_A/\Delta x)\cdot\Delta t} \times (1 - h_{\text{three-wall,D}}\cdot h_{..,A}) \tag{B20}$$

$$p_{\text{three-wall,other}} = \frac{(1/3)\cdot[-\ln(h_{\text{three-wall,D}})]}{[-\ln(h_{\text{three-wall,D}})] + (s_A/\Delta x)\cdot\Delta t} \times (1 - h_{\text{three-wall,D}}\cdot h_{..,A}) \tag{B21}$$