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Airborne Human Odorants: Detection, Dispersion and Characterization

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**MARCH 2012
Interim Report**

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14. ABSTRACT This project concentrates on characterizing how VOCs emitted by humans interact and propagate in the environment. In humans, the axillae are a unique source of human odor. In addition to a high density of eccrine glands, the axillae contain large numbers of sebaceous and apocrine glands. The interactions between the cutaneous microflora and skin secretions lead to a complex mix of odorants, several of which are unique to humans. We have begun our investigation of how human-derived odorants emanate into the vapor phase. Our instrumentation has been calibrated for several odorants and how their vapor phase concentration changes with time in a small sealed system. In addition, we have created, a computational model for how human axillary odorants may emanate from the axillae into a room (experimental chamber) under know experimental conditions.					
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Airborne Human Odorants: Detection, Dispersion and Characterization

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Progress report for September 1, 2011 to December 31, 2011

The volatilization and dispersion of human VOCs depends on several factors: 1) the molecular properties such as saturated vapor pressure, Henry law constant, air/octane partition coefficient, etc. The human odorants we have chosen for study are emitted from the body in axillary sweat which is a complex mixture of water, protein, lipids and other small, VOCs. All of these properties and interactions are unknown, however, we will assume initially, that these odorants, because of their highly oxidized structures (e.g. they are acids) will remain stable in the vapor phase. With this assumption we have focused on how these compounds disperse through air movement caused either by active ventilations or by natural convections (diffusion). We have employed diverse experimental approaches to begin this research.

To allow the quantification of various human odorants we first calibrated the gas chromatography-mass spectrometry system that will be employed to quantify odorants collected from various headspaces.

Experiment 1: a.) Calibration of GC-MS system was performed by injecting small quantities of known concentrations of each compound under study (in chloroform or other appropriate solvent). To date, the instrument has been calibrated for the following compounds: dimethylsulfone, E-3-methyl-2-hexenoic acid (3M2H), 6-heptenoic acid, and 7-octenoic acid. Completion of calibration curves for these compounds has allowed us to quantify the amount of these VOCs found in headspaces of sealed systems of known volumes.

A typical calibration curve is shown in **Figure 1** for, dimethylsulfone.

Figure 2 shows how the concentration changes in the vapor phase, over time, in a fixed (0.50 L) volume.

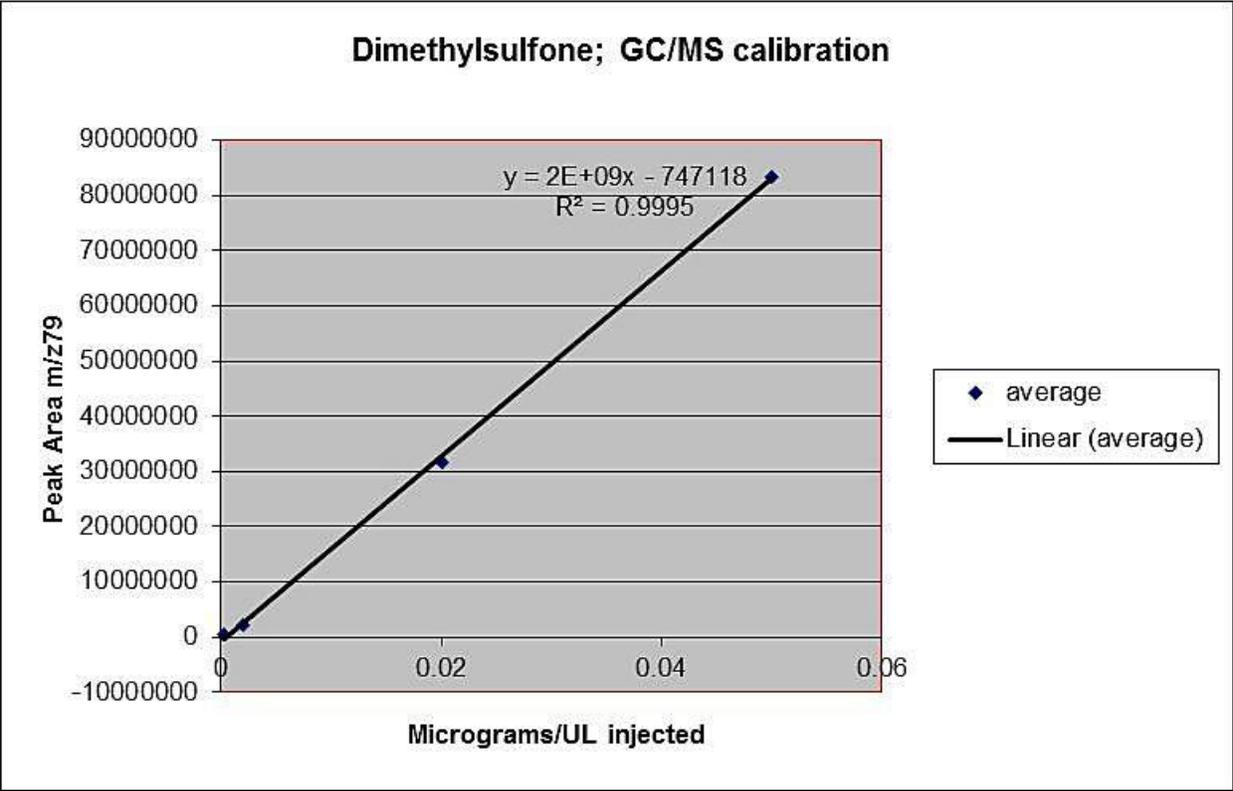


Figure 1. Dimethylsulfone (DMS) Calibration curve for dimethylsulfone, a mammalian metabolite reflective of metabolism of sulfur-containing amino acids.

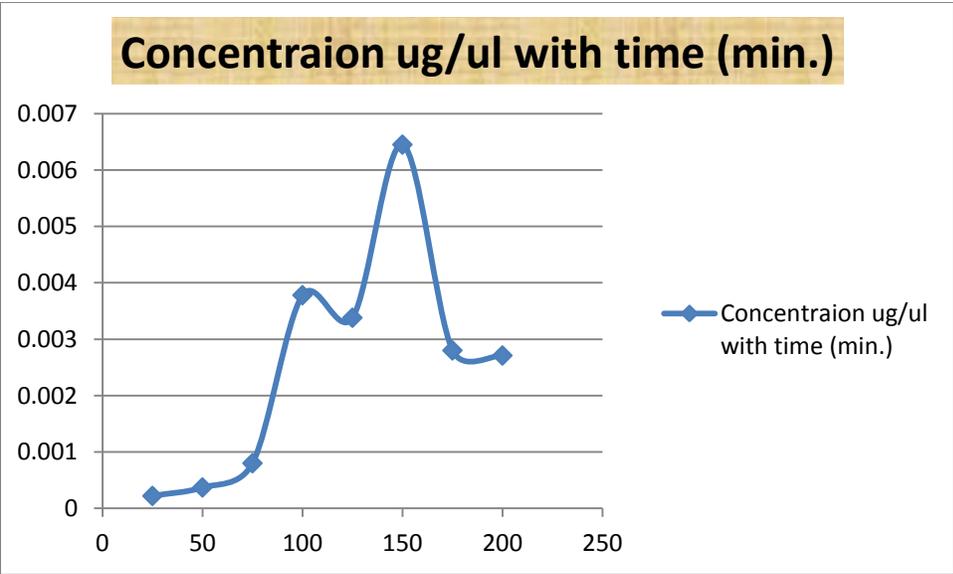


Figure 2. Vapor phase concentration of dimethylsulfone with time, in a small fixed volume.

Experiment 2) Quantifying human signature odorant propagation in an environmental chamber (250 sq foot).

We have setup computational models of the Monell Center’s environmental chamber where our indoor experiments will be conducted, to hopefully assist future experimental design, e.g. placement of odor monitor sites, expected standoff time, etc.

Method: The dimension of the chamber and the locations of the fresh air inlets and exhaust (three inlet on the ceiling and one exhaust at the lower side wall) were precisely replicated in silico (**Figure 2.1**). A widely acceptable mathematical method, the finite volume method, was used to simulate room air movement and odor propagation. This method works by dividing the air space into many small and simple volumes, e.g. tetrahedral, polyhedron, prism, etc. The final model for our room contains about 3 million volumes (elements). Within each volume, the nonlinear and higher order fluid dynamic equations can then be approximated with linear equations, thus greatly simplify the computational task. Obviously, it is likely that with more and finer elements, the linear approximation would be closer to the real solution. Thus, we have compared simulation results in models with 400k, 1million and 3 million elements, and concluded the results reached convergency at 3 million elements, that is further more elements does not improve the numerical accuracy significantly. There are also different mathematical schemes to linearize the fluid dynamic equations based on various flow conditions, e.g. laminar, turbulent, etc. The renormalization group K-eps turbulence model, which has been previously reported to perform best for indoor airflow than other two-equation turbulence models (Chen, 1995 and Posner et al 2003), is applied here to capture airflow.

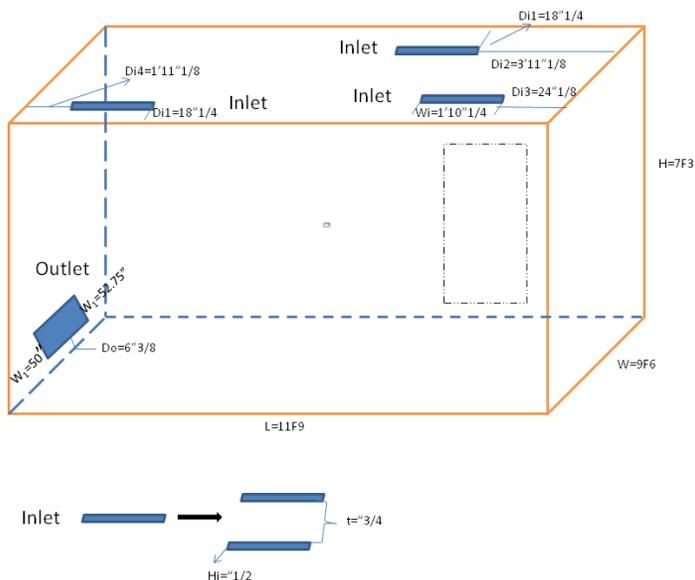


Figure 2.1. Diagram of the computational replication of the chamber. Each air inlet contains two parallel slits of 1/2” wide and 3/4” apart.

The initial simulation is conducted under an air exchange rate of 6 ACH (air exchange per hour), which is about mid range for ASHER (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Guideline-2001 (4-12 ACH). Room is assumed to be in constant temperature of 25 C.

Results: The following graphs (**Figure 2.2** and **Figure 2.3**) show the air velocity (m/s) in three parallel planes cut across the three axes (x, y, z).

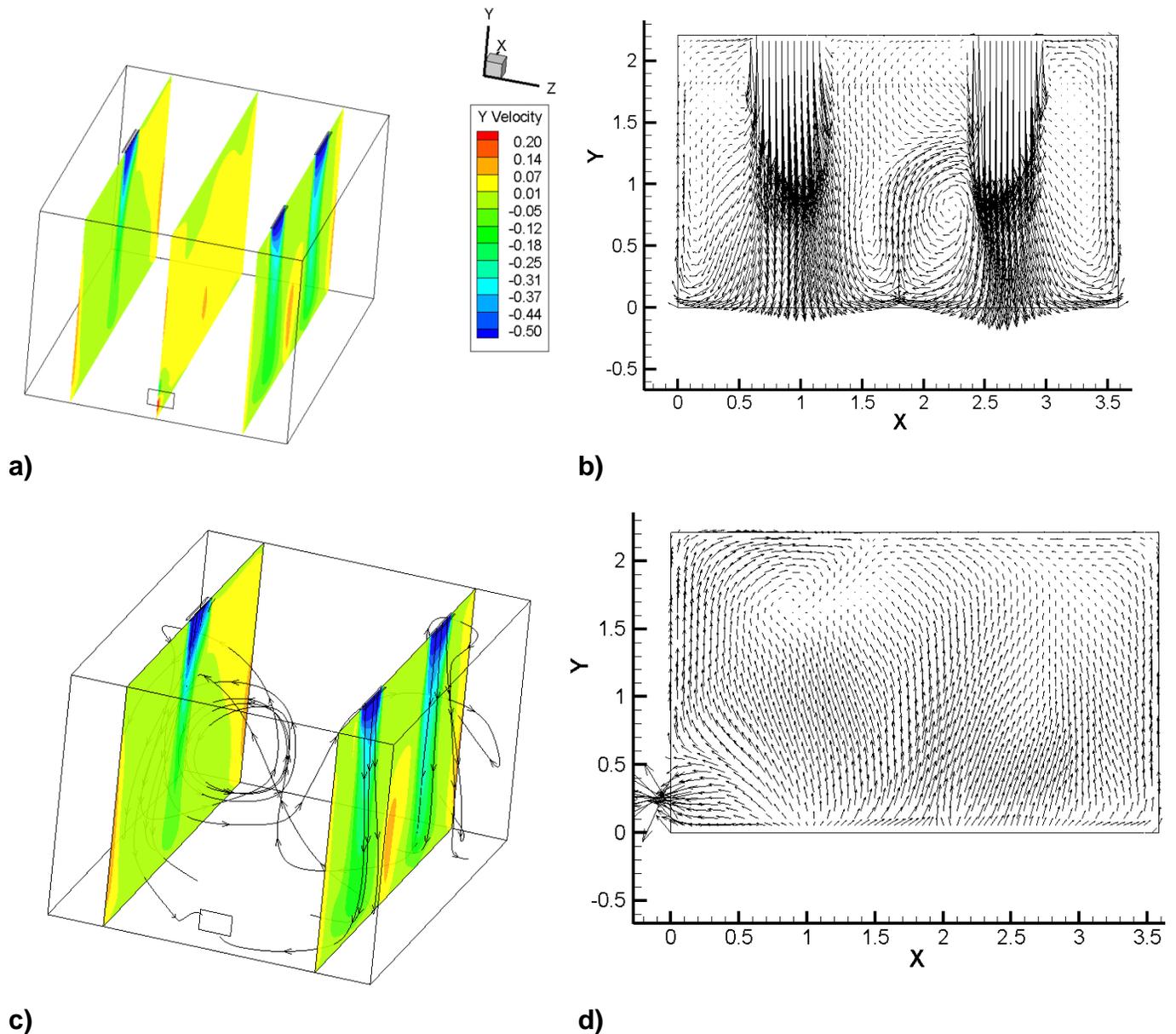


Figure 2.2. (a) Planes across z axis. Negative Y velocity means the flow towards floor, which is apparent on the two of planes that cut right along inlet slits. (b) air flow vector plots of the right most plane of (a), where the two air inlet slit were shown. Vectors show recirculation of air along the walls and between two air inlets. (c) flow vector in the middle

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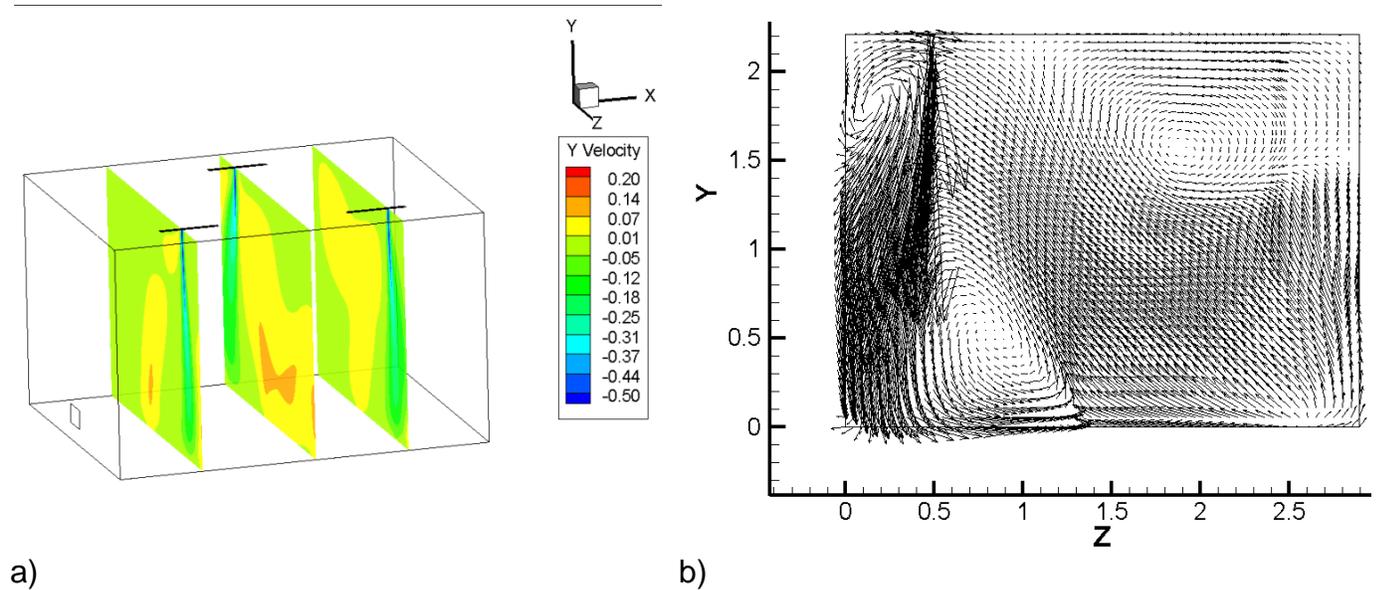


Figure 2.3. (a) planes across x axis and cut across three inlets. (b) air flow vector plots of the middle plane in (b), which shows intense recirculation of air between the inlet and wall.

We further simulated in **Figure 2.4** the situation where a pseudo odor vapor source of 100ppm is released with constant rate of 100ml/s in the middle of the room, approximately 1.5m from the floor, roughly at the height of the chest or arm pit. In the future, an odor evaporation profile obtained from experimental 1, will be used to capture realistic human signature body odor releases.

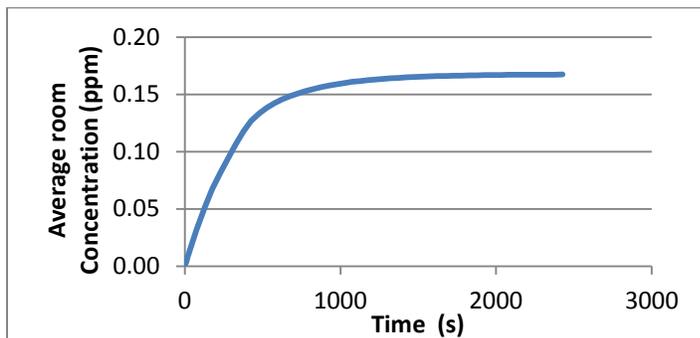


Figure 2.4. Simulated release of 100 ppm odor vapor source

The overall averaged room air concentration rise to plateau after at least 1000 s under the current room ventilation. If assuming perfect mixing condition, the concentration in

the room should rise to 0.263 ppm in theory, which was never reached. Thus, a significant portion of the fresh air was not well mixed with the room air before they exit the room.

9 virtual sites were setup to monitor the room odor concentration spreading in the middle z plane that cut across the outlet (see **figure 2.5a**). Compared to the average room concentration, various room regions contain high odor concentrations that are not well mixed with fresh air or with rest of the room air (**Figure 2.5 b**). The highest concentration level is at PC2, which is right above the source; the 2nd highest is PA1 near outlet; the 3rd highest PC1; and the 4th PA3. From the above air flow patterns and attached video, we can see that the source point is located in or near an air pocket of a vortex (by accident), thus for the first 250 seconds or so, the odor propagation is very much contained within that pocket, after which it then spreads/jumps into a second bigger pocket of air/vortex that is located near the outlet. That is why we see PC2, which is located in the first pocket, rises sharply and quickly, whereas, PA1, PC1, PA3, which are located in the second pocket, rise with a bump after 250 seconds. The attached video shows odor propagation at 3 planes across at source point. PC3, which is right below the source point, is only the 5th highest, much lower than PC2, probably because it is outside the first pocket and endured more washout from the inlet.

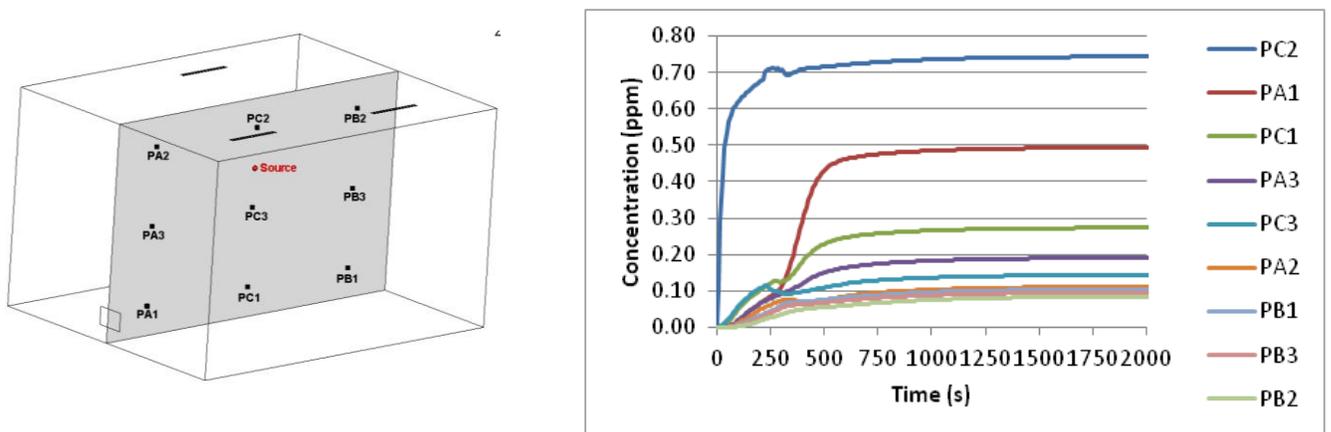


Figure 2.5 a) 9 virtual sites monitoring room b) Room regions containing high odor concentrations

Summary

The above simulation indicate that even within a well ventilated room, the propagation of odor can be very non-uniform and depend heavily on the location of source, monitor sites and their relationship to the ventilation inlet and outlet. The standoff distance and time may vary significantly depending on these locations. In our trial case, for a location moderately away from the source (~half room size), a considerable delay (~ 250 s) may be expected before encountering the bulk odor. For some locations (the half room away from the source and outlet, PB 1,2,3 in our setup), the concentration of odor may never reach ~40% of expected -under well mixing assumption- level.

Future Work:

We plan release a target odor in the chamber as we've simulated to validate the computational results.

Chen, Q. 1995. Comparison of different k-eps models for indoor air flow computations. Numerical heat transfer Part B, Fundamentals, 28(3), 353-369.

Posner, J.D., Buchanan, C.R., and Dunn-Rankin, D. 2003. Measurement and prediction of indoor air flow in a model room. Energy and buildings 35 (5): 515-526.