Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting Information

Effects of Room Airflow on Accurate Determination of PUF-PAS Sampling Rates in the Indoor Environment

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Quality Assurance and Control

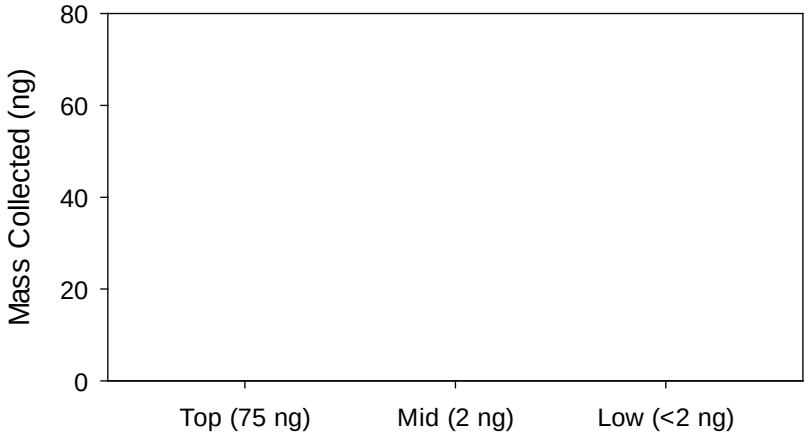


Figure S1: Results from the breakthrough test on an active sampling PUF-plug showing no PCBs above typical lab blank levels (~2 ng) penetrate past the first third of the PUF-plug for our set flowrate and sampling period.

Active Air Sampling Results

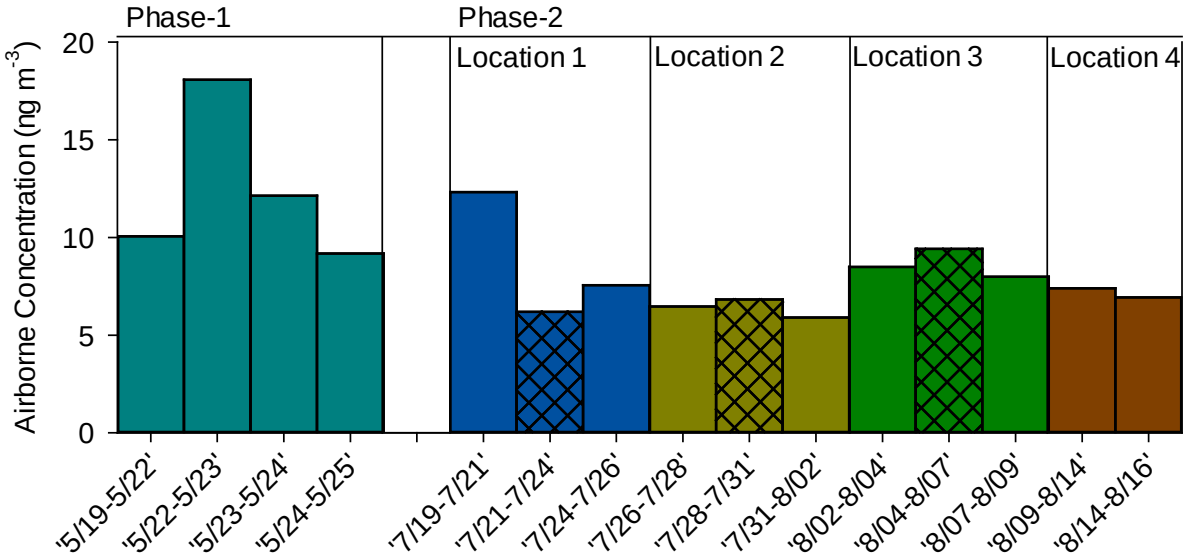


Figure S2: Average airborne concentration determined from the low-volume sampling during the two phases of the study. The checkered bars denote samples collected when the HVAC system was off for >90% of the time and each color represents a different location in the study.

Anemometer Data

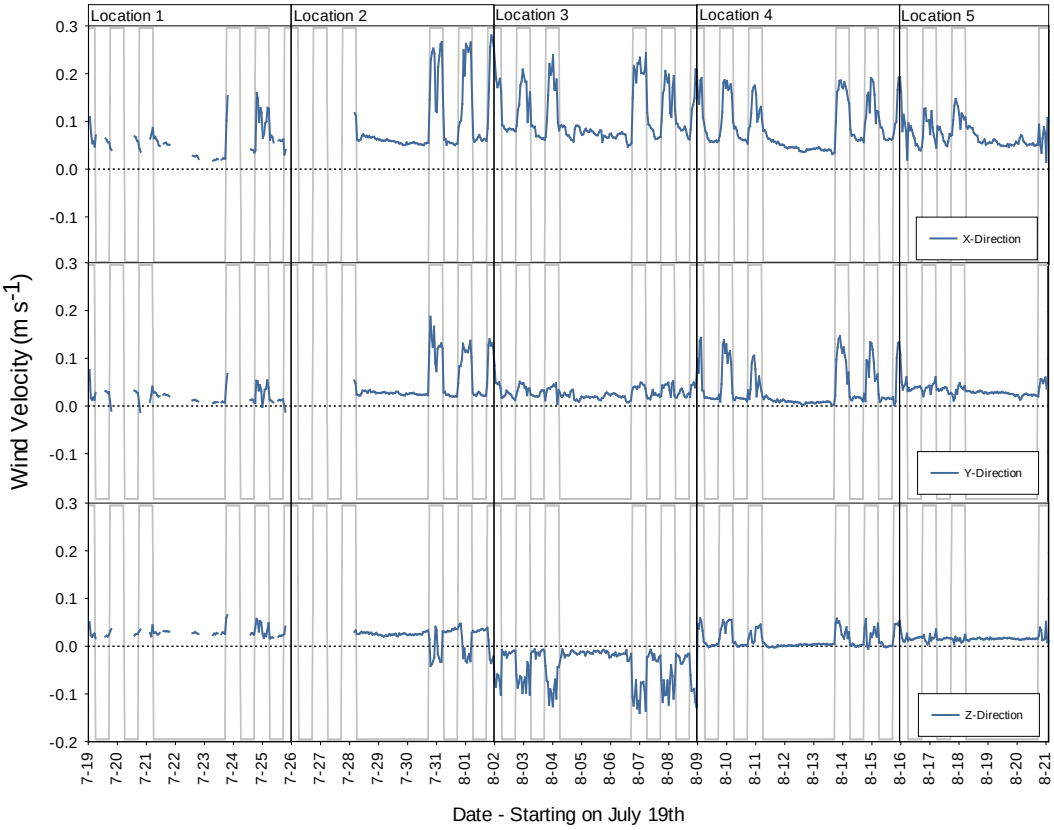


Figure S3: Airflow velocities in all three-vector directions from the 3D sonic anemometer data during phase-2 of our study. The grey shading represents times when the HVAC system was on while the white shading represents times when the HVAC system was off.

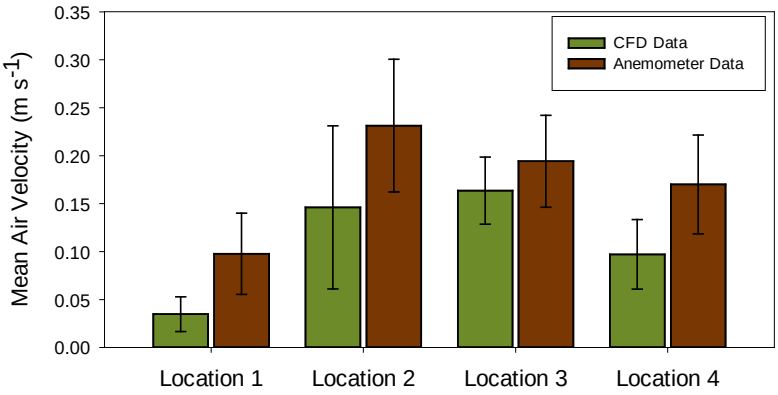


Figure S4: Comparison of the time-series anemometer data to a spatial distribution from the CFD model of the room to verify our model showing approximate agreement.

Uptake Study (Phase-1)

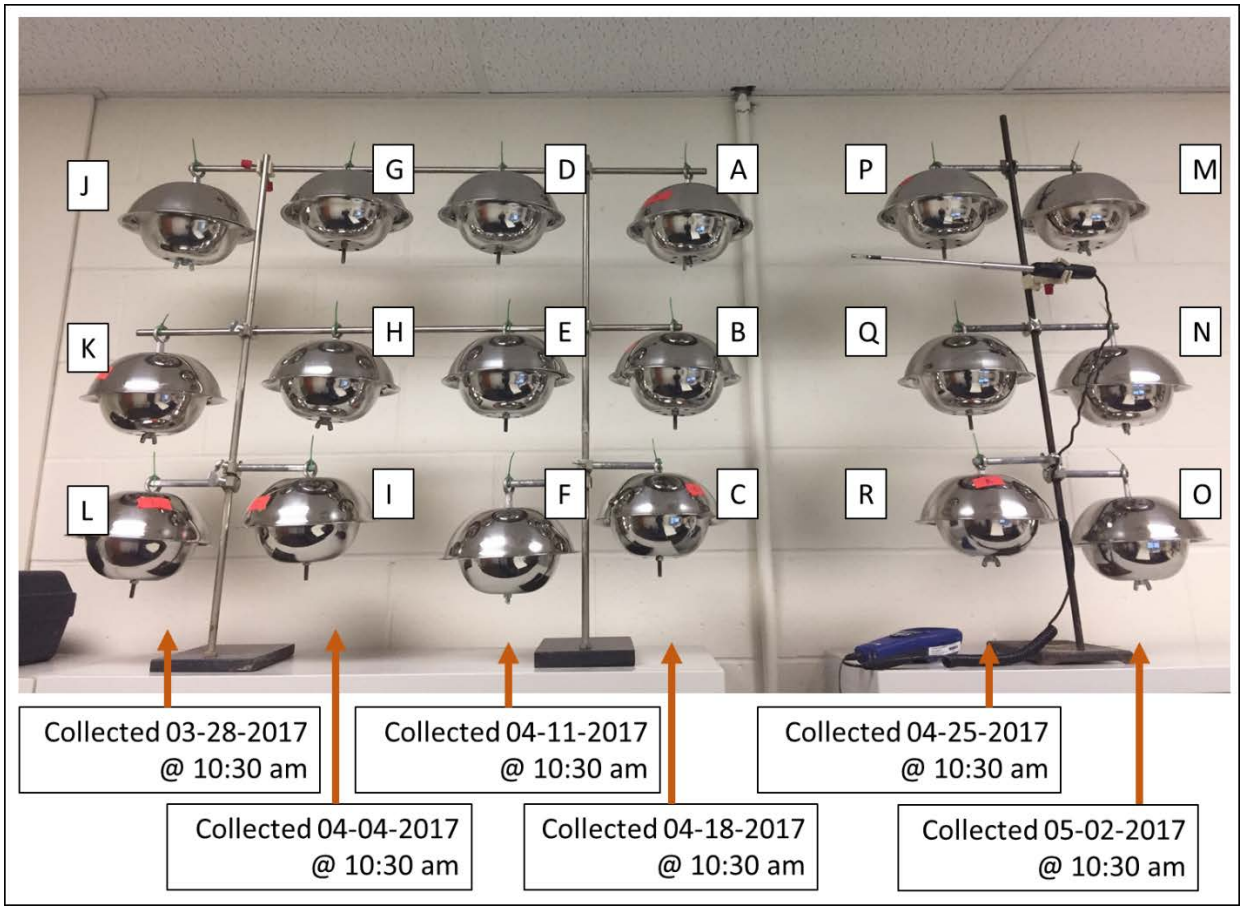


Figure S5: Sampler layout for the 6-week uptake study in the study room. The left side of this schematic represents the northernmost end of the bookcase.

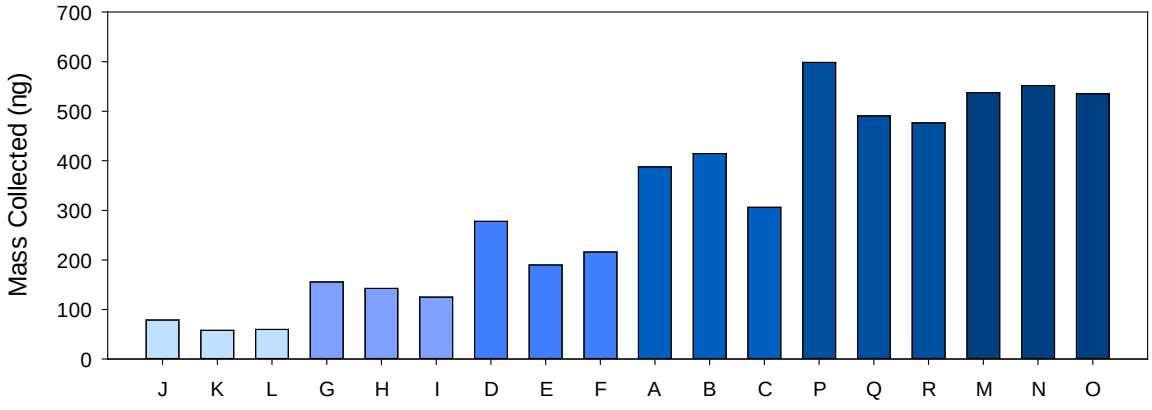


Figure S6: Total mass of PCBs collected on each PUF-PAS sample sampled during phase-1 of this study.

Spatial Study (Phase-2)

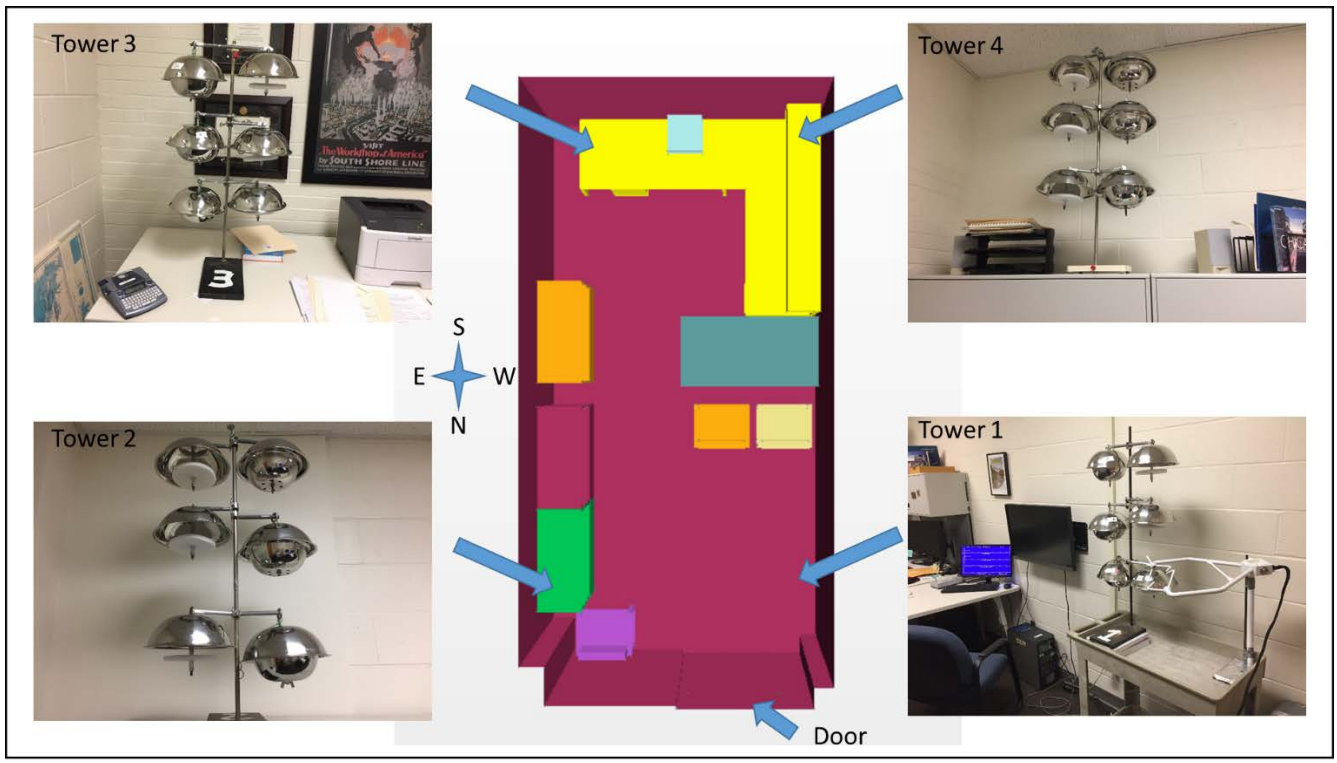


Figure S7: Sampler layout and room floor plan for the 4-week spatial study. The bottom side of this schematic represents the northernmost end of the room. Phase-1 of this study was conducted on the bookcases on the eastern side of this room.

Table S1: Summary of the average experimental and modeled sampling rates (38 congeners) for both sampler designs at the four locations throughout the test room.

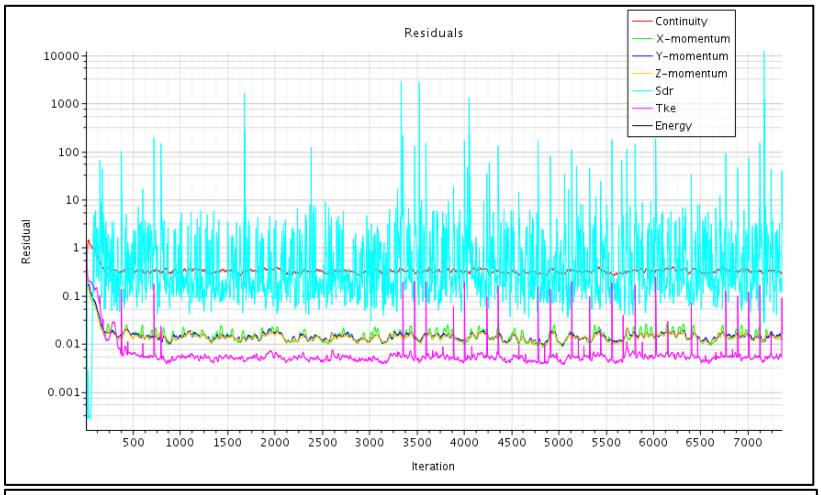
			Accumulation[1] Rate (ng d^{-1})		Rs (Experimental)		Location Specific Parameters					
							Rs (Predicted)		Residual		Percent	
			mean	*Std*	mean	*Std*	mean	*Std*	mean	*Std*	mean	*Std*
DB-dome	1	A	0.72	*0.64*	2.26	*0.24*	1.00	*0.04*	1.26	*0.22*	55%	*4%*
		B	0.60	*0.54*	1.88	*0.23*	1.01	*0.04*	0.87	*0.21*	46%	*6%*
		C	0.83	*0.73*	2.57	*0.24*	0.96	*0.04*	1.61	*0.22*	63%	*3%*
	2	A	0.21	*0.18*	0.80	*0.15*	1.03	*0.04*	0.25	*0.13*	35%	*21%*
		B	0.24	*0.21*	0.89	*0.10*	0.93	*0.04*	0.10	*0.04*	12%	*5%*
		C	0.21	*0.18*	0.78	*0.11*	1.16	*0.04*	0.38	*0.10*	51%	*17%*
	3	A	0.36	*0.32*	1.32	*0.14*	1.09	*0.04*	0.23	*0.15*	17%	*9%*
		B	0.45	*0.41*	1.61	*0.15*	1.14	*0.04*	0.47	*0.16*	29%	*6%*
		C	0.41	*0.36*	1.48	*0.14*	1.28	*0.05*	0.21	*0.15*	13%	*8%*
	4	A	0.16	*0.14*	0.64	*0.08*	1.03	*0.04*	0.39	*0.10*	63%	*21%*
		B	0.25	*0.21*	0.94	*0.11*	0.95	*0.04*	0.10	*0.06*	11%	*6%*
		C	0.18	*0.16*	0.70	*0.09*	1.06	*0.04*	0.36	*0.11*	55%	*20%*
Average			0.39	*0.44*	1.32	*0.64*	1.05	*0.10*	0.52	*0.48*	36%	*23%*
Room-Avg			na	*na*	na	*na*	1.08	*0.04*	0.53	*0.39*	38%	*16%*
HF-dome	1	D	0.94	*0.82*	2.90	*0.26*	2.48	*0.09*	0.42	*0.21*	14%	*6%*
		E	0.92	*0.82*	2.84	*0.28*	2.53	*0.10*	0.32	*0.20*	11%	*6%*
		F	0.76	*0.68*	2.36	*0.21*	2.39	*0.09*	0.13	*0.11*	6 %	*5%*
	2	D	0.70	*0.61*	2.58	*0.41*	2.57	*0.10*	0.25	*0.28*	9 %	*8%*
		E	0.71	*0.63*	2.64	*0.41*	2.33	*0.09*	0.33	*0.36*	11%	*10%*
		F	0.75	*0.66*	2.75	*0.39*	2.89	*0.11*	0.31	*0.19*	11%	*6%*
	3	D	0.90	*0.78*	3.22	*0.30*	2.72	*0.10*	0.52	*0.31*	15%	*7%*
		E	0.86	*0.75*	3.15	*0.32*	2.84	*0.11*	0.35	*0.32*	11%	*8%*
		F	0.93	*0.80*	3.40	*0.35*	3.18	*0.12*	0.31	*0.34*	8 %	*8%*
	4	D	0.62	*0.53*	2.35	*0.20*	2.56	*0.10*	0.26	*0.15*	11%	*7%*
		E	0.59	*0.51*	2.23	*0.16*	2.38	*0.09*	0.20	*0.12*	9 %	*6%*
		F	0.59	*0.51*	2.24	*0.17*	2.64	*0.10*	0.41	*0.19*	19%	*9%*
Average			0.77	*0.68*	2.72	*0.48*	*2.62*	*0.26*	*0.32*	*0.26*	*11%*	*8%*
Room-Avg			na	na	na	na	2.69	0.10	0.35	0.28	13%	*9%*

1

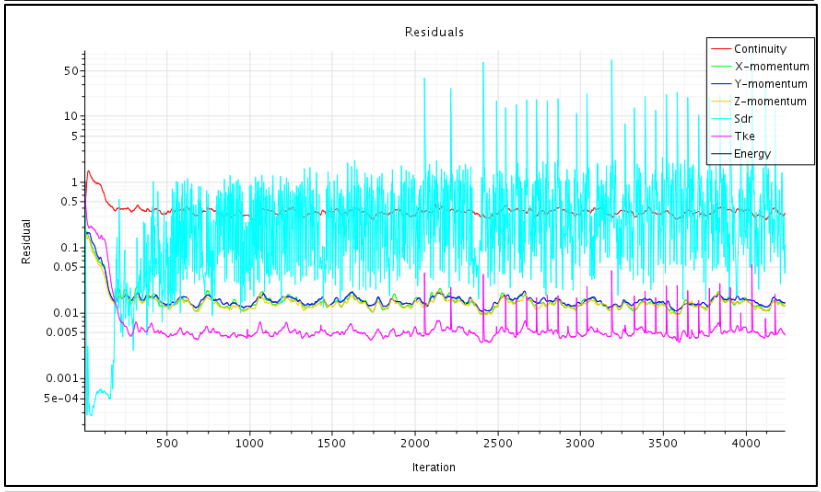
[1] PCB accumulation was calculated by dividing the collected mass by deployment time. [2] The Empirical R_s was calculated by dividing the accumulation rate by the average Low-Volume airborne concentration. [3] The room averaged input parameters were calculated from anemometer data and set bimodal (on vs. off). [4] The location specific parameters used the CFD results to adjust the room average parameters to more accurately represent the specific location. [5] The residual was calculated as |empirical R_s – Predicted R_s|. [6] The residual percent was calculated as the residual divided by the empirical R_s.

Computational Fluid Dynamic Results

1)



2)



3)

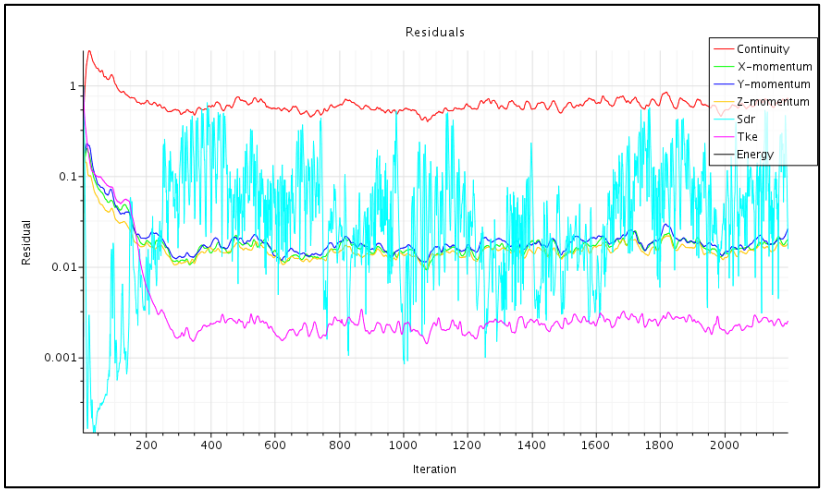


Figure S8: Computational Fluid Dynamic (CFD) residuals demonstrating convergence for our 3 main simulations; 1) room with door closed, 2) room with door open and 3) room with samplers and PUF included.

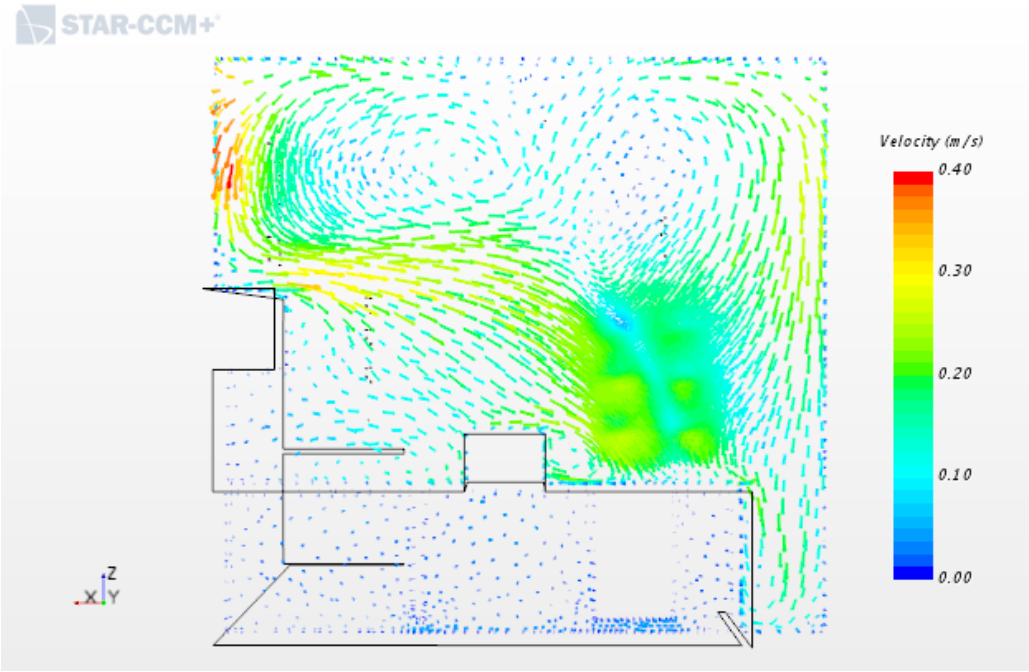


Figure S9: Vector Field demonstrating downdraft at position 3.

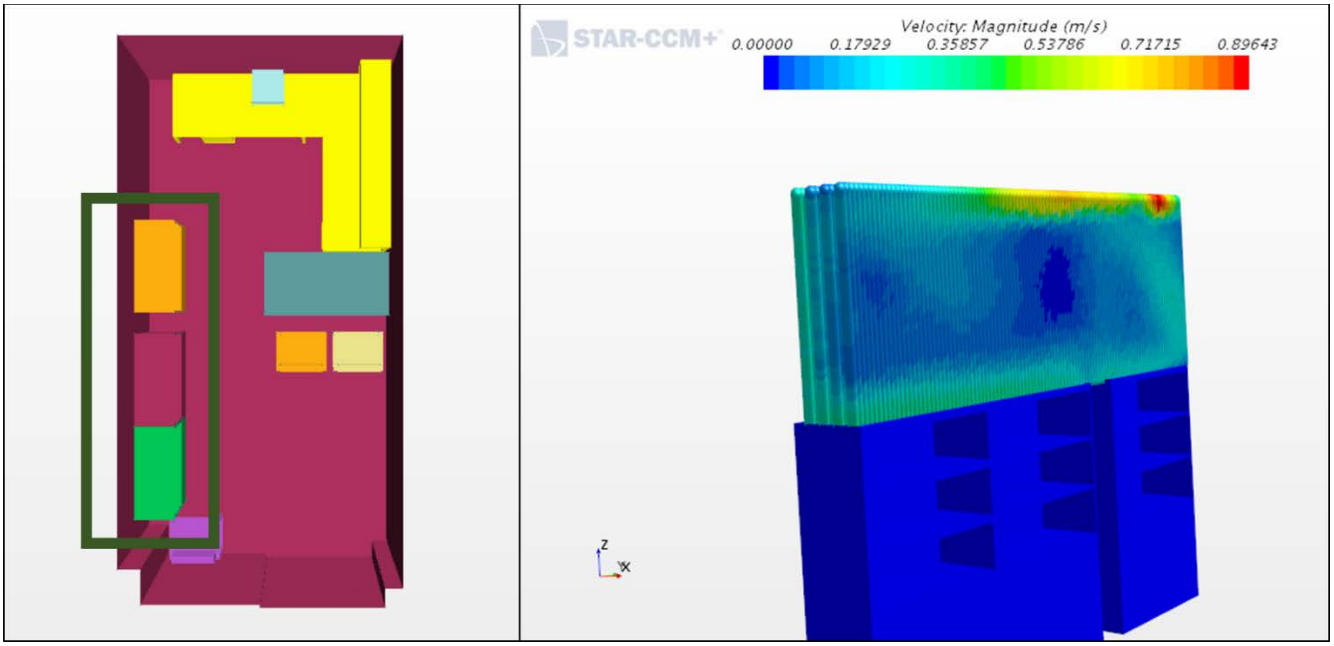


Figure S10: Schematic showing the study area we used to examine the placement of a sampler in the room and the effects of being near a wall/surface.

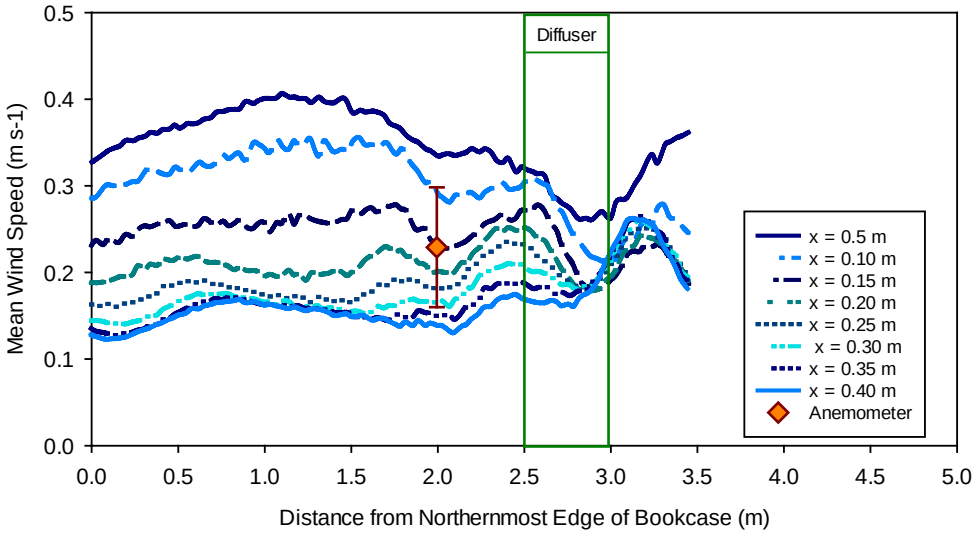


Figure S11: Horizontal profiles showing the influences of mixing from higher velocities at locations nearer to the HVAC air diffuser generated from the CFD model in our study zone. The x direction denotes distances from the wall. The anemometer data that corresponds with this location was also included to show the general agreement between the 3D sonic anemometer data and the CFD.

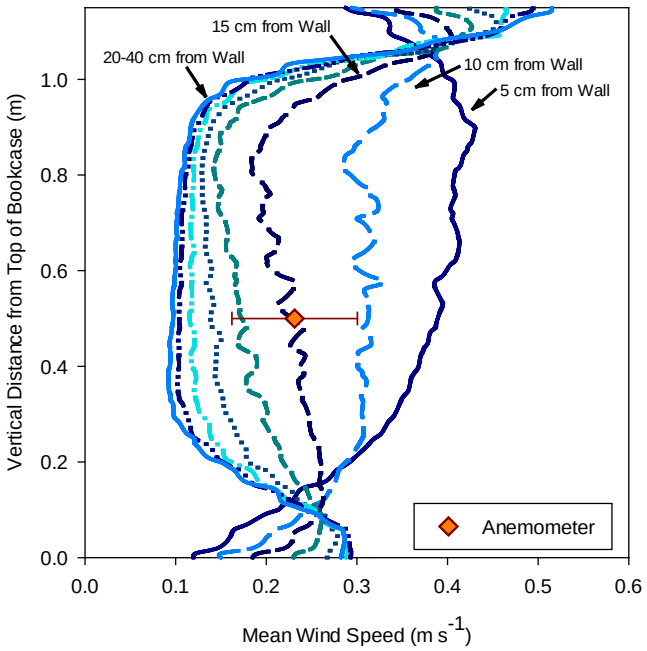


Figure S12: Vertical profiles showing the effects of turbulent mixing along the ceiling and surface of the bookcase and the convergence of airflow to room average parameters at increasing distances from the respective surfaces generated from the CFD model in our study zone. The x direction denotes distances from the wall. The anemometer data that corresponds with this location was also included to show the general agreement between the 3-D sonic anemometer data and the CFD.

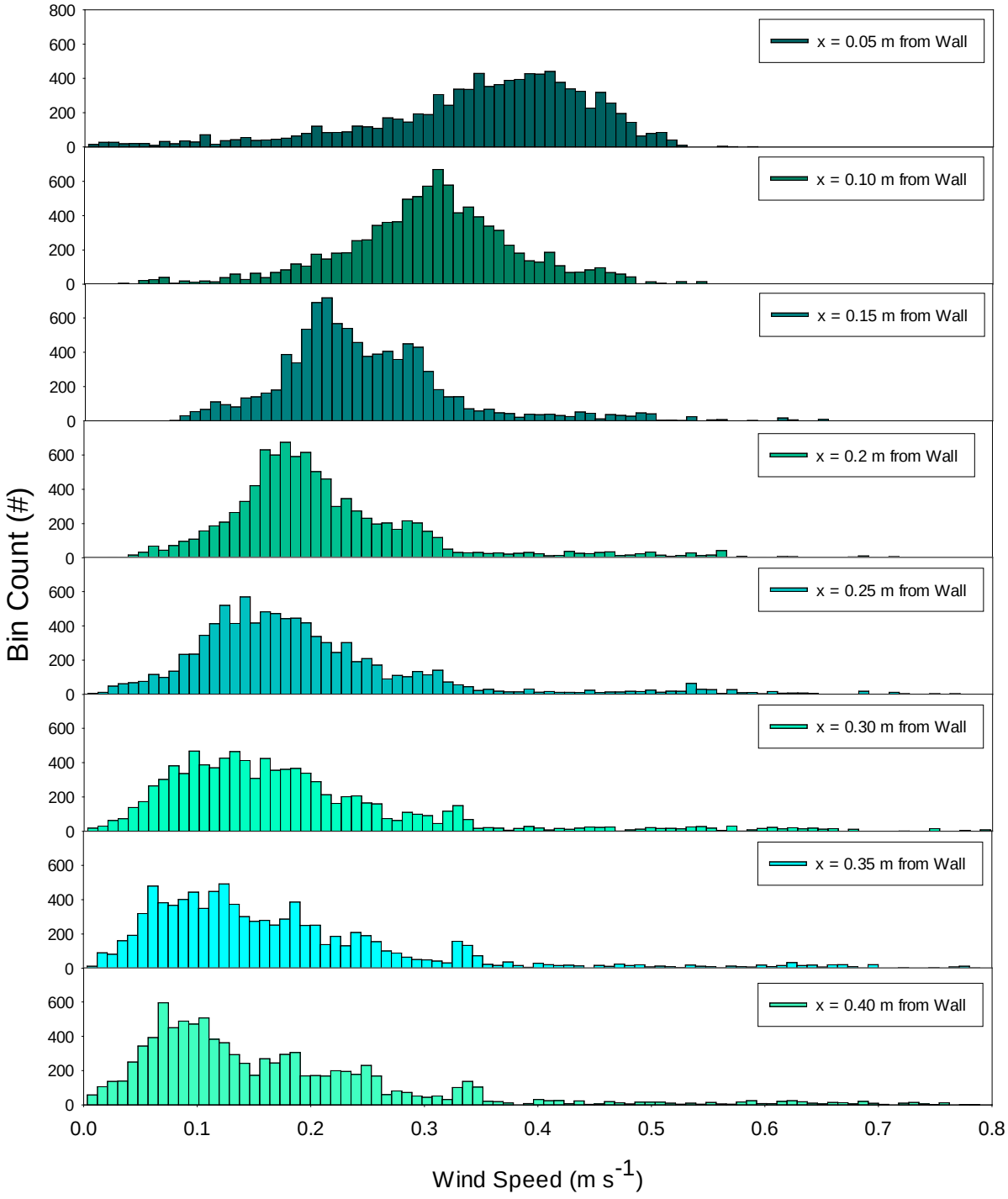


Figure S13: Histograms from the CFD model showing the convergence of airflow to room average parameters at increasing distances from the wall (x direction).

Effects of Door Changes on Airflow

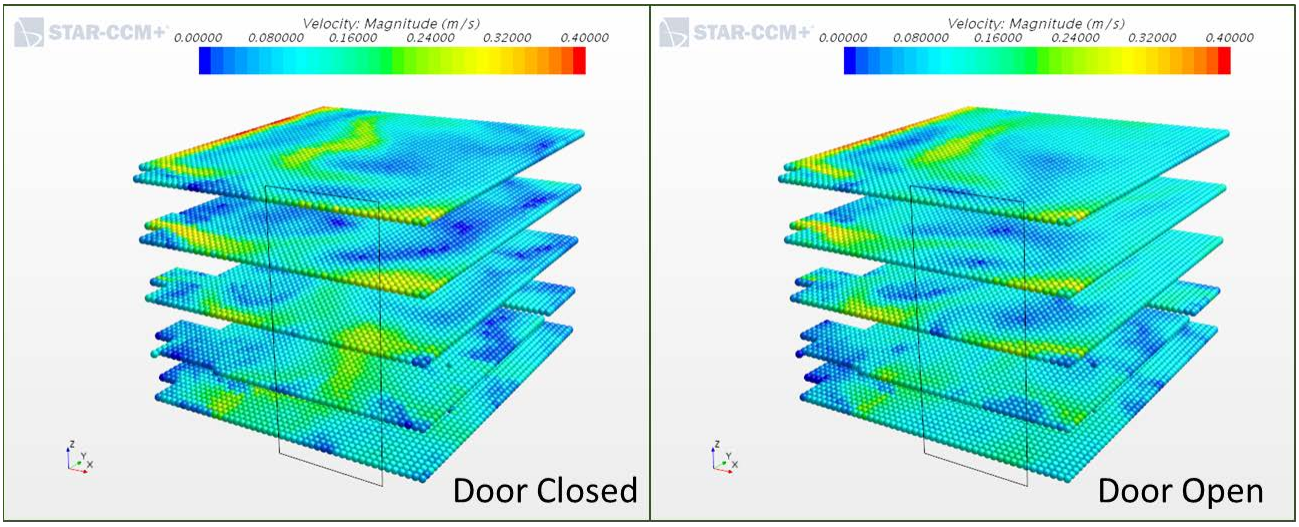


Figure S14: Schematic showing the study area we used to examine the placement of a sampler in the room and the effects of being near a door opening and closing.

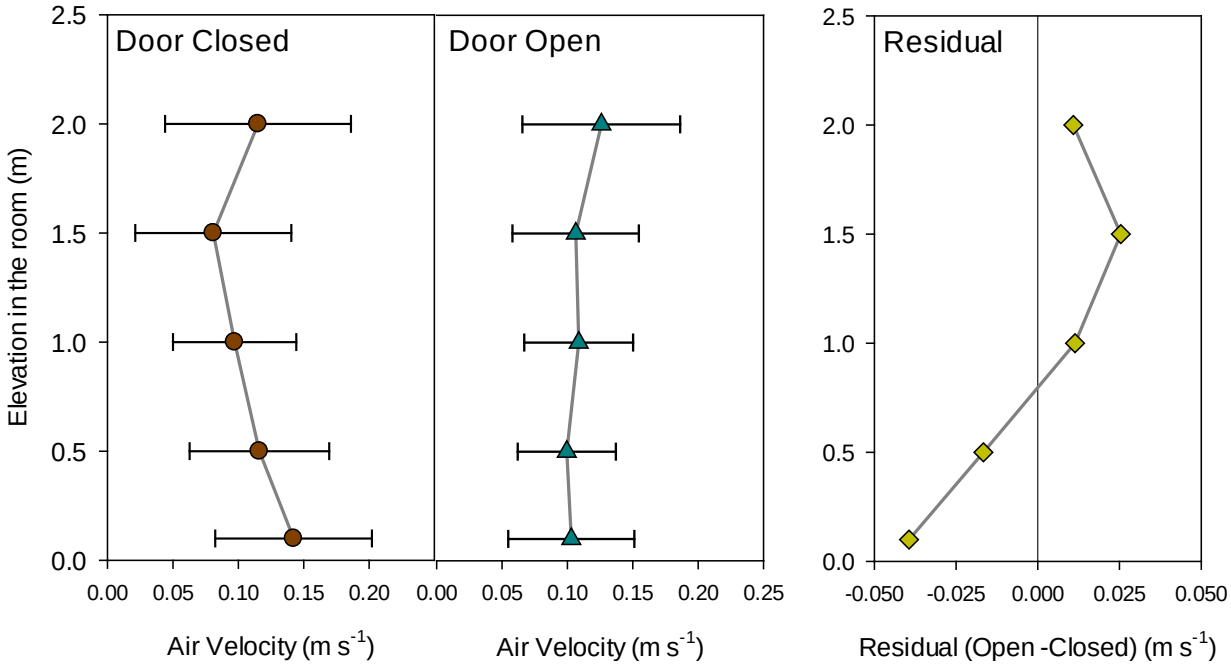


Figure S15: Vertical profiles from a CFD model showing the effects of the door being open or closed on the area immediately surrounding the door.

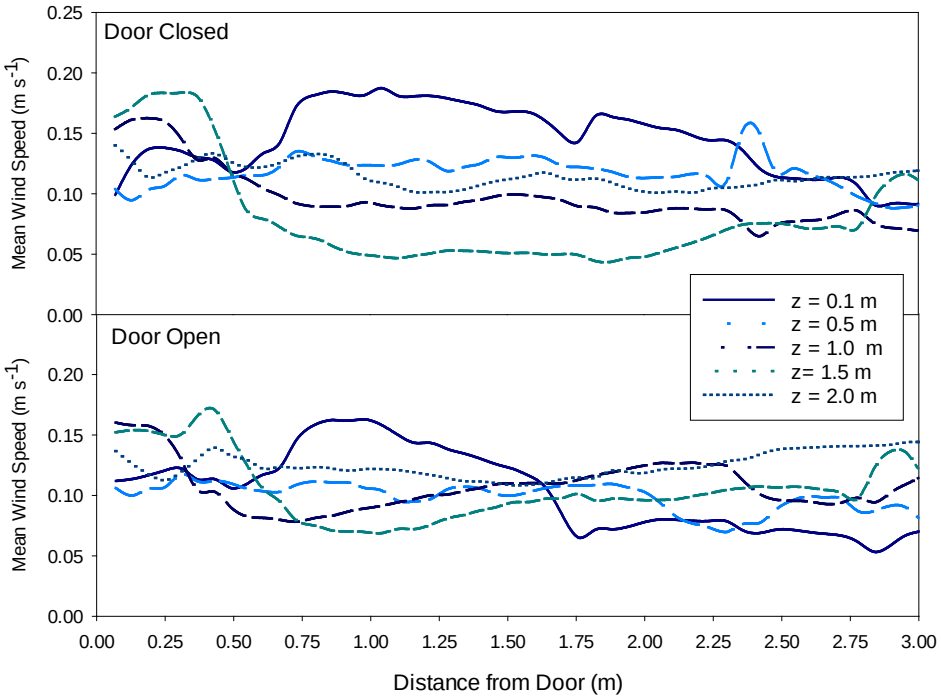


Figure S16: Horizontal profiles from a CFD model showing the effects of the door being open or closed at increasing distances from the door and at difference heights above the ground in the room (z direction).