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### **Publication Date**

2002

# MIXING OF A POINT-SOURCE INDOOR POLLUTANT: NUMERICAL PREDICTIONS AND COMPARISON WITH EXPERIMENTS

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## ABSTRACT

In most practical estimates of indoor pollutant exposures, it is common to assume that the pollutant is uniformly and instantaneously mixed in the indoor space. It is also commonly known that this assumption is simplistic, particularly for point sources, and for short-term or localized indoor exposures.

We report computational fluid dynamics (CFD) predictions of mixing time of a point-pulse release of a pollutant in an unventilated mechanically mixed isothermal room. We aimed to determine the adequacy of the standard RANS two-equation ( $k$ - $\epsilon$ ) turbulence model to predict the mixing times under these conditions. The predictions were made for the twelve mixing time experiments performed by Drescher *et al.* (1995). We paid attention to adequate grid resolution, suppression of numerical diffusion, and careful simulation of the mechanical blowers used in the experiments. We found that the predictions are in good agreement with experimental measurements.

## INDEX TERMS

Air transport, Microclimates, Exposure assessment, Air and pollutant transport modeling and measurement, Modeling indoor pollutant concentrations.

## INTRODUCTION

Indoor air quality investigations usually assume a uniform distribution of pollutants throughout the interior space. This assumption of instantaneous mixing offers some compelling advantages in domain of its validity. For experimental purposes, the measurement of the concentration at only one point can be used to obtain the overall concentration throughout the room. In modeling studies, the assumption leads to governing equations that are either systems of ordinary differential equations or algebraic equations, whose numerical solutions are straightforward in contrast to the partial differential equations that must be solved if one takes real mixing into account.

However, particularly for point sources, and for short-term or localized indoor exposures, this assumption proves too simplistic for the initial period of the mixing of the pollutant in the room air. Lambert *et al.* (1993) showed, for example, that the levels of respirable suspended particles and nicotine were respectively 40% and 65% lower in no-smoking sections of restaurants than in the smoking sections. The mixing problem has two aspects: (1) how to determine the conditions under which the well-mixed approximation is inappropriate, and (2) how to model pollutant concentrations when the well-mixed approximation is inappropriate. We earlier addressed the first question experimentally for rooms mixed with natural or forced convection (Baughman *et al.* 1994, Drescher *et al.* 1995). A “mixing time” is defined for a

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point pulse release of a pollutant in the room, under particular flow conditions. At times beyond the mixing time one can safely use the well-mixed assumption. At times earlier than the mixing time, the well-mixed assumption is a poor approximation.

Previous work on modeling imperfectly mixed pollutant concentrations aimed for the introduction of an additional mixing factor (Hoegg, 1972) (Ishizu, 1980). More recently, a two-compartment model was applied, artificially defining a small virtual space around the source (e.g., an area of workplace pollutant emissions) also with a uniform concentration, but different from that in the rest of the room (Furtaw, 1996). Although construction allowed for initial concentration build-up near the source, comparisons with experiments showed that concentrations near the source exceeded the predictions of this modeling approach. In the current work, we focus not on improving approaches to model exposure under poorly mixed conditions, but on determining the mixing time beyond which the well-mixed assumption is valid, and before which it is a poor approximation.

Computational fluid dynamics (CFD) solves the partial differential equations governing pollutant mixing and can provide solutions with high spatial and temporal resolution. With the improvements in CFD methods and increased computer power, CFD is increasingly common in research. Nevertheless, making accurate CFD predictions of room airflow remains a difficult territory, requiring great care in defining the settings and numerical properties of the model.

Most of the previous work on the CFD simulation of contaminant dispersion in a room was performed without corresponding experiments (Baker and Kelso, 1990). Gadgil *et al.* (2000) provide a brief review. Yaghoubi *et al.* investigated mixing of pollutants using simulations with varied emissions from a pollutant source, cooling and heating locations, and incoming air temperatures (Yaghoubi *et al.*, 1995). Roy *et al.* (1994) used a CFD code to predict contaminant dispersion in a kitchen-hood geometry.

The specific goal of this research was to explore the adequacy of the standard ( $k$ - $\epsilon$ ) turbulence model for predicting the mixing time of a point-source release, by comparing CFD predictions with experiments releasing a point pulse of Carbon Monoxide (CO) in an isothermal room with forced convection airflow. We simulated a series of 12 experiments releasing a pulse of CO from a point-location into a mechanically mixed unoccupied room, carried out by Drescher during her Ph.D. thesis (Drescher, 1994).

## **MIXING TIME THEORY**

The characteristic mixing time  $t_{mix}$  is defined as the interval from the time of point-pulse release of the pollutant into the room to the time at which the standard deviation of the pollutant concentration  $C_i(t)$  (measured at  $N$  monitoring points in the room,  $i=1, \dots, N$ ) drops permanently below 10% of the arithmetic mean concentration  $\bar{C}(t)$  of all sensors.

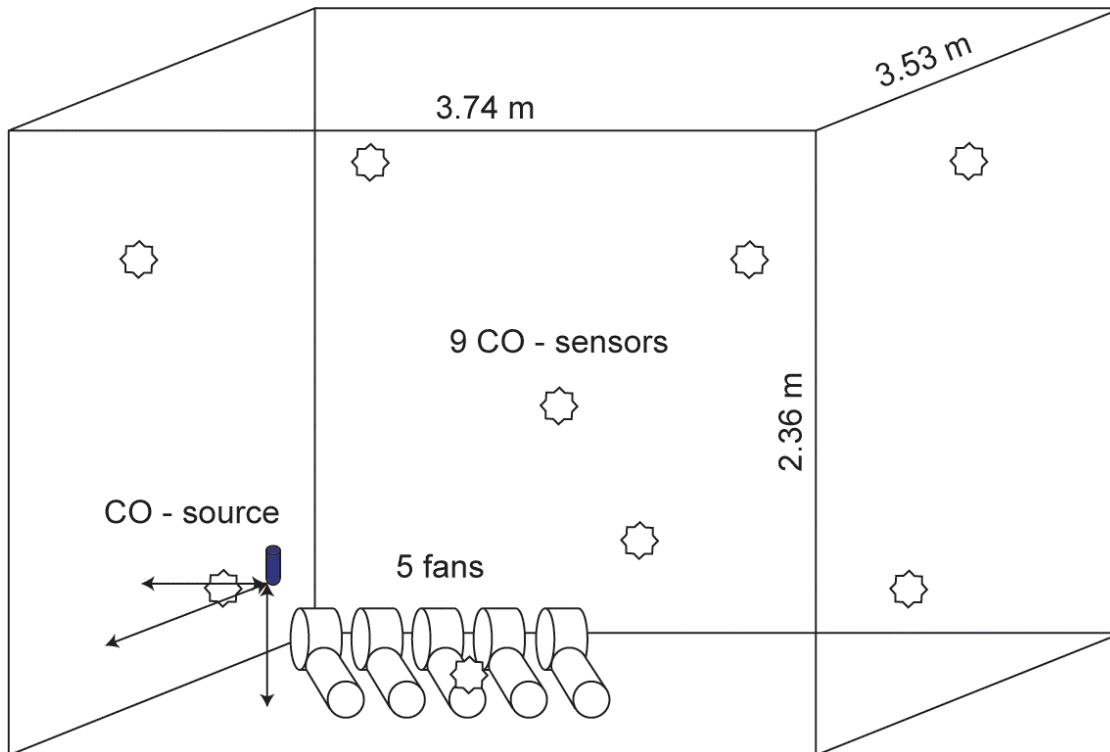
In the Drescher series of experiments,  $N=9$  sensors were used, selected such that the mixing time calculated from their monitored values is the same as that calculated from a denser network of 41 sensors used by Baughman *et al.* (1994). Since the CO injection was not truly instantaneous (it took 20 seconds), the time interval was measured from the midpoint of the duration of CO injection. Engineering analysis shows that under conditions of forced convection,  $t_{mix}$  should be proportional to the inverse of the cube root of mechanical power  $P$ , deposited into the room air by the array of blowers.

$$t_{mix} = c * \frac{M^{1/3} L^{2/3}}{P^{1/3}} \quad (1)$$

where  $c$  is the constant of proportionality,  $M$  denotes the mass of the air in the room and  $L$  is a characteristic dimension of the room. The term on the right-hand side is also known as power parameter  $p$ , and has units of time.

### GEOMETRICAL SETTINGS

Figure 1 displays the schematic for the experimental room, which measured 3.53m x 3.74m x 2.36m high (31m<sup>3</sup>). Metal foil covered the windows to block sunlight. The temperatures at the walls and at different heights in the middle of the room differed from the average temperature by amounts ranging from 0.25 to 1 Kelvin with an average of 0.59 Kelvin. The influence of natural convection was neglected in the CFD simulations, and we apply a correction to experimental mixing time to remove the small influence of natural convection, before comparison with predictions. Five independently powered identical centrifugal fans, each fitted with a 60 cm long plastic exhaust pipe, were placed 3 cm above the ground with their plastic exhaust pipes parallel to one another and to the floor. At the start of each experiment, 1.5 l of pure CO was released over a period of 20 seconds through a perforated syringe. The CO concentrations at various locations in the room were monitored with nine sensors, and each of the twelve experiments was repeated once.



**Figure 1.** Schematic model of the experimental room

In the CFD simulations, the physical space occupied by the blowers (which refers to the fans and pipes together) was excluded from the computational domain. Appropriate boundary conditions modeled the blower intakes and exhausts. Pollutant mass leaving the computational space by entering a blower intake immediately reappeared at the blower exhaust and re-entered the computational space. Infiltration through the walls, experimentally

measured to range from 0.03 to 0.08 air changes per hour, was ignored. A small area on the room surface was defined as a pressure boundary to improve stability of the solution procedure. This allowed a small (but negligible) amount of pollutant to leave the room during the simulated experiments. The syringe was simulated as the combined surface of the holes ( $12\text{cm}^2$ ), releasing CO at a speed of  $6.29\text{ cm/s}$ .

## NUMERICAL METHODS

Most of the room space was discretized with a coarse  $10\times 10\times 10\text{ cm}$  mesh, except near the boundaries and near the blower jets. An inner large block of cells surrounding and enclosing the blowers was aligned with the exhaust pipes of the blowers to avoid imposing the grid orientation on the exhaust jets. The final working grid had 130,942 nodes. The fans and attached pipes were simulated using block structures with  $5\text{mm}$  resolution at the ends of the blower pipes where the highest velocities were reported. The walls of the room and the outside of the blowers were defined as impermeable non-slip boundaries (except for the small pressure boundary area mentioned above). The blower inlets and exhausts were defined to have prescribed flows with fixed velocity profiles and with pollutant concentrations coupled to each other through user-subroutines. The grid quality was verified by testing the resulting predictions for independence of the grid size, time-step and turbulence parameters. A constant time step size of  $0.1\text{ sec}$  was used for each simulation.

The Navier-Stokes equations were solved using a commercial code based on a finite-volume fully implicit method and selecting the standard (high Reynolds number) RANS two-equation ( $k-\varepsilon$ ) turbulence model. In this work, the MARS (Monotone Advection and Reconstruction Scheme) differencing scheme was chosen, because it is second-order accurate. The solution algorithm applied was SIMPLE (Semi Implicit Method For Pressure Linked Equations) for the calculations of the steady-state velocity fields (without pollutant) and PISO (Pressure Implicit Split Operator) for the transient calculations of the pollutant dispersion in the room (with fixed velocities and turbulence parameters).

The chosen convergence criterion was that the residuals for all calculated dependent variables decreased at each cell below a value of  $10^{-4}$  for the steady state calculations. Iterations to reach convergence for the steady state ranged from 1817 to 4855, requiring 10 to 35 hours processing time on a server with  $2\text{GB}$  RAM and two processors. The transient calculations required half as much processing time.

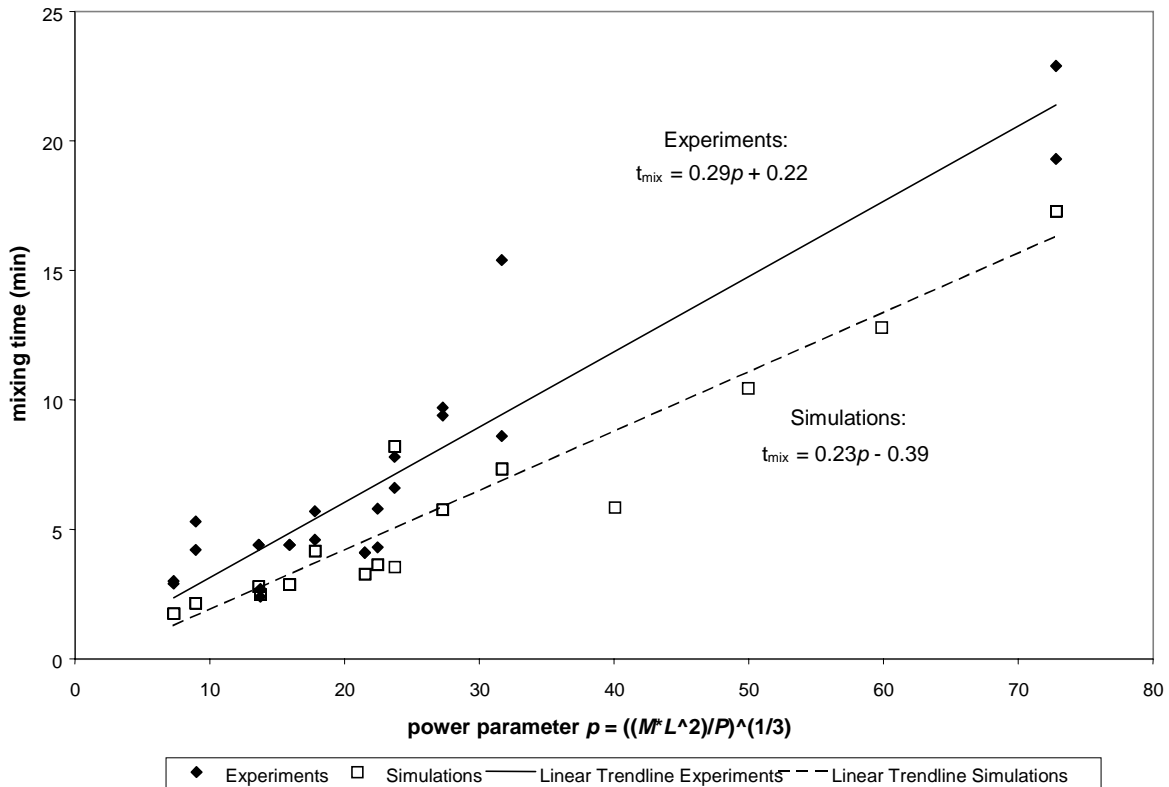
## COMPUTATIONAL RESULTS

Drescher *et al.* performed 2 replicates of 12 experimental set-ups. The number of blowers operated and the average velocity of the air jets at the blower exhausts (and therefore also at the inlets) varied from one setup to another. CFD computations were performed for all 12 setups. Three additional computations were performed to obtain predictions for a gap left in the experimental dataset regarding the power parameter values. Since the simulations were performed isothermally, the experimental data were corrected for the small influence of natural convection before comparison with simulation results. The total mechanical power deposited into the room air by the blower jets ranged from  $0.001\text{ W}$  to  $0.985\text{ W}$ .

Typical predictions of concentration over time for the nine different sensors displayed a high initial peak concentration, as the plume of pollutant passed each sensor for the first time, and several smaller secondary peaks from recirculation of the plume, until the concentration at all sensors locations converged toward the fully mixed state. Further details are omitted for brevity.

## COMPARISON WITH EXPERIMENTS

Detailed experimental data were available about the fully developed turbulent velocity fields at the blower pipe exhausts, which was essential in simulating them correctly. Data from continuous temperature measurements at each wall supported our decision to conduct the simulations isothermally. The mixing times obtained from the experiments (two experiments per setup, adjusted for natural convection) and predicted from the simulations were compared as a function of the power parameter  $p$  (1), displayed in Figure 2.



**Figure 2.** Mixing times as a function of the power parameter  $p$ , experiments and simulations. Each experiment was replicated twice, yielding two experimental points for each power. Experimental values are shown corrected for the small effect of natural convection.

## DISCUSSION

As can be seen in Figure 2, there is significant variability in the experimental results. The two values of mixing time for identical setups, obtained from replicate experiments, differ on average by 18%. The constant of proportionality,  $c$ , between the power parameter and the mixing time (expressed in seconds, not in minutes as depicted in Figure 2) agrees reasonably well for experimental data and simulation results. For the experiments  $c$  is  $15 \pm 5.2$ , and for the simulations  $12 \pm 3.0$ . These results demonstrate the ability of the High-Reynolds number ( $k-\epsilon$ ) turbulence scheme to adequately predict the experimental mixing times, under the conditions tested in the setups.

We also find a good correspondence between the mixing times of the simulations and the turbulent parameters averaged over the flow field. Again, details are omitted for brevity.

## CONCLUSION AND IMPLICATIONS

In this work, we found that the standard ( $k-\epsilon$ ) turbulence model, using a carefully generated grid, carefully designed boundary conditions and the MARS solution algorithm, suppressing

numerical diffusion, gives mixing time predictions within 15% of experimental measurements over an order of magnitude range in mixing time.

In future work, it would be useful to explore the capability of a low-Reynolds number ( $k-\epsilon$ ) turbulence model to predict mixing times, and also to determine the extent to which the mixing time value is a property of the given airflow setup in the room, and whether it is independent of the location of the point pulse release. Finally, predictions of mixing time under non-isothermal conditions also need to be explored and tested against experimental data.

## ACKNOWLEDGEMENTS

The first author would like to thank Elizabeth Finlayson for her support in the use of the commercial CFD simulation tool Star-CD. This work was supported by the Office of Nonproliferation Research and Engineering, Chemical and Biological National Security Program, of the National Nuclear Security Administration under U.S. Department of Energy Contract No. DE-AC03-76SF00098.

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