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Performance of Deterministic Workplace Exposure Assessment Models for Various Contaminant Source, Air Inlet, and Exhaust Locations

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Contaminant concentration estimates from simple models were compared with concentration fields obtained by computational fluid dynamic (CFD) simulations for various room and source configurations under steady-state conditions. Airflow and contaminant distributions in a 10 × 3 × 7-m room with a single contaminant source on a 1-m high table were simulated using CFD for steady, isothermal conditions. For a high wall jet inlet, simulations were performed for nine room air exhaust locations and eight source locations. For a ceiling diffuser inlet the impact of two exhaust locations and eight source locations were investigated. Because CFD treats determinants of contaminant transport explicitly and agreed well with experimental results, it was used as the standard for comparison. Parameters of the one- and two-zone completely mixed models (CM-1 and CM-2) and the uniform turbulent diffusivity model (UD) were determined from CFD simulation results. Concentration estimates from these were compared with CFD results in the breathing zone (BZ) plane (1.5 m above the floor) for the entire BZ, the source "near field," and the source "far field." In the near field the mean percentage difference between the model concentration estimates and the CFD results for all room configurations were −21.9, 32.3, and 126% for the CM-1, CM-2, and UD models, respectively, with standard deviations of 26.8, 111, and 103%. In the far field the mean percentage difference between the model estimates and CFD results were −4.8, −2.3, and −36.3%. The CM-1 model had generally the best performance for applications such as occupational epidemiology for the conditions and configurations studied. However, CM-1 tended to underestimate the near field concentration; thus, CM-2 was judged to be better in the near field when underestimation is undesirable, such as when determining compliance with occupational exposure limits. The agreement of CM-2 estimates with CFD results in the near field was more variable than that of the CM-1. The UD model performed poorly on average in both near and far fields, and the difficulty in accurately estimating the turbulent diffusivity presents a significant impediment to UD model use for exposure estimation.

Keywords: computational fluid dynamics, exposure assessment, models

Models describing the relationship of contaminant emission rate (G), dilution airflow rate (Q), and the airborne contaminant concentration (C) in an enclosed space are important tools for estimating worker exposure. They are especially useful for making retrospective estimates and predicting future exposure during process design. However, most such models now in use are based on simplistic assumptions regarding airflow and contaminant transport, and the errors resulting from these assumptions have not been systematically evaluated. Previous evaluations have been on a case-by-case basis so that generalization to other circumstances is not possible. Thus, industrial hygienists are forced to make numerous untested assumptions or utilize uncertain safety factors to deal with model inaccuracies. Two basic model types are considered here.

COMPLETELY MIXED (CM) MODELS

These models assume that the contaminant concentration in a room, or portions of a room, may be treated as uniform. This assumption permits the development of formulas for a variety of circumstances from a contaminant mass balance equation (which sets contaminant accumulation in a defined "control volume" over a given time period equal to the inputs minus the losses of contaminant over that period). However, no workroom with localized sources and dilution air exchange has perfectly uniform concentration. Thus, it is important to understand the impact of nonuniform concentration on errors in estimating exposure.

Recognizing that concentrations in a room, especially close to a contaminant source, are not uniform, Lidwell and Lovelock[1] recommended in 1946 the use of a mixing factor to account for deviations from the completely mixed assumption. For a room with a constant clean dilution airflow rate of Q, a volume of V, and no emissions, they described the change of concentration C at a fixed point within the room as:

$$C = C_0 e^{-\Phi t} \quad (1)$$

where Φ = the mixing factor, t = time, and C_0 = the concentration at the point at $t = 0$.

For a well-mixed room, $\Phi = Q/V$. Lidwell and Lovelock recognized that Φ is a function of position within the room and may be greater than or less than Q/V.

In 1960, Brief[2] recommended using a "mixing" factor to adjust dilution ventilation flow rates computed assuming a room is completely mixed:

$$q_{eff} = mQ/V \quad (2)$$

where q_{eff} = the effective number of air changes per unit time, and m = the mixing factor, ranging from ⅓ to $\frac{1}{10}$.

In the selection of m, Brief[2] considered contaminant toxicity and the locations of inlets, outlets, and sources, as well as mixing. Thus, m is more accurately termed a "safety" factor. Jayjock[3] described the use of a similar mixing factor to compute the effective ventilation rate from the actual dilution airflow rate. He then used the effective ventilation rate to estimate concentration in both the steady-state and nonsteady-state exposure scenarios.

In reviewing corrections for nonuniform mixing, Mage and Ott[4] demonstrated that the use of m for exposure assessment is not appropriate when applied to an entire room, because the contaminant mass balance is violated. The National Research Council[5] report on exposure assessment, assessing the state-of-the-art in 1991, concluded that the development of models more sophisticated than the one-zone model (CM-1) was not justified because flow patterns are uncertain, and sources and sinks are difficult to characterize. Nevertheless, some efforts have been made to deal with the shortcomings of the CM model. The next level of sophistication of the CM model is to utilize multiple zones within a space, each of which is assumed to be completely mixed. This was suggested by Hemeon,[6] more recently discussed by Heinsohn,[7] and used to illustrate the deficiencies of using mixing factors by Nicas.[8]

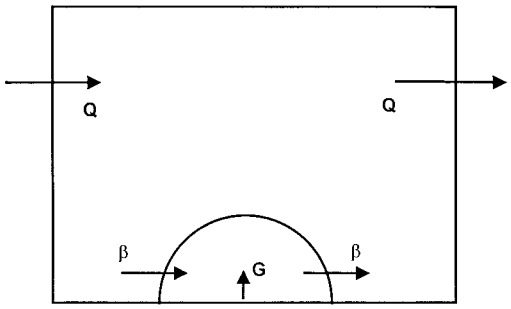

FIGURE 1. Schematic representation of the two-zone model used here, which assumes each zone is completely mixed (CM-2 model)

A commonly used two-zone model (CM-2) is illustrated in Figure 1. At steady-state with clean dilution airflow, the concentration of the two zones may be calculated as follows:

Source zone:
$$C_s = \frac{G}{Q} + \frac{G}{\beta} \quad (3)$$

Room zone:
$$C_r = \frac{G}{Q} \quad (4)$$

where
C_s = the source zone concentration at steady state
C_r = the room zone concentration at steady state
Q = the flow rate of clean dilution air into the room zone
β = the flow rate of air exchange between the two zones
G = the contaminant emission rate

The source zone is usually a cubic or hemispheric space enclosing the source. The room zone is all portions of the room outside the source zone, not including exhaust ducts.

Although the two-zone model is used increasingly, significant questions remain regarding its application. The means for determining β is poorly understood. Also, the size and shape of the near-field zone often are selected arbitrarily. However, little research has been performed in these important areas.

UNIFORM DIFFUSIVITY (UD) MODELS

UD models generally are applied close to a contaminant source (in the "near field"), where significant concentration gradients exist. These models assume that contaminant transport away from the source is due to turbulent diffusion, the intermingling and mixing of parcels of air (eddies), resulting in a net movement of contaminant from high to low concentration regions. Under turbulent flow conditions, the ratio of the turbulent diffusion rate to the concentration gradient is called the turbulent diffusivity.

A typical formulation of this model for isotropic diffusion from a point source on a flat surface was derived by analogy with heat transfer[9] and is given in Equation 5:[10]

$$C = \frac{G}{2\pi Dr}\left[1 - \text{erf}\left(\frac{r}{\sqrt{4Dt}}\right)\right] \quad (5)$$

where
D = the turbulent diffusivity
r = distance from the source
t = time after emission begins
erf = the error function

Application of this model, while taking concentration variations into account, presupposes that contaminant transport is the same in all directions from the source. This is seldom true in real workrooms because the combined actions of mechanical ventilation and natural convection usually establish convective flow past the source in some consistent direction. Under such conditions contaminant concentration distribution near the source usually resembles an outdoor air pollution plume, rather than the concentric concentration hemispheres predicted by Equation 3. Thus, workroom conditions often do not comply with the assumptions inherent in this model. Nevertheless, the accuracy of this approach has not been thoroughly evaluated.

Here the BZ concentration estimates from the simple models described above were compared with computational fluid dynamic (CFD) simulation results for various hypothetical workroom configurations at steady-state.

METHODS

To evaluate the commonly used exposure assessment models, the concentration throughout a workroom must be determined by some method that will serve as a standard of comparison. There are two basic approaches for accomplishing this: monitoring contaminant concentration in a space with controlled airflow, or using mathematical methods to estimate the concentration field. CFD, the numerical solution of the fundamental equations governing fluid flow and contaminant transport, was used here because CFD allowed rapid exploration of the effects of a variety of room configurations, flow rates, and emission rates, and provided finely resolved concentration estimates throughout the rooms.[11]

Accurate CFD simulation of a particular workroom requires careful characterization of inlet flow patterns, sources, and thermal boundary conditions. It also relies on assumptions including the treatment of turbulence and near-wall fluid phenomena. Thus, validation of CFD methods for such simulations is required. Here the authors used CFD to obtain insight into the behavior of hypothetical workrooms, not to predict the behavior of a specific room. Nevertheless, several types of validations were undertaken, including comparison with observations from full-size rooms under controlled conditions and comparison with observations from a scale model of the workroom simulated here.

CFD Accuracy and Validation

Many studies have considered broadly CFD's ability to predict concentration or velocity, but few deal with accuracy in detail. Emmerich,[12] reviewing numerous applications of CFD for indoor environments, found somewhat mixed success. However, it appears that careful use of CFD can accurately simulate flow in single compartments, even in spaces with combined radiative and convective heat transfer. Inaccurate characterization of boundary conditions seems to have been a major cause of the differences between CFD results and observation.

Here solution methods were validated for grid independence, physical plausibility, and ability to simulate experimental data. Grid independence was checked by comparing CFD results from a 30 × 24 × 36 grid with results from a 60 × 24 × 36 grid. As a measure of physical plausibility, the average exhaust concentration was compared with G/Q. Under the steady-state conditions studied here, they should be nearly equal.

The external validations relied primarily on a comparison of CFD-simulated tracer gas concentrations with experimental concentrations for a 1 × 0.7 × 0.3-m scale model of the rooms simulated here, constructed according geometrical and kinematic similarity criteria. These efforts were discussed in greater detail elsewhere.[13,14]

CFD Simulations

Airflow and contaminant distribution in a 10 × 3 × 7-m room with a single contaminant source on a 1-m high table were simulated using CFD for 22 different configurations of air inlet, air outlet, and source locations. To ensure that conditions explored represent those that may be reasonably found in real work areas, the hypothetical workroom was designed according to ventilation guidelines from Awbi,[15] ISO,[16] and ASHRAE.[17] Design rationale was presented elsewhere.[14] The effects of two different dilution air inlets were explored: (1) a 1.4-m by 0.6-m high wall jet centered horizontally, and (2) a 0.6 × 0.6-m, 3-vane ceiling diffuser.

A standing work surface was represented by a 1-m cube at the center of the room with an 0.2-m square opening in the center of the cube's upper surface serving as the contaminant source. The 1-m surface height was chosen because it is nearly midway between two recommended heights for a standing workplace. A height of 107 cm is recommended for light assembly, writing, and packing tasks, and a height of 91 cm is recommended for tasks requiring large downward or sideward forces.[18]

For the wall jet inlet and centered source table, simulations were performed for nine exhaust locations (Figure 2). For the wall jet inlet and a single exhaust outlet location, simulations were performed for eight source locations (Figure 3). For the ceiling diffuser inlet, simulations were carried out for five of these same source locations (Figure 4). (Fewer source locations were used for the ceiling diffuser because the configuration with the diffuser in the center of the ceiling has more planes of symmetry than the wall jet configuration.) The simulation conditions include a contaminant emission of 2.33×10^{-5} m³/sec and a dilution airflow rate of 14 m³/min (4 ACH), yielding a G/Q value of 100 ppm. The following conditions were employed for all simulations: (1) gas phase, neutrally buoyant contaminant, (2) steady-state, (3) negligible contaminant sinks, (4) no mechanical stirring (e.g., from fans in room or worker movements), (5) negligible emission velocity, (6) air outlet not close to source (i.e., no intentional local exhaust), (7) isothermal conditions (no heat sources or air supply buoyancy), (8) no obstructions in the room except the work table, (9) clean dilution air, (10) uniform inlet velocity, normal to the inlet fac, and (11) no consideration of worker-body wake effects.

The numerical simulations were performed with commercial CFD software (structured Fluent, V. 4.2, Fluent Inc., Lebenon, N.H.), which uses the control volume method and the SIMPLE algorithm described by Patankar.[11] The k-turbulence model was chosen to reduce run times, as it requires less computational effort than more sophisticated models. The room simulation used a uniform grid of 0.2-m cubic cells. The solution was considered converged if the sum of the normalized residuals for each conservation equation was less than 10^{-5}. The turbulence intensity was taken

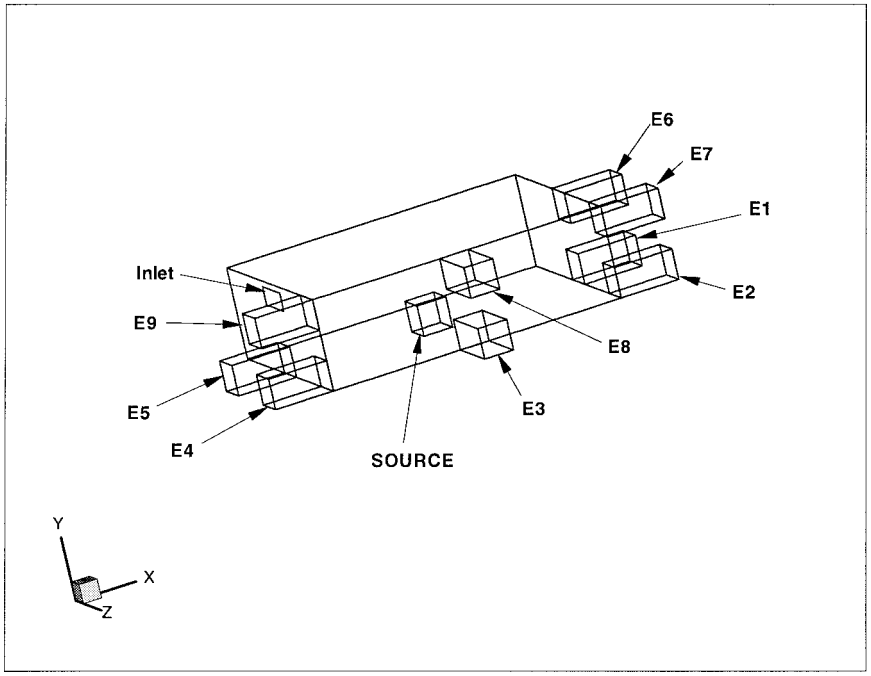

FIGURE 2. Locations of dilution air exhausts studied for the wall jet air inlet

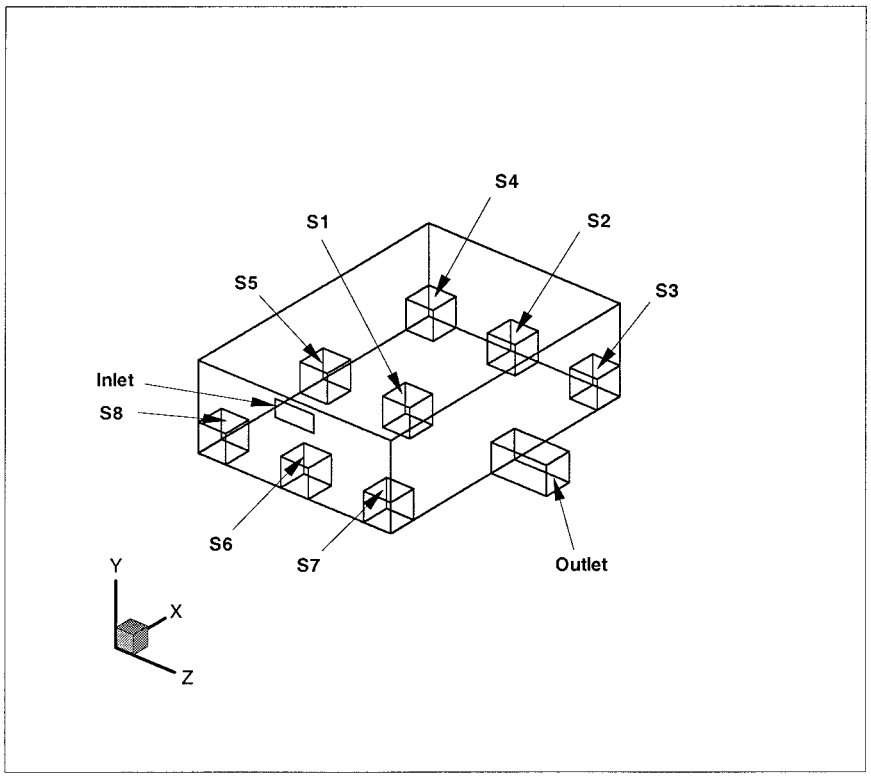

FIGURE 3. Locations of contaminant sources studied for the wall jet air inlet

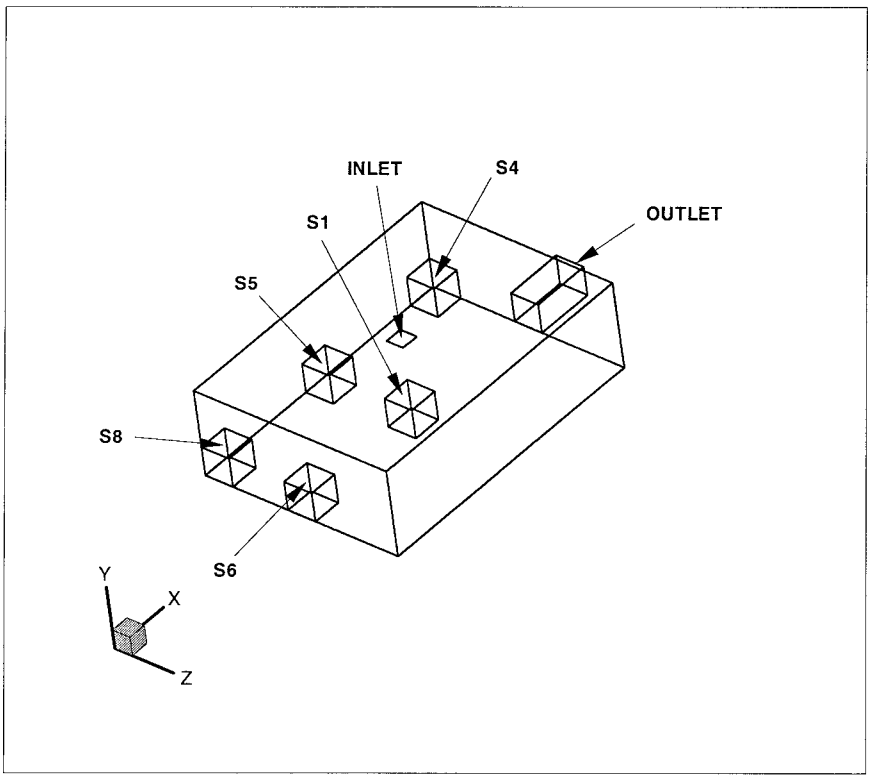

FIGURE 4. Locations of contaminant sources studied for the ceiling diffuser air inlet

to be 10%, a common practice when this quantity is not measured. The characteristic length scales were set at 1.4 m, the width of the inlet (no grill present), for the wall jet, and at 0.038 m (1.5 inches), the distance between vanes for the ceiling diffuser.

Simple Model Estimates

Comparison between simple model concentration estimates and CFD simulation results focused on the BZ plane, here defined as a plane 1.5 m above the floor. This is the average BZ height of the median male and median female in the United States.[19]

In industrial hygiene practice the assumption that a workroom is completely mixed is frequently employed.[20] In specifying the dilution airflow rate needed to comply with an occupational exposure limit, the flow rate calculated as $Q = G/C$ is multiplied by a safety factor accounting for incomplete mixing. However, the use of a safety factor to calculate the concentration to which workers are exposed yields an upper bound estimate.[20] When exposure is assessed for occupational epidemiologic research, the objective is to estimate the most likely exposure level, not the upper bound. A specific worker's exposure may be greater than or less than G/Q, the CM-1 estimate; in fact, the room mean concentration can be greater or less than G/Q, depending on whether more dilution air or more contaminant is "short circuited" to the exhaust before mixing with the room contents.[4,14] Thus, mixing is generally ignored when calculating the most likely exposure using deterministic models. For these simulations, the emission rate and the dilution airflow rate were constant. Therefore, the CM-1 model concentration estimate—100 ppm—was the same for all simulations.

The values of the CM-2 and UD model parameters were determined as an industrial hygienist would in a practical application, except that the data were taken from CFD simulations instead of from measurements. The rate of air exchange between the source and room zones in the CM-2 model was based on the simulated air velocity field. Here the CM-2 source zone was a 1-m radius hemisphere concentric with the source opening. The average air speed just upwind of the source zone was determined from CFD results. The CM-2 exchange rate, β, for each simulation was calculated as the product of the average air speed and the cross-sectional area of the hemispheric source zone. The zone cross-section was corrected for truncation for sources close to room walls and for air direction. For each simulation, eddy diffusivities, Ds, were calculated from the simulation emission rate and concentrations values at locations both within the room air boundaries and 2-m from the source center along lines parallel to the three major room axes. The average D from locations meeting these criteria for each simulated room was used to calculate the UD model concentration estimates for that room.

Comparisons

For each room simulated, the CM-1, CM-2, and UD concentration estimates and the percentage differences between these simple model estimates and CFD concentrations were calculated at each of the 1700+ CFD solution nodes individually within the full BZ plane using a computer program written specifically for this purpose. The program then calculated the mean, minimum, and maximum percentage differences separately for the BZ near field, BZ far field, and the entire BZ. For CM-2, note that BZ near field includes some points from the CM-2 source zone and some from the CM-2 room zone.

TABLE I. Percentage Difference Between CM-1 and CFD

	Entire BZ				Near-Field BZ				Far-Field BZ			
Configuration[A]	N	Mean	Min	Max	N	Mean	Min	Max	N	Mean	Min	Max
WJ-E1 (=WJ-S1)	1715	20.5	−76.4	67.8	172	3.6	−76.4	60.4	1543	22.4	−58.7	67.8
WJ-E2	1715	−11.0	−54.5	38.4	172	−3.7	−54.5	38.4	1543	−11.8	−49.5	30.2
WJ-E3	1715	−34.7	−63.3	−4.3	172	−30.1	−63.3	−4.3	1543	−35.2	−60.7	−9.1
WJ-E4	1750	−6.4	−60.7	36.2	172	−7.0	−60.7	36.2	1578	−6.3	−53.8	27.9
WJ-E5	1750	−1.7	−54.4	58.9	172	27.2	2.7	58.9	1578	−4.8	−54.4	58.9
WJ-E6	1715	−30.7	−78.4	−7.8	172	−34.4	−78.4	−7.8	1543	−30.3	−67.7	−11.5
WJ-E7	1715	−12.9	−48.3	45.6	172	1.0	−48.3	45.6	1543	−14.4	−43.8	36.7
WJ-E8	1715	−33.5	−70.1	−5.7	172	−33.5	−70.1	−5.7	1543	−33.5	−65.0	−8.3
WJ-E9	1750	−9.7	−67.0	24.8	172	−0.7	−21.9	22.0	1578	−10.7	−67.0	24.8
WJ-S2	1715	−14.9	−83.6	28.0	114	−32.4	−83.6	16.1	1601	−13.7	−43.3	28.0
WJ-S3	1715	171.0	−77.0	404.0	84	−11.7	−77.0	114.0	1631	180.0	−65.9	404.0
WJ-S4	1715	−37.2	−77.5	−13.4	75	−48.5	−77.5	−19.0	1640	−36.6	−71.6	−13.4
WJ-S5	1715	−39.6	−91.1	−14.5	114	−52.8	−91.1	−20.9	1601	−38.6	−81.5	−14.5
WJ-S6	1715	−15.5	−89.9	21.4	114	−37.1	−89.9	7.1	1601	−13.9	−79.5	21.4
WJ-S7	1715	15.6	−95.1	89.6	84	−70.1	−95.1	11.8	1631	20.0	−84.2	89.6
WJ-S8	1715	−14.2	−80.5	15.8	75	−41.7	−80.5	2.6	1640	−13.0	−68.7	15.8
CD-S1	1715	1.6	−91.3	23.0	172	−15.7	−91.3	18.3	1543	3.6	−17.0	23.0
CD-S4	1715	−10.1	−52.0	13.4	75	−15.5	−32.9	−4.3	1640	−9.8	−52.0	13.4
CD-S5	1715	−13.7	−83.4	18.3	114	−40.8	−83.4	12.5	1601	−11.7	−74.5	18.3
CD-S6	1715	−20.1	−93.6	22.1	114	−59.6	−93.6	−28.6	1601	−17.3	−73.6	22.1
CD-S8	1715	−30.7	−80.0	6.3	75	−56.0	−80.0	−41.9	1640	−29.5	−78.2	6.3

[A]WJ = wall jet; CD = ceiling diffuser; S# = source location; E# = exhaust location.

RESULTS

Validation

Grid independence was demonstrated. The mean node-to-node difference between the concentrations from the $30 \times 24 \times 36$ cell grid and the concentrations from a grid with twice as many cells was only −0.3%. Thus, to shorten the computation time, the coarser of the two grids was used. The mass balance of the contaminant in these two runs was checked by integrating the contaminant concentration across the outlet duct. The averages were compared with G/Q. Agreement was within 1% for both grids.

For the scale model chamber, the mean simulated concentrations at three elevations within the chamber were compared with the mean observed concentrations at these levels. The mean for the uppermost elevation was significantly different from the observed mean ($p \leq 0.05$). The overall means and the means at the chamber middle and lowest levels were not significantly different. Graphical comparison of experimental isobutylene concentrations and the simulated concentrations showed that the CFD-derived concentration distributions agreed well with the observed data.[14] Overall, this validation exercise demonstrated that the CFD approaches used here, including the grid characteristics and the treatment of turbulence and boundary conditions, performed well in modeling a chamber geometrically and kinematically similar to the simulated rooms. Thus, it appears that CFD is a valid means of generating plausible concentration distributions for these hypothetical rooms.

CM-1 Model

Table I presents summary statistics for point-by-point percentage differences of CM-1 from CFD concentration estimates for the entire room, the source "near field" and the source "far field." Here, the near field is defined as the portion of the BZ within 1.5 m horizontal distance of the source center. The far field is the remainder of the BZ. Each simulation represents a different room configuration as shown in Figures 2 through 4.

Table I shows that the CM-1 BZ concentration on average underestimated the CFD concentration over the entire BZ for all but three of the room configurations studied. This suggests that incoming dilution air is more likely to "short circuit" the room than contaminant emissions for the two common air inlet types studied. For comfort purposes, air typically is introduced to a room so that the highest air velocities are along the ceiling and down the walls. Because exhaust vents often are located in the walls, a significant portion of dilution air may reach the exhaust before mixing with room contents, reducing the effectiveness of this airflow for exposure control. Examination of the CFD airflow patterns downwind of the source show that the mean percentage difference is positive (i.e., CM-1 overestimates CFD) only when a large portion of the contaminant plume from the source was carried directly to an exhaust opening. The WJ-S3 configuration is the most extreme example of this, as demonstrated by the stream traces (i.e., paths of hypothetical, massless particles injected into the flow field at the source) in Figure 5, which show the most likely paths of contaminant leaving the source.

The maximum values in Table I indicate that CM-1 underestimated concentrations throughout the entire BZ for five configurations. These were all rooms with wall jet inlets and with exhaust and source located so that a significant amount of incoming dilution air reached the exhaust before reaching the source. Also, the CM-1 model underestimated the CFD results by a greater degree in the near field than in the far field, simply because CFD concentrations in the near field generally are higher than in the far field, whereas the CM-1 model estimated a single concentration for the entire room.

CM-2 Model

Because concentrations generally are higher near a source, the CM-1 model appears to underestimate exposure of workers stationed near a source, as demonstrated above. The CM-2 model

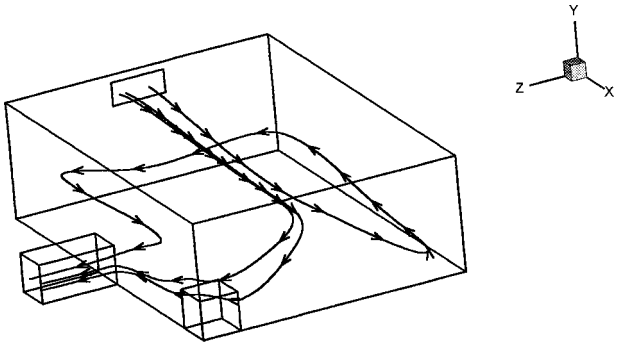

FIGURE 5. Stream traces for wall jet air inlet and source location S3. A stream trace is the most probable path taken by a gas molecule released at a specific location within the room and was estimated by CFD simulation.

allows near-field concentration to be higher than the concentrations in the rest of the room. Table II presents summary statistics of the percentage differences between CM-2 and CFD concentration. Examination of the mean differences for the entire BZ in Tables I and II shows that CM-2 behaves very much like CM-1. The CM-2 mean differences regressed versus the CM-1 mean differences yielded a straight line with slope of 0.93, an intercept of −7.1%, and a regression coefficient of 0.99. This agreement is anticipated because the concentration estimates for CM-1 and CM-2 are nearly the same for the far field, which encompasses more than 90% of BZ, a horizontal plane 1.5 m above the floor.

For the near field, the average percentage difference shows that the CM-2 model tended to overestimate the CFD concentration, in one instance by an average of 191%. Clearly, the inlet used has a significant impact on the mean difference. For 4 of the 5 ceiling-diffuser configurations and for only 1 of the 16 wall-jet configurations, CM-2 underestimated, on average, the CFD simulated near-field concentrations. Examination of the minimum and maximum percentage differences for the near field showed that CM-2 had a much wider range of differences than CM-1, twice overestimating CFD near-field levels by more than an order of magnitude. Although the CM-2 concentration estimates were uniform within the near-field zone, CFD simulated distributions generally formed a plume of high concentration downwind of the source and had relatively low concentration levels upstream. Thus, use of the CM-2 model resulted in a very wide range of percentage difference from CFD results for the near field, as shown in Table II.

UD Model

Like the CM-2 model, the UD model accounts for higher concentrations near a contaminant source. In contrast with the CM-2 model, UD model concentration decreased continuously with the inverse of distance from the source. Table III shows summary statistics for the percentage differences of the UD estimates from the CFD simulated concentrations. The mean differences for the entire BZ are all negative. Thus, unlike the CM-2 model, the UD model underestimated, on average, the CFD-simulated values for all configurations studied.

In the near field, the UD model generally overestimated the CFD results, often by more than a factor of two. The mean difference between UD and CFD estimates was negative for one configuration only, WJ-S7, where the source was in a corner on the same side of the room as the outlet. The simulation predicted that a significant portion of the airflow along the near wall in Figure 3 would enter the outlet duct, thus depleting the return circulation along the near wall and greatly reducing dilution of the contaminant plume in the near corner. The maximum differences in the near field were much higher than those for the CM-1 model, but lower than those for the CM-2 model. In general, the performance of the UD model in the near field was characterized by overestimation of CFD concentration by factors of 2 to 6.

TABLE II. Percentage Difference Between CM-2 and CFD

	Entire BZ				Near-Field BZ				Far-Field BZ			
Configuration[A]	N	Mean	Min	Max	N	Mean	Min	Max	N	Mean	Min	Max
WJ-E1 (=WJ-S1)	1750	30.7	−52.0	470	172	67.4	−52.0	470	1578	26.7	−45.6	77.4
WJ-E2	1750	−2.9	−32.3	296	172	45.6	−27.2	296	1578	−8.2	−32.3	51.2
WJ-E3	1750	−29.2	−50.2	181	172	5.8	−47.7	181	1578	−33.0	−50.2	3.0
WJ-E4	1750	1.4	−36.8	305	172	43.4	−36.0	305	1578	−3.2	−36.8	47.1
WJ-E5	1750	7.1	−24.0	347	172	65.5	−22.9	347	1578	0.8	−24.0	75.4
WJ-E6	1750	−24.4	−60.2	234	172	8.1	−60.2	234	1578	−28.0	−57.0	0.9
WJ-E7	1750	−4.9	−30.5	298	172	50.1	−24.4	298	1578	−10.8	−30.5	60.1
WJ-E8	1750	−27.8	−51.4	201	172	5.8	−51.4	201	1578	−31.5	−51.4	4.2
WJ-E9	1750	−2.8	−45.5	295	172	29.6	−45.5	295	1578	−6.3	−44.0	34.2
WJ-S2	1750	−6.9	−51.7	399	128	41.2	−51.7	399	1622	−10.7	−34.8	40.8
WJ-S3	1750	187.0	−59.9	1180	94	191.0	−59.9	1180	1656	187.0	−56.0	474.0
WJ-S4	1750	−30.5	−66.3	369	84	49.1	−66.3	369	1666	−34.5	−65.1	−12.9
WJ-S5	1750	−35.0	−83.8	309	114	−5.1	−83.8	309	1636	−37.1	−79.5	−13.6
WJ-S6	1750	−10.7	−89.2	416	114	30.5	−89.2	416	1636	−13.5	−79.5	31.5
WJ-S7	1750	25.6	−91.0	1160	84	70.6	−91.0	1160	1666	23.4	−81.9	119.0
WJ-S8	1750	−6.6	−73.0	705	75	74.6	−73.0	705	1675	−10.3	−67.7	26.1
CD-S1	1750	2.9	−71.8	170	172	1.9	−71.8	170	1578	3.0	−17.6	23.3
CD-S4	1750	−8.1	−49.3	95	84	18.1	−25.2	95.3	1666	−9.4	−49.3	13.3
CD-S5	1750	−11.8	−77.3	125	114	−17.6	−77.3	125	1636	−11.4	−70.5	18.1
CD-S6	1750	−18.8	−80.3	44	114	−46.3	−80.3	44.5	1636	−16.9	−73.6	22.2
CD-S8	1750	−28.4	−75.0	82	75	−14.6	−74.0	82.9	1675	−29.0	−75.0	7.2

[A]WJ = wall jet; CD = ceiling diffuser; S# = source location; E# = exhaust location.

TABLE III. Percentage Difference Between UD and CFD

	Entire BZ				Near-Field BZ				Far-Field BZ			
Configuration[A]	N	Mean	Min	Max	N	Mean	Min	Max	N	Mean	Min	Max
WJ-E1 (=WJ-S1)	1750	−10.6	−57.0	378	172	123.0	−28.9	378	1578	−25.2	−57	116
WJ-E2	1750	−3.8	−63.6	563	172	189.0	23.2	563	1578	−24.9	−63.6	149
WJ-E3	1750	−7.9	−64.4	523	172	171.0	16.9	523	1578	−27.4	−64.4	124
WJ-E4	1750	−6.0	−62.7	517	172	167.0	5.4	517	1578	−24.9	−62.7	132
WJ-E5	1750	−4.6	−59.7	591	172	194.0	30.1	591	1578	−26.3	−59.7	161
WJ-E6	1750	−8.3	−58.9	446	172	149.0	−0.7	446	1578	−25.4	−58.9	113
WJ-E7	1750	−0.6	−62.8	637	172	214.0	32.1	637	1578	−24.0	−62.8	172
WJ-E8	1750	−8.0	−59.6	503	172	163.0	21.0	503	1578	−26.7	−59.6	129
WJ-E9	1750	−9.0	−62.4	455	172	142.0	−1.2	455	1578	−25.4	−62.4	119
WJ-S2	1750	−32.1	−79.3	215	128	97.3	22.5	215	1622	−42.3	−79.3	113
WJ-S3	1750	−13.0	−78.5	362	94	90.7	−51.6	362	1656	−18.9	−78.5	130
WJ-S4	1750	−38.8	−84.8	357	84	155.0	−3.6	357	1666	−48.6	−84.8	101
WJ-S5	1750	−34.6	−75.5	322	114	86.3	−48.5	322	1636	−43.0	−75.5	84.7
WJ-S6	1750	−43.8	−80.5	283	114	64.2	−73.5	283	1636	−51.4	−80.5	97.5
WJ-S7	1750	−42.9	−74.7	102	84	−25.8	−74.7	102	1666	−43.7	−71.6	88.8
WJ-S8	1750	−38.6	−83.8	287	75	101.0	−24.0	287	1675	−44.8	−83.8	112
CD-S1	1750	−30.5	−71.2	193	172	45.4	−54.7	193	1578	−38.7	−71.2	43.4
CD-S4	1750	−44.0	−75.9	381	84	159.0	29.8	381	1666	−54.3	−68.2	59.4
CD-S5	1750	−44.7	−73.2	232	114	44.9	−61.5	232	1636	−51.0	−64.1	61.2
CD-S6	1750	−37.5	−68.2	101	114	23.7	−57.4	101	1636	−41.8	−73.2	51.8
CD-S8	1750	−42.2	−64.1	340	75	118.0	−28.5	340	1675	−49.4	−75.9	46.1

[A]WJ = wall jet; CD = ceiling diffuser; S# = source location; E# = exhaust location.

The eddy diffusivities calculated from the CFD-simulated concentration fields are listed in Appendix I. The D values tend to be toward the lower end of the range reported of industrial workrooms. Because the aim of this study was to explore the effects of inlet type, and source and exhaust locations, some principal determinants of room turbulence, airflow rate and room size, were the same for all simulations. Thus, room Reynolds number was constant and D varied only moderately in these simulations.

Discussion

Table IV presents an overview of the percentage differences between the models' concentration estimates and CFD simulation results. In the near field, the CM-1 model underestimated CFD concentrations by an average of 22% over all the simulations. The near-field estimates from the CM-2 and UD models overestimated CFD concentrations by 32 and 126%. For estimating near-field concentrations, the CM-1 and CM-2 models were similar in absolute accuracy based on their agreement with CFD results, but CM-1 underestimated and CM-2 overestimated the CFD near-field concentrations. In the near field, the CM-2 model provided a margin of safety on average, but its percentage difference from CFD had much greater variability than the CM-1 model. In the far field, the CM-1 and CM-2 concentrations were essentially the same. Therefore, their ability to estimate CFD concentration results is also the same. On average, the UD model greatly overestimated near-field CFD concentrations and underestimated far-field CFD concentrations. In both regions of the BZ plane, the UD model had worse average performance than the CM-1 and the CM-2 models.

TABLE IV. Summary Statistics of Percentage Difference of Model from CFD Concentration Estimates Over All Simulations

	Near Field		Far Field	
Model	Mean	SD	Mean	SD
CM-1	−21.9	26.8	−4.8	29.5
CM-2	32.3	111	−2.3	31.4
UD	126	103	−36.3	28.4

The relative model performance can be understood by comparing concentration distributions for typical simulations. Figure 6 shows the concentration distributions produced by CFD, the CM-2 model, and the UD model for two simulations using source location S5, one with a wall jet inlet and the other with a ceiling diffuser. (Because the CM-1 model assumes that the concentration is uniform throughout the workroom, the CM-1 estimate is not shown). The principal difference between CFD and the simpler models is its ability to account for the complex interaction of velocity and contaminant concentration, predicting a plume of contaminant blowing downwind from the source. This plume mixes with and is diluted by room air. The localized momentum of airflow entering a room and the circulation of air within a room produces patterns of contaminant distribution generally more complex that those resulting from point source emissions to the outdoor air. For the CM-2 and UD models, the shape of the concentration contours is determined not by consideration of airflow patterns but by the simplifying assumptions inherent in model formulation.

Appropriate application of these models depends on the purpose for estimating exposure. For some applications, such as occupational epidemiology, the objectives are to achieve the most accurate exposure estimate possible, and to characterize the errors associated with these estimates. As a basis for setting occupational exposure limits (OELs), a "neutral bias" (small absolute error) is desirable because overestimation can lead to excessively lenient OELs and underestimation can lead to overly stringent OELs. In occupational epidemiology, random errors in exposure may lead to classification errors and a greater risk of accepting a false null

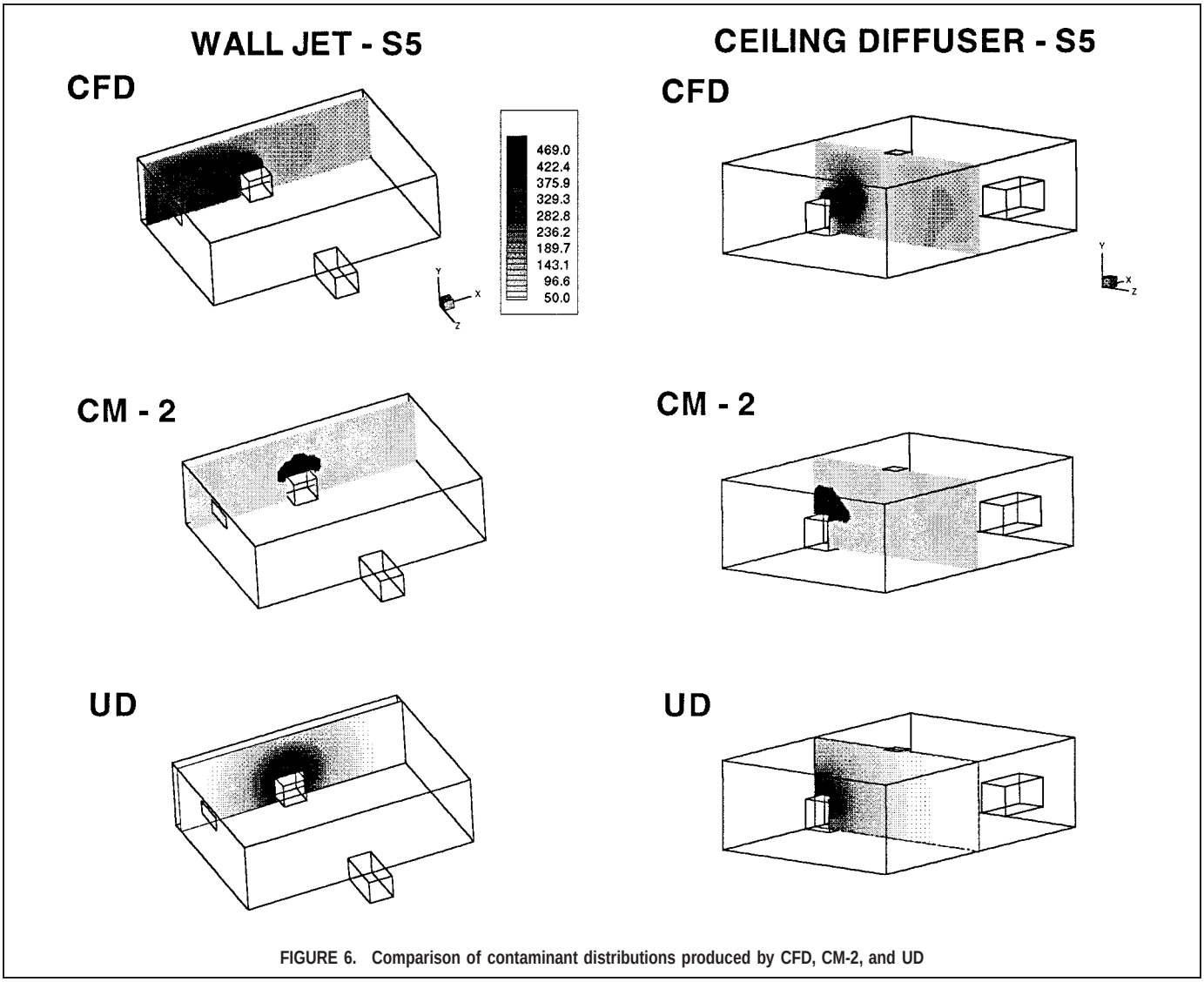

FIGURE 6. Comparison of contaminant distributions produced by CFD, CM-2, and UD

hypotheses. Such applications contrast with the exposure estimation to protect workers from overexposure, or to judge compliance with an OEL. For these purposes, models that overestimate exposure are acceptable because they maintain a margin of safety, whereas models that underestimate exposure may lead to worker overexposure.

Appropriate use of these models also requires thorough consideration of their assumptions, strengths, and limitations. The CM-1 model requires the least information, only G and Q. The flow rate often may be measured easily, but emission rates are more difficult to determine accurately. For emission caused by evaporation of a liquid, the emission rate is highly dependent on airflow patterns near the source. Thus, any measurement approach that affects airflow near such a source can change the emission rate. Rate estimates based on material consumption are often averaged over long time periods, preventing consideration of temporal variation of emissions. For the room configurations studied, the assumption of uniform room concentration in CM-1 produced an underestimation of concentration on average, especially in the near field. However, the percentage difference between CM-1 and CFD results was less variable than this difference for the CM-2 and UD models. Therefore, CM-1 appears to be a reasonable choice for obtaining the most accurate exposure estimate, or when the information available is limited to G and Q.

Unlike the CM-1 model, the CM-2 model produced an average overestimation of CFD concentrations in the near field. The percentage agreement of CM-2 with CFD concentration was more variable than CM-1. Nevertheless, for the conditions studied here CM-2 appears to be more appropriate than CM-1 for near-field worker protection and compliance determination because it provided a margin of safety. However, the near-field CM-2 concentration estimate approaches the CM-1 estimate as the ratio of β to Q increases. The near-field concentration ratio of CM-2 to CM-1 equals 3.0 at $\beta/Q = 0.5$, 2.0 at $\beta/Q = 1.0$, 1.5 at $\beta/Q = 2$, and 1.1 at $\beta/Q = 10$. Thus, in rooms where $\beta/Q > 10$, the difference between the CM-1 and CM-2 estimates is less than 10%.

A major difficulty in applying the CM-2 model is the estimation of β. Sometimes β may be based on air velocity measurements. First, the airflow direction near the source must be determined, for instance, with a "smoke" tube. Then the average air speed upstream of the source zone is determined. For hemispheric source zones, various authors[6,8] have suggested that the average air speed should be multiplied by half the surface area of a hemisphere (πr^2) to calculate β. However, this would be correct only if the mean velocity normal to the hemisphere surface were used. The mean component of velocity normal to a hemispheric surface

is difficult to determine. A more direct approach is to use the cross-sectional area of the hemisphere as viewed from the direction of airflow. For horizontal airflow and a source away from the walls and other obstructions, the cross-sectional area of a hemispheric source zone is $\pi r^2/2$. Using the average velocity upwind of the source zone, this method produces a β one-half that calculated using the surface area, and thus a higher source zone concentration estimate.

The UD model did not perform well in these comparisons, greatly overestimating the CFD near-field concentrations and underestimating the CFD far-field concentrations, on average. Like the CM-2 percentage differences from CFD results, the UD percentage differences varied greatly within the near field. These performance characteristics result from the intrinsic constraints of this model. Two of its principal assumptions are that contaminant transport is by turbulent diffusion only and that pollutant transport is independent of direction from the source. For these assumptions to be correct, there must be no persistent convective flow patterns near the source. Paradoxically, the turbulence necessary for eddy diffusion in rooms is created and maintained principally by convective airflow. Because most work areas have some convective flows (mechanical, natural, or both), which significantly affect contaminant distribution even at low air speeds, few conform to these assumptions. As is evident from Equation 5, the UD concentration changes with the inverse of distance from the source. As pointed out above, this overestimated the upwind near-field concentrations. Also, the UD estimate continues to decrease with distance, even though mixing in the far field tends to reduce the concentration gradients, resulting in underestimation far from the source. In addition, far-field accuracy suffers because the UD model does not take the effect of dilution airflow into account.

Like the CM-2 model, a parameter must be determined to use the UD model. The turbulent diffusivity, D, can be based on measured concentrations and estimated emissions for a specific workroom. However, if measurements of C are available, the use of a mathematical model may be superfluous for exposure assessment. Estimates of D for various workrooms have been reported, ranging from 0.1 to 11 m^2/min,[21–25] but no relationship between D and physical room characteristics has been developed. Also, when the UD model was used to estimate emission factors of hexavalent chromium from plating baths, deviation from the fundamental assumptions due to factors such as the presence of multiple sources and convective transport by cross-drafts, were thought to prevent valid estimation of emission rate and eddy diffusivities for some time periods.[24] Finally, there has been little effort to define the errors in measured D values. Thus, problems determining D are now a significant impediment to using the UD model for exposure assessment as acknowledged by Jayjock.[20]

CONCLUSIONS

The conclusions of this study are subject to various limitations. Although a wide range of exhaust and source locations and two very common air inlet types were studied, workrooms can differ in many ways from the configurations and conditions simulated, including in room shape and dimensions; thermal characteristics; the presence of fans, moving workers, and machines; buoyant contaminant plumes; and temporal variation. The performance of these deterministic models may be different for cases not simulated. Although quantitative agreement of models with CFD would probably be altered by changes in configurations and conditions, the fundamental qualitative characteristics of model behavior is unlikely to be affected. For instance, these models will still not be able to account for the effect of convection on contaminant distribution.

In addition to differences between real and simulated rooms, CFD is not able to predict exactly the velocity and concentration for any particular room. Although the CFD approaches have been validated, the simulation results are not perfect. Nevertheless, moderate inaccuracies of CFD simulation results should have little impact on model evaluations because the values of G, Q, β, and D employed in the simple models were based the CFD simulations.

For the source near field, CM-1 appears to be superior to other models for exposure assessment applications such as occupational epidemiology and setting OELs required, because CM-1 estimates were the most "neutrally biased" and their differences from CFD results had the lowest variability. Also, CM-1 requires knowledge of only emission rate and flow rate. For exposure assessment performed to ensure worker protection or to determine compliance with an OEL, the CM-2 model is preferable for room configurations and conditions like those simulated here because CM-2 overestimated CFD results and thus provides a margin of safety. The need to estimate β, the air exchange rate between the source zone and the room zone, limits applicability of CM-2, especially in retrospective and prospective exposure assessment. In the far field, CM-1 and CM-2 performed nearly identically.

The UD model performed poorly on average in both near and far fields. The mathematical relation between concentration and distance from the source did not agree well with CFD-simulated contaminant distribution patterns. In addition, the difficulties in accurately estimating D, the turbulent diffusivity, present a significant impediment to UD model use for exposure estimation.

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APPENDIX I. Eddy Diffusivity Values Calculated From CFD Simulation Results

Configuration	D, m²/min
High Wall Jet Inlet	
E-1	1.15
E-2	0.87
E-3 (S-1)	0.65
E-4	0.90
E-5	0.97
E-6	0.67
E-7	0.86
E-8	0.64
E-9	0.86
S-2	0.81
S-3	1.39
S-4	0.57
S-5	0.60
S-6	0.88
S-7	0.89
S-8	0.68
Ceiling Diffuser Inlet	
S-1	1.20
S-4	0.82
S-5	1.00
S-6	0.65
S-8	0.53