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Modeling Contaminant Exposure and Indoor Air Quality in a Single-Family House

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Synopsis

In this study, computational fluid dynamics (CFD) and a variety of mixing models is used to evaluate the indoor air quality in a small single-family house. CO_2, CO, NO_2, formaldehyde (HCHO), and vapor are tracked throughout the house to determine the concentration levels, occupational dosing, and personal exposure for a family of two adults and two children. Variations in metabolic activity, smoking, gas stove cooking, and showering make exposure very dependent on the individual's location in the house due to pollutant migration. Door positions have a significant role in exposure, where the comparative difference in exposure may be as much as 38%. The mixing models predict the average exposure of contaminants within approximately 30% of the CFD models, but the nuances of the flow pattern are not easily observable.

Keywords CFD, mixing model, infiltration, contaminant exposure

List of Symbols

A	area [m^2]
C	concentration [ppm]
C_d	discharge coefficient
C_o	room concentration [ppm]
C_s	constant outdoor contaminant concentration [ppm]
ΔH_{npl}	distance between lowest part of opening to neutral pressure plane [m]
N	source generation rate [m^3/s]
Q	airflow rate [m^3/s]
t	time [s]
T_i	indoor temperature [K]
T_o	outdoor temperature [K]
V	space volume [m^3]
$\dot{V}$	volume flow rate [m^3/s]

Introduction

New, stricter building codes for energy conservation mandates tighter building construction, which directly reduces the amount of available fresh air from infiltration. This decrease in fresh air is a subject of intensive study as health becomes a progressively sensitive issue. Mechanical ventilation is a system increasingly implemented to respond to and aid these burgeoning trends to reduce the risk of overexposure to indoor pollutants.

In order to understand the impact of pollutants on human health, it is necessary to perform assessments of the actual exposure to these household contaminants. As personal exposure monitors are sometimes cumbersome to use and do not provide predictive data for unbuilt domains, alternative methods are quite necessary when assessing certain precautionary liabilities. Therefore the employment of the CFD and mixing models are undertaken when analyzing complex floor plans, accounting for combustion byproducts, to more accurately assess the effectiveness of the ventilation system.

Since the indoor flows are quite complex and the transport of contaminants is highly dependent on these room airflows, often a perfect mixing model is used to determine an average room contaminant concentration level. The clear advantage of such a model is its simplicity, which is calculable by hand. The heavy tradeoff stems quite clearly from the fact that it assumes instantaneous and complete mixing of the volume in which the contaminant source is located, in effect averaging a value throughout the whole room. It is clear from both numerical and experimental results that there are definitive stratifications or non-uniformities (when the airflow rate is low) in the distribution of pollutants [1]. Through better approximations of the equations that govern fluid flow, CFD provides better insight into the actual distribution of contaminants. Though expensive, this method provides a clearer understanding of pollutant transport and personal exposure. This paper provides a comparison of the personal exposure to indoor pollutants obtained with the mixing and CFD models for a single-family house.

Research Approach

House Plan and Occupancy Scenario

The single-family house shown below in Figure 1 consists of a dining/living room/kitchen area (47.2m^2), two childrens' bedrooms (11.1m^2 and 10.5m^2), a bathroom with a shower (9m^2), a hallway (7.1m^2), and a master bedroom (15m^2), each containing a variety of everyday furniture. The house has a total floor area of 100 m^2.

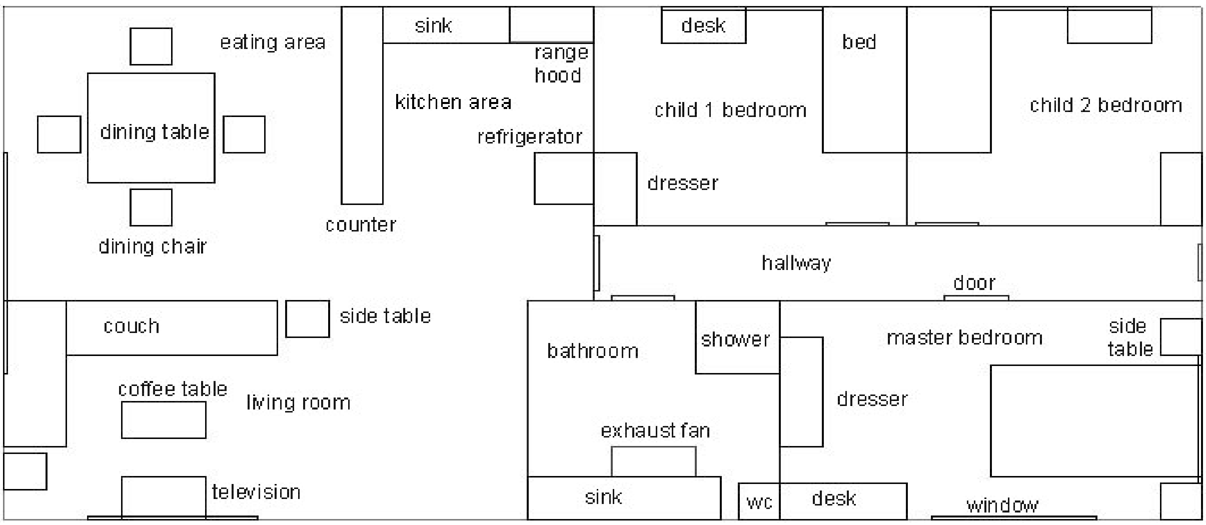

Figure 1 Single-family house layout

The occupation of each person throughout the day is shown in Figure 2. Between 0900h-1800h, the parents work and the children attend school, so nobody is at home.

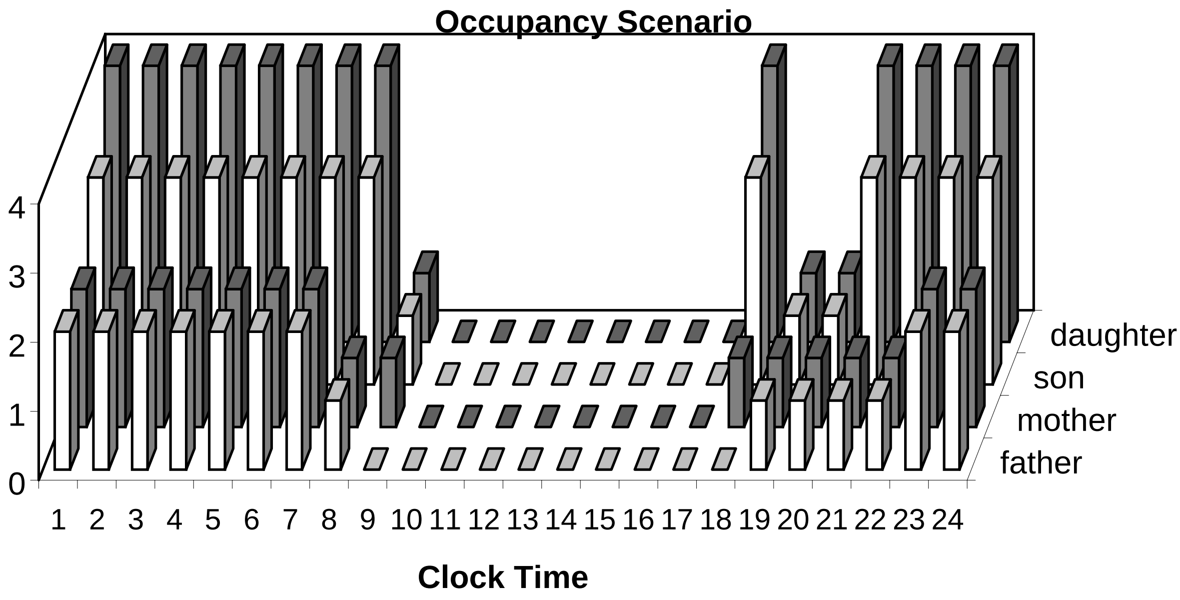

Figure 2 Occupancy scenario: (0) not at home (1) dining/living room/kitchen area (2) master bedroom (3) son's bedroom (4) daughter's bedroom

The pollutant source strengths in the house are assumed in Table 1 and Table 2.

	Outside [ppm]	Gas cooking [g/kJ]	Cigarette Smoking [g/s]	Adult awake (asleep) [g/s]	Child awake (asleep) [g/s]
CO_2	307.4	0.045	0.00065	0.0099 (0.0066)	0.0066 (0.0022)
CO	0.116	0.00005	0.00011	0	0
NO_2	0.064	0.000011	0.0000018	0	0
HCHO	0.00896	0	0.0000037	0	0

Table 1 Pollution source strengths

	Adult awake (asleep) [g/h]	Child awake (asleep) [g/h]	Breakfast [g/person]	Dinner [g/person]	Shower [g/person]
Vapor	55 (30)	45 (15)	50	300	300

Table 2 Vapor source strengths

The two mechanical extraction devices used in the house include a fixed rate bathroom exhaust, and a variable rate kitchen range hood. The bathroom exhausts at a rate of 45m^3/h, while the range hood exhausts at 45m^3/h throughout the day, and 120m^3/h during cooking, when the range top gives off 1.28kW/m^2 of heat. Baseboard convectors condition the interior space with a heat flux of 200W/m, keeping the indoor temperature between 18-20ºC.

Infiltration of outdoor air occurs at cracks around the windows, where the flow rate is proportional the window area. A global rate of 0.44 air changes per hour (ACH) throughout the house is assumed for moderate infiltration.

Mixing Models

The personal exposure of the occupants to various indoor pollutants in the house is studied by using two types of flow simulation models: mixing models and a CFD model. The differential form of a perfect mixing model based on mass balance is described as

$$V\frac{dC}{dt} = -\dot{V}\left(C - C_s\right) + N \qquad (1)$$

An integrated form of this equation is

$$C(t) = C_s + \frac{N}{\dot{V}} + \left(C_o - C_s - \frac{N}{\dot{V}}\right)\exp\left(-\frac{\dot{V}t}{V}\right) \qquad (2)$$

A single zone model will predict mixing within one room only. The large opening model essentially connects each room of the apartment to each of the other rooms via an open doorway. The transference of airflow and contaminants occurs due to internal stack effect; stratification and a temperature difference between each of the individual rooms and the hallway will induce flow, thus exchanging the room contents with that of the rest of the apartment. The rest of the apartment then exhibits perfect mixing, where the contaminants are equitably dispersed based on the floor area of each of the remaining rooms. The following equation describes the flow due to stack effect:

$$Q = C_d A\sqrt{2g\Delta H_{npl}\left(T_i - T_o\right)/T_i} \qquad (3)$$

The whole house model treats the entire house as a singular perfectly mixed space, whereas it is a conglomeration of partitioned rooms when employing the other mixing models. This is the simplest of the mixing models, as the rooms need not be treated as separate entities. The reason for the employment of this method is to drastically gain simplicity, most likely at the expense of accuracy.

CFD Model

The CFD model solves the conservation equation of mass, momentum, energy, and species concentrations with a renormalized (RNG) k-ε turbulence model [2]. The advantage of using CFD for the assessment of exposure lies in its ability to clearly model and approximate real situations. However, the fine resolution leads to increased expenditure of resources, thus taking a long time to complete the evaluation.

Comparison Technique

A comparison of CFD and hand calculated mixing models use mechanical ventilation systems and infiltration
to ascertain the differences that affect exposure. The numerically computed concentrations and dosages are compared to those calculated by a single-zone perfect mixing model, a multi-

zone large opening model, and a whole house mixing model to determine the legitimacy and the necessity for the use of CFD to assess such complex systems and interior layouts. This paper compares the results of five cases:

1. Base case: CFD simulation with the doors closed when the room is occupied
2. Open door: CFD simulation with the doors closed only when occupants are sleeping, otherwise, the doors are open
3. Single-zone mixing: mixing model that treats each room as a separate entity
4. Large opening: mixing model that treats rooms as an interconnected network of spaces, exchanging pollutants by stack effect flows through open doorways. The door positions are the same as the open door CFD case.
5. Whole house: mixing model that treats the whole house as one single entity

To be examined are the effects of the position of the door on the migration of pollutants, and whether or not simplified mathematical models (which may be computed by spreadsheets) suffice in providing accurate contaminant exposure over a twenty-four hour period. Of singular importance in the employment of the mixing models is to dramatically cut down the time for the assessment of contaminant exposure. Where the completion of CFD calculations in this case are on the order of days or weeks, a mixing model performs an equivalent evaluation in hours. The main assessments are the base case versus a single-zone perfect mixing model, the base case versus an open door CFD model, and the open door CFD simulation versus both the large opening and whole house models.

Although mixing models are simple, computational tools better predict the nuances of the real situation through the iterative solution to algebraic simplifications of the Navier-Stokes equations; simple mixing models cannot resolve such detail. And although the solutions may not be correct in every way, CFD achieves accuracy in modeling real circumstances through more practical approximations in the specifics of the simulation.

Measurement Location

It is important to select the correct location for data extraction for the numerical simulation. Due to thermal buoyancy from metabolic heat generated by the occupants, there is a boundary layer of fresher air that clings to the body as it travels upward to the breathing zone; as such, the inhaled air is different from the ambient air at the same height [3]. Since low infiltration generally produces low airflow velocities, and natural convection is dominant, exposure is influenced by entrainment in the human boundary layer [4]. It is therefore more accurate to obtain the pollutant data somewhere below the facial region, as cleaner air tends to be transported upwards to the breathing orifices.

Results and Discussion

Base Case vs. Single-Zone Mixing Case

When comparing the CFD results with those of the well-mixed model, it is clear that there are areas of very good correlation, and also times when the comparative patterns are all but lost. Although there are visible differences in the models, the inclusion of exposure over the whole day tempers these disparities to exhibit smaller differences than may be otherwise imagined.

There exists a noticeable departure from the well-mixed exponential growth pattern in the master bedroom between 2300h-0700h, as shown in Figure 3. This is attributable to the changes in the airflow pattern in the room. The mother generally receives a smaller dosage of CO_2 compared to the father since she sleeps closer to a window that generates a lateral infiltration, thus carrying contaminants emitted by the mother into the breathing zone of the father.

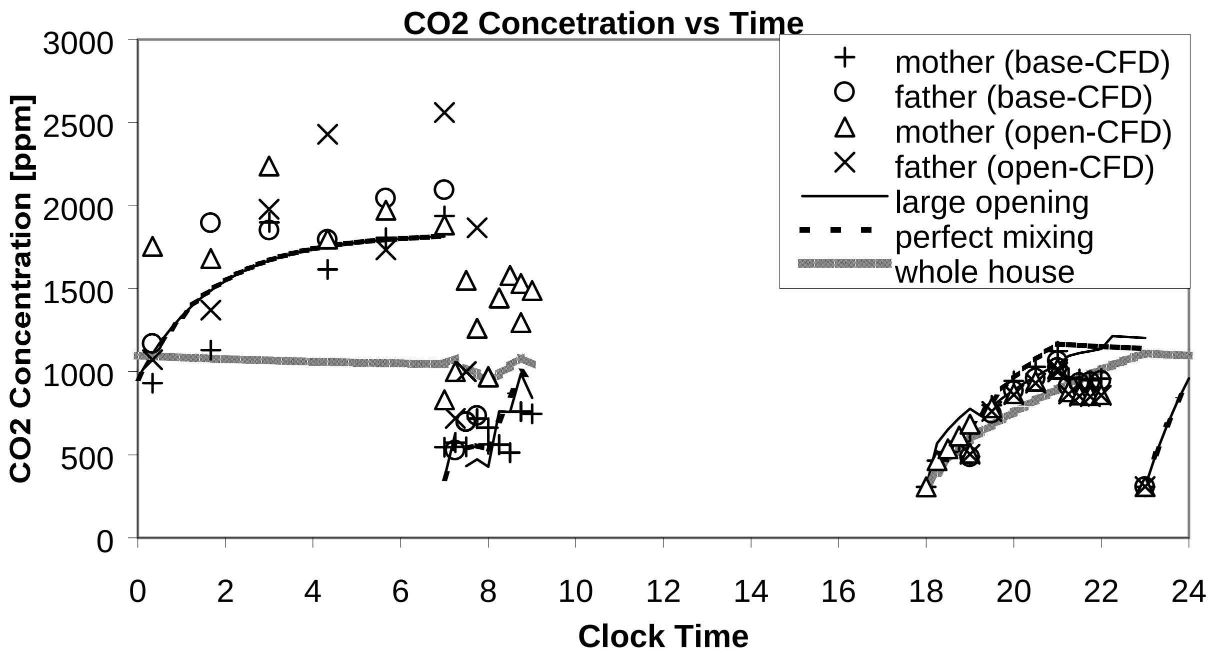

Figure 3 CO_2 concentration for the parents throughout the day

During dinner, the congregation of many heat sources generally gives rise to effective mixing, exhibited by the contaminants generated by the occupants (e.g. CO_2 and vapor). The locus of relatively contaminated air is centered around the dining table, and due to the effects of the range exhaust ventilation, much of the pollutants will tend to migrate towards this sink and away from the living room area (refer to Figure 1). When the mother and father move from the kitchen to the living room after dinner at 2100h, there is a shift down between the well-mixed model and the numerical data for CO_2. This constant shift occurs since the parents move upstream from their previous location, thereby moving into cleaner, fresher air. Since the perfect mixing model would not account for differences in exposure due to changing locations, the realization of this effect can only be under numerical or empirical observation.

Larger differences are seen when comparing those pollutants that are naturally associated with combustion (CO and NO_2). The mother and father experience both the largest dosage of CO and the greatest difference between the CFD and mixing model. This can be attributed mostly to the close proximity to which they are in contact with environmental tobacco smoke (ETS) from cigarettes. Although the mother is the primary cook in the house, the combustion by-products from the gas stove do not affect her quite as much as the cigarette smoke due to two main reasons:

1. The local range hood exhaust above the stove helps to extract and expel a large portion of the contaminants that emanate from it (as witnessed by the large departure between the mixing model and CFD results
2. Cigarette smoke emits more CO per second than does the gas stove. Comparing the maximum exposure of the mother to the gas stove for an hour while cooking dinner and an hour's worth of exposure to the CO from fifteen minutes of smoking, the mother is exposed to three and a half times as much CO from the cigarette compared to the stove.

Between 1800h-2100h and 0800h-0900h, the mother experiences gross under-representation of about 45-50% comparing the CO and NO_2 concentration of the numerical simulation to that found using the mixing model as shown in Figure 4. During the main time periods of cooking, this under prediction is due to the local exhausting of contaminants during and immediately following cooking. In addition, because of the heat produced at the stove surface, the range exhaust performance is enhanced by buoyancy capture, where a large density difference induces high degrees of natural convection to sweep contaminants toward the exhaust [5]. As well, this confluence incurs entrainment of the surrounding air, helping to prevent dispersion and diffusion of these contaminants. Perfect mixing of combustion contaminants never occurs in these situations.

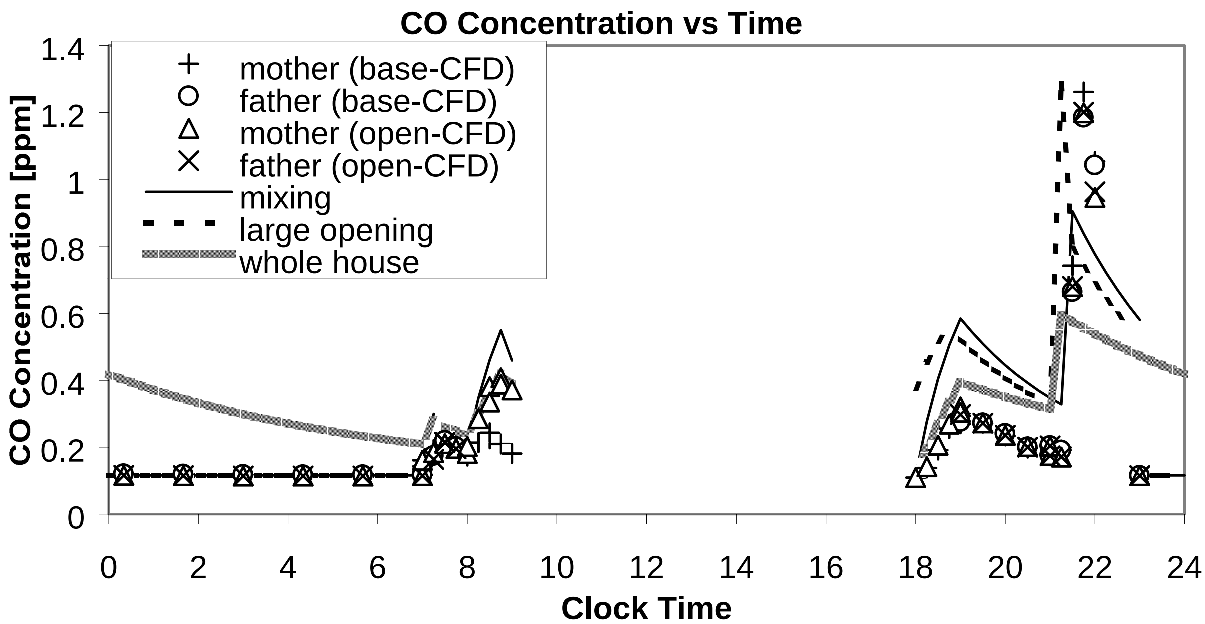

Figure 4 CO concentration for the parents throughout the day

The mixing curve for the parents never matches the CFD results for CO during smoking due to the large volume of air with which the smoking contaminants are diluted in the mixing model. Smoking releases a larger proportion of CO than any other contaminant (compared to cooking). During cooking, however, the range hood exhaust runs at three times the normal flow rate to extract cooking pollutants locally by a combination of buoyancy and velocity capture, the resolution of which may be observed using the numerical code. Localized exhaust does not play a role in helping to reduce the amount of exposure to smoking pollutants since the sources are located so remotely; therefore the concentration of contaminants is greater than predicted by the mixing model.

The exhibition of HCHO is very similar to CO for the parents during the period of smoking. Since it is only emitted during the burning of cigarettes, HCHO exerts a sudden large influence during this period. During dinner, the levels of CO in the dining room/living room area have a chance to disperse to a relatively low level after cooking, and HCHO is not even introduced during this period. When smoking begins, a large burst of contaminant emission occurs (CO and HCHO) that is traced by the CFD simulation, but is lost through the dispersion of a large volume of air for the mixing case.

Table 3 shows the percent difference in exposure over one day between the computational and perfect mixing models for this base case scenario. CO_2 and water vapor have good correlations, while the CO juxtaposition is greatly dissimilar.

Pollutant	Mother	Father	Son	Daughter	Average % Difference
CO_2	27.5	14.7	21.2	19.3	20.7
CO	54.2	48.9	27.0	54.6	46.2
NO_2	37.0	38.1	32.4	30.2	34.4
HCHO	13.7	18.4	22.4	20.6	18.7
Vapor	30.0	19.3	13.9	14.5	19.4
				Average	27.9

Table 3 Exposure difference comparing base case CFD and single-zone mixing model

In general, the differences in exposure correlate well in pairs, where the differences between models for the mother and father are of similar magnitude; the son and daughter are also similarly complemented. However, as will be seen later, the base case CFD and single-zone perfect mixing model exhibits the largest difference between two models of comparison. This occurs mainly from the fact that a mixing model comparison to that obtained from a numerical simulation is quite different. When comparing the open door CFD model and the other mixing models, the values already show a degree of inflation across the board. This sort of comparison might show better correlations may not be of true essence.

Base Case vs. Open Door Case

The reason for this specific investigation is to find whether or not the openings of the doors contribute to faster or easier migration of pollutants. The childrens' bedroom doors are modeled open at all times that they are not sleeping since privacy becomes an issue during that period. The door to the master bedroom is closed at all times, since there is no occupation of the room during the parents' waking hours.

The migration of CO into the childrens' bedrooms between 1800h-2200h occurs because the sources of CO are in the kitchen (stove top) and the living room (cigarette smoke), and the open doors allows the transportation of these pollutants into the rooms since the ventilation and infiltration extends weakly to these areas (Figure 5). Thermal stratification and stack effect tends to enhance the migration of contaminants to areas of low concentration. This trend is exhibited by all pollutants associated as by products of combustion, since the source locations are in the kitchen or living room, outside the childrens' bedrooms.

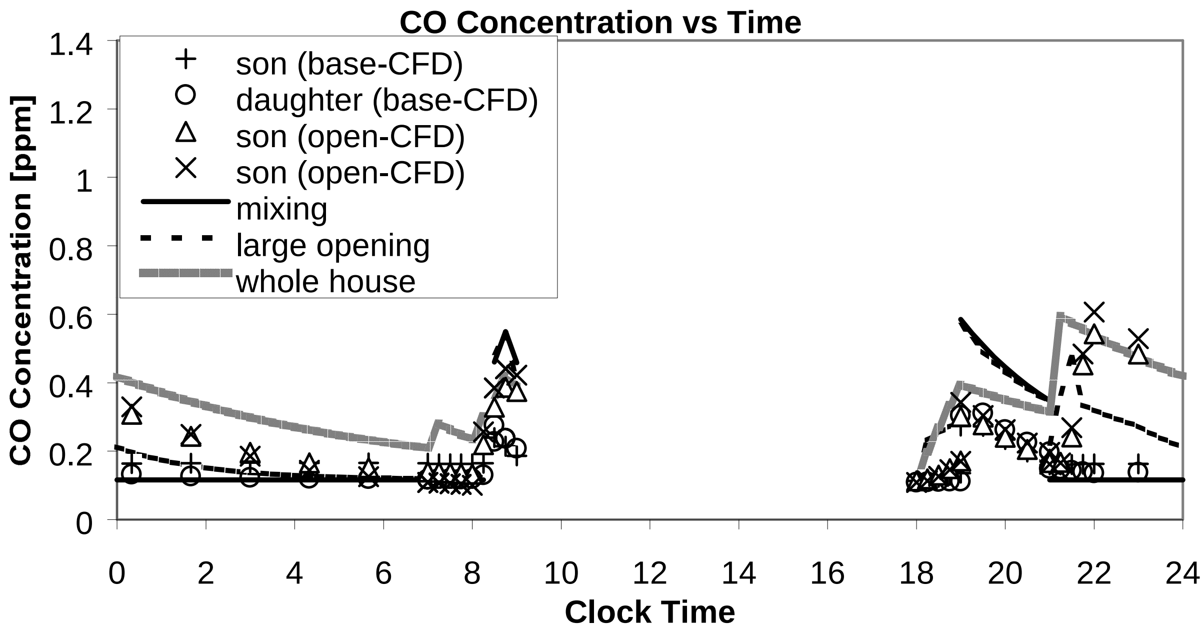

Figure 5 CO concentration for the children throughout the day

During the period that the father smokes, there are observably striking differences in each combustion contaminant assessment, since the childrens' doors are open. Although not aided by large buoyant forces (compared with the stove) the contaminants generated by cigarettes are traced substantially to the childrens' rooms. This effect is directly attributable to contaminant migration and interaction between the rooms through the openings as only strong heat sources that induce buoyancy aids in effective mixing [6].

Table 4 shows the percent difference of exposure for each occupant when comparing the base case and the open door case.

Pollutant	Mother	Father	Son	Daughter	Average % Difference
CO_2	23.6	3.5	63.6	61.0	37.9
CO	3.0	-1.7	39.6	69.2	27.5
NO_2	3.7	0.2	5.4	6.0	3.8
HCHO	2.1	0.4	59.3	44.0	26.5
Vapor	-13.9	-31.0	13.0	25.0	-1.7
				Average	18.8

Table 4 Exposure difference comparing base case CFD and open door CFD

Large spaces tend to temper any major fluctuations in contaminant influx, while the influences observed in smaller spaces are quite immediate. Since the holistic parameters of the two cases are the same, it is quite evident that the opening of doors (or the addition of weak sources, as another way to think about it) plays a significant role in the outcome of daily exposure. It is intuitive that the son and daughter experience the most difference between the cases, as their occupational habits are most drastically changed, exposing them to more contaminants. Though not often a design parameter, the position of the doors should be noted when attempting to predict the exposure to pollutants.

The assessment of pollutant migration trends becomes less and less evident throughout the course of the evaluation period. This is due to the fact that the cause of certain differences in comparative results becomes less apparent due to the previous hours' error. After twelve hours, cumulative error propagation and increasing uncertainty makes it very difficult to recreate a base point upon which to make a standard of comparison. Thus it is only of use that the absolute values calculated and recorded are compared, without a rigorous analysis of the reasons for discrepancy.

Open Door Case vs. Large Opening & Whole House Case

In addition to the single-zone perfect mixing model, a comparison of the open door CFD model to a large opening and whole house model is one that is somewhat analogous to the base case CFD and single-zone mixing model. Since the doors are open when the room occupants are not sleeping in the large opening model, it is one that switches between the single-zone model when the occupants are sleeping, (since the conditions are exactly the same for the large opening case as the perfect mixing case) and the large opening model when the room is occupied and the doors are open. When there are no occupants in the room it should act as a sink, drawing in a small portion of the contaminants generated in other rooms.

Inflated concentrations of the open door and mixing model cases compared to that of the base case results in smaller perceived differences in exposure. This inflation results from the fact that before the occupants go to sleep for the night, some exchange of contaminants occurs in the large opening case that does not previously in the perfect mixing model. This difference thus propagates throughout the rest of the night and into the next morning, since there are extra contaminants that must be diluted. Ultimately the large opening case will over predict the open door CFD scenario.

Although it may seem that the large opening model should match well with the open door case, it is not observably so. The situation that incurs the most significant difference is during times of cooking when the kitchen range hood is on. Stratification and buoyancy capture are the main reasons for the disparities in contaminant exposure. A compiled table of percent differences between the open door CFD case and the large opening case is shown in Table 5.

Pollutant	Mother	Father	Son	Daughter	Average % Difference
CO_2	2.2	9.4	-14.5	-13.3	-4.0
CO	52.7	53.1	15.0	16.6	34.4
NO_2	34.3	36.9	43.8	40.3	38.9
HCHO	17.0	21.1	-13.4	-4.8	5.0
Vapor	40.0	56.4	-2.8	-13.4	20.1
				Average	18.8

Table 5 Exposure difference comparing open door CFD and large opening mixing model

Where great simplicity is gained in the whole house model, accuracy is concurrently lost. In general, this model will also over predict the exposure since walls and partitions used in all other models tends to hinder the migration of contaminants, and keep it out altogether when there are sources external to a closed room. Although it may seem that the numbers correspond well for the comparison of the two models, it is noticeable that the contaminant concentrations deviates greatly from the CFD case. These large deviations tend to cancel out in the final estimation, leaving a lower, but misleading difference in exposure, as evidenced by Table 6 below.

Pollutant	Mother	Father	Son	Daughter	Average % Difference
CO_2	3.1	10.8	-26.0	-25.9	-9.5
CO	91.5	116.6	66.3	62.9	84.3
NO_2	32.2	37.9	25.6	22.8	29.6
HCHO	11.3	17.8	-23.1	-16.3	-2.6
Vapor	-14.3	-3.1	7.6	-2.2	-3.0
				Average	19.8

Table 6 Exposure difference comparing open door CFD and whole house mixing model

Conclusions

There is sufficient evidence to observe a considerable discrepancy between the exposures predicted by the well-mixed models than that obtained through CFD analyses. This is especially true when considering the transport of contaminants that are byproducts of combustion, as mixing models do not explicitly account for stratification and the efficiency in local exhausting for occupants situated close to strong sources. Generally, contaminants such as CO_2 and vapor are well predicted (when averaged over the five trials) by the perfect mixing model.

It is evident that the position of doors has an impact on the amount of occupational exposure to contaminants. It is not a trivial matter as it may incur differences in exposure of up to 38% when compared to closed door situations.

On the whole, the mixing models predict exposure with more than 70% accuracy compared to the CFD cases. If not interested in the specifics of the channels of exposure, then these mixing models might suffice since CFD imposes severe time limitations. Because design change evaluations need to be quick and easy, ensuring that a gamut of variations be tried and evaluated, the CFD method hinders the ability for designers to achieve the necessary rapid turnover. Therefore, mixing may be practical enough to predict differences between designs, but not the specific exposure values. However, the most accurate assessment is through CFD, and the mixing models are recommended for conceptual design tools while the CFD model must be a final evaluation tool.

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