Supplementary Information: Evaluation of a four-zone indoor exposure model for predicting TCPP concentrations in a low-energy test house

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S1. Erroneous measured temperature and airflow data

Throughout the years of data collection, intentional and unintentional events caused the data acquisition systems to record erroneous data for indoor air temperatures, HVAC temperatures, and HVAC airflows. One example of an intentional event includes a data acquisition system being shut down in order to troubleshoot or update NZERTF equipment. One example of an unintentional event includes an error in the data acquisition system resulting in blank data. These erroneous data points were replaced with either the previous/following day's data from the same timeframe or by averaging the data points before and after the erroneous data point. The number of erroneous data points are summarized in Table S.1.

Table S.1. Number of erroneous data points by calendar year.

Year	# of hrs/yr	Indoor Temperatures						HVAC Temperatures				HVAC Airflow	
		Living Area		Attic		Basement		Return		Supply		HP/SDHV	
2013	4416*	84	1.9 %	84	1.9 %	84	1.9 %	111	2.5 %	111	2.5 %	48	1.1 %
2014	8760	245	2.8 %	245	2.8 %	253	2.9 %	253	2.9 %	253	2.9 %	27	0.3 %
2015	8760	218	2.5 %	218	2.5 %	218	2.5 %	218	2.5 %	218	2.5 %	2	0.0 %
2016	8784	294	3.3 %	294	3.3 %	538	6.1 %	1497	17.0 %	719	8.2 %	133	1.5 %
2017	8760	22	0.3 %	21	0.2 %	70	0.8 %	77	0.9 %	77	0.9 %	0	0.0 %
2018	8760	1267	14.5 %	1263	14.4 %	1656	18.9 %	1143	13.0 %	1143	13.0 %	4	0.0 %
TOTAL	**48240**	**2130**	**4.4 %**	**2125**	**4.4 %**	**2819**	**5.8 %**	**3299**	**6.8 %**	**2521**	**5.2 %**	**214**	**0.4 %**

* Data acquisition system started on July 1st, 2013

S2. CONTAM model and input

The CONTAM model represented the 1st floor, 2nd floor, and the attic as separate zones. Figure S.1 is a graphical representation of the CONTAM 1st floor model. To produce airflow values for the living zone for inputs into the IECCU model the CONTAM airflows for the 1st floor and 2nd floor were combined for Simulation 1 and 2. For Simulation 3, the CONTAM airflows for the 1st floor, 2nd floor and attic were combined to generate IECCU living zone airflows.

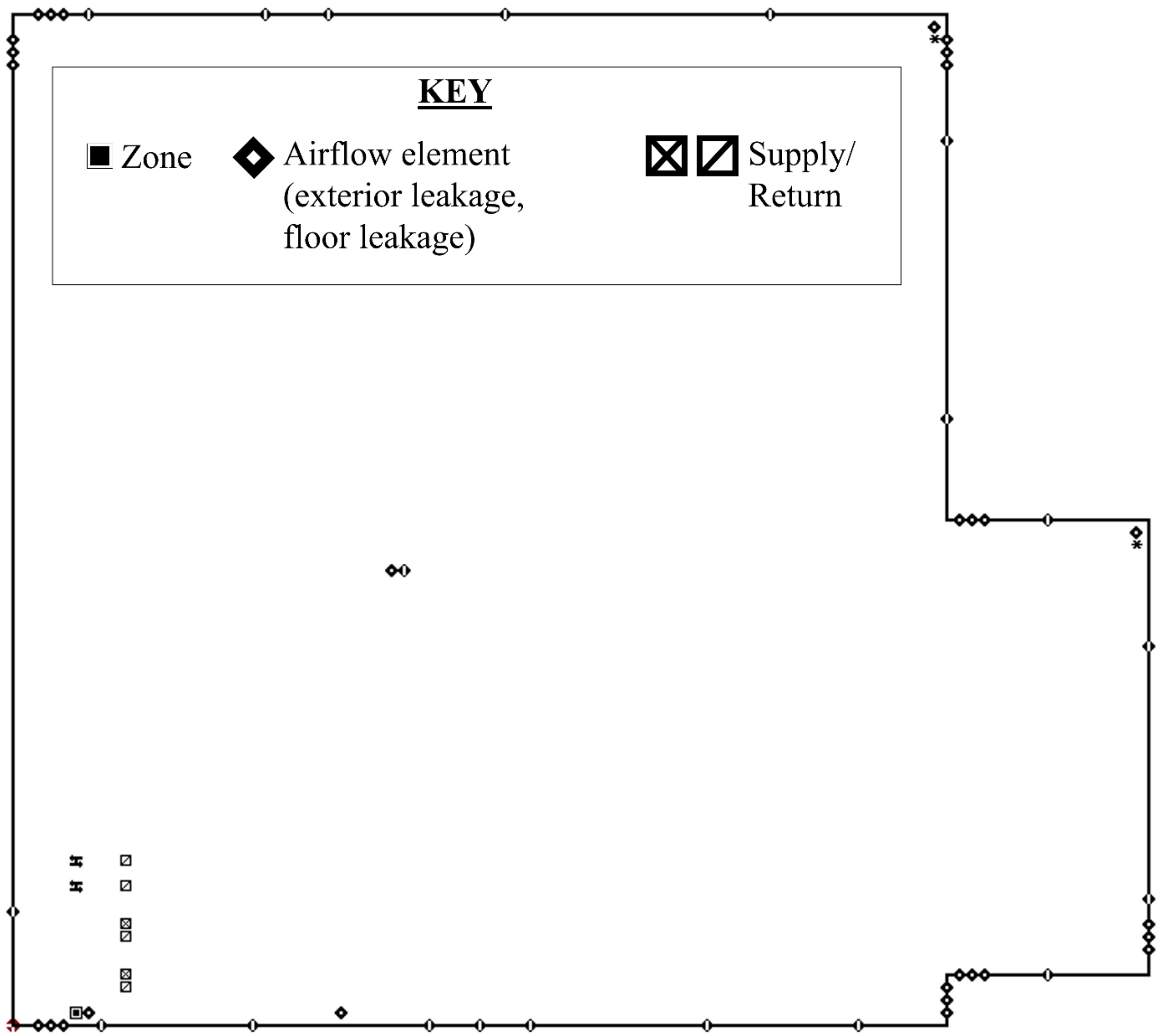

Figure S.1. CONTAM model of the NZERTF (1st floor) for deriving airflow input for IECCU. Other levels are not shown, but are similar.

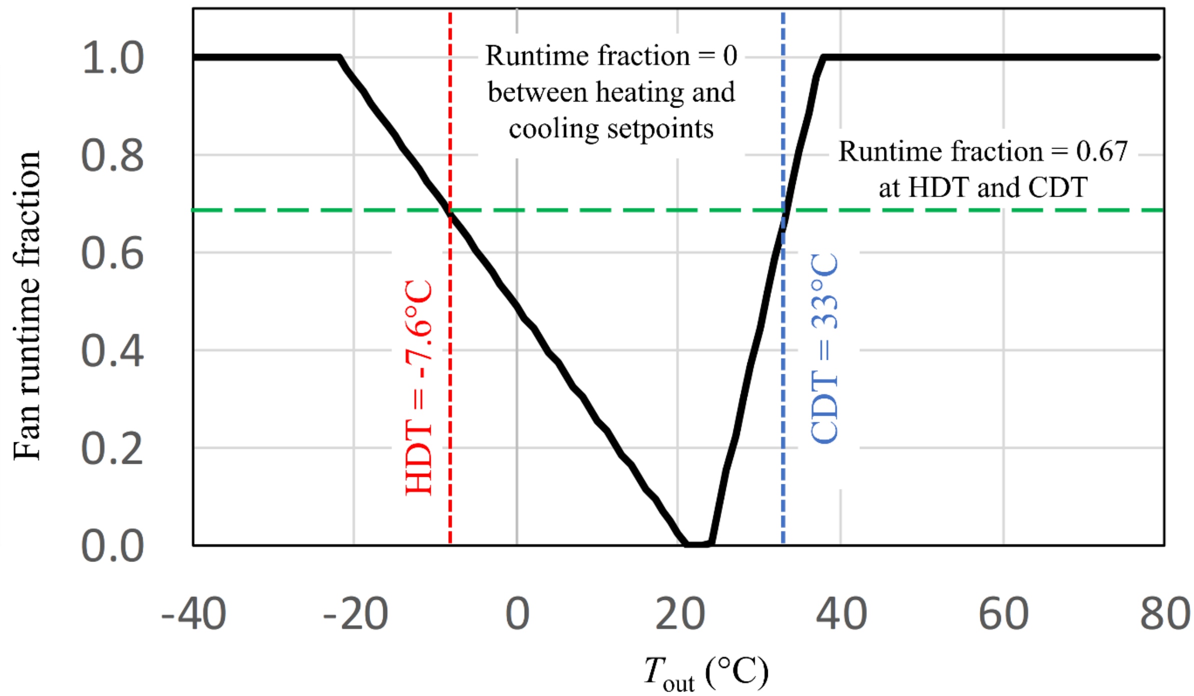

Figure S.2. Assumed runtime fraction of HVAC system for “design” input data.

S3. Input temperature and airflow

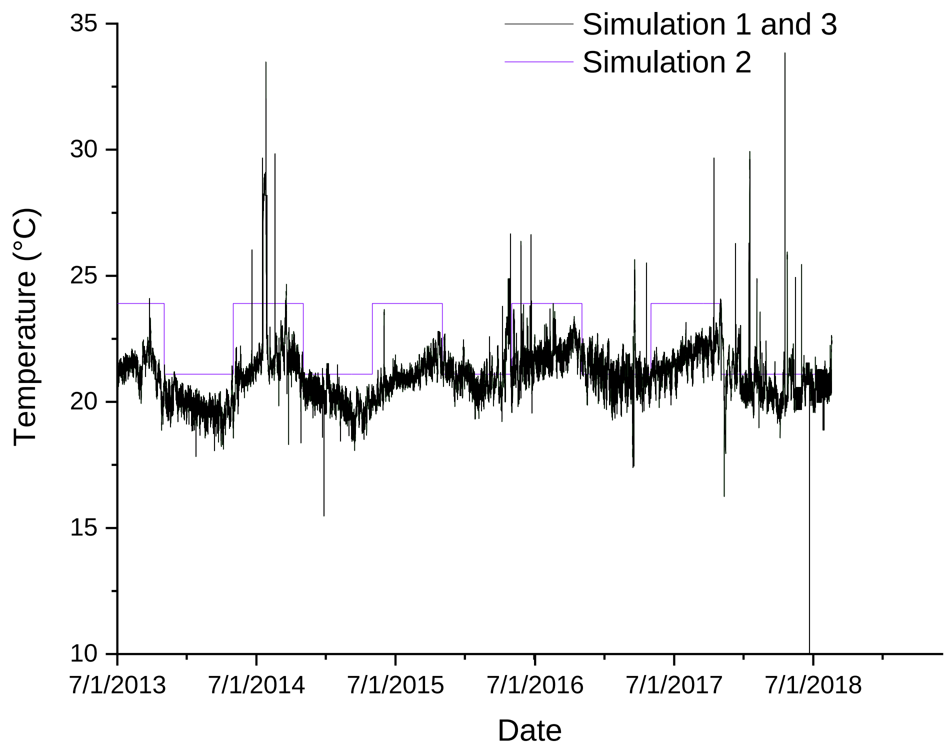

Figure S.3. Temperature in the basement zone for Simulation 1 and 3 (measured data) and Simulation 2 (design data).

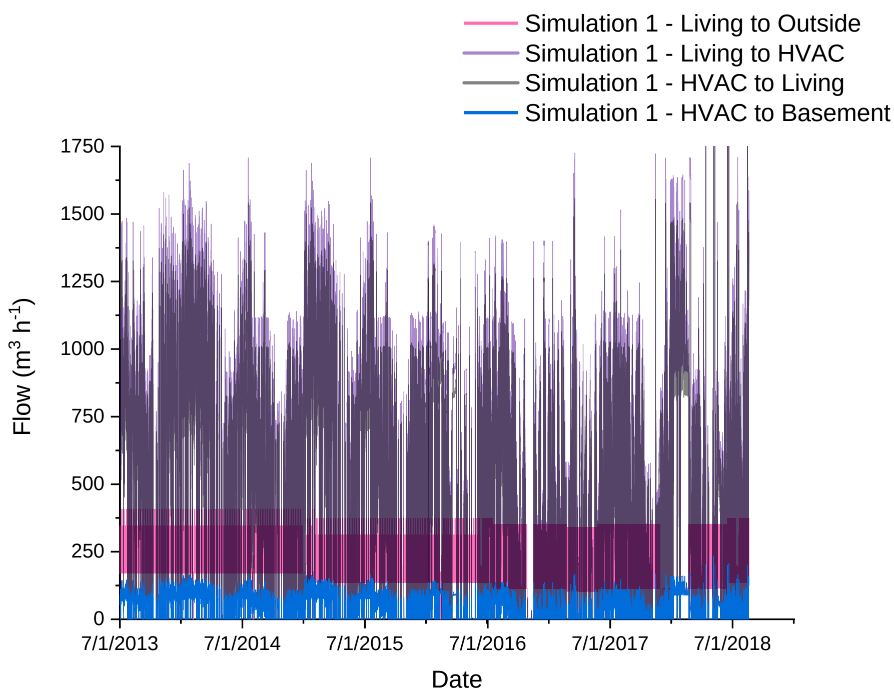

Figure S.4. Four largest input quantified airflows for Simulation 1.

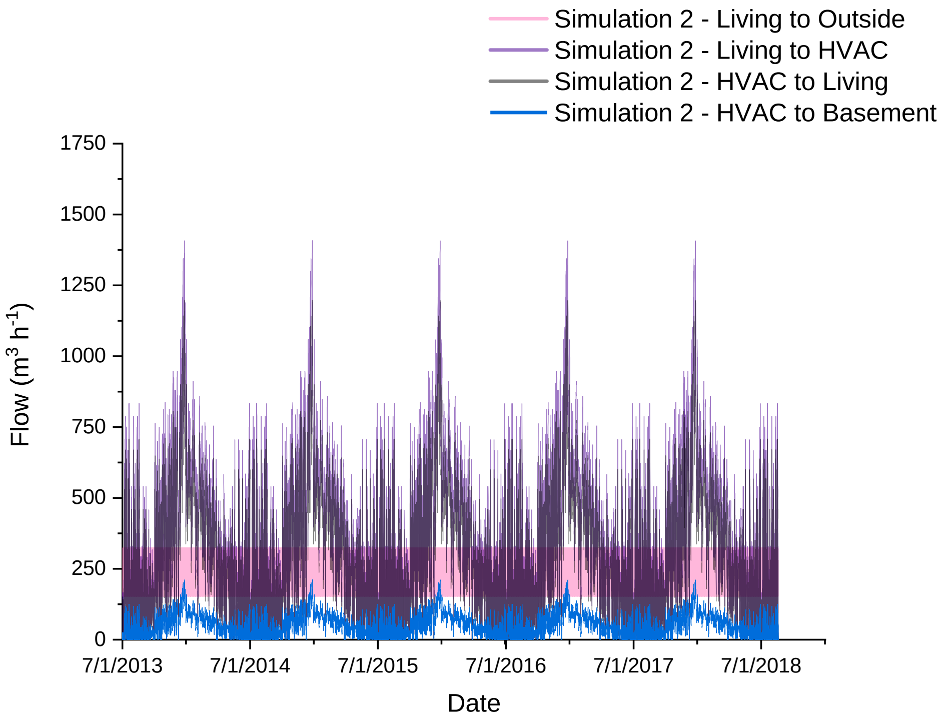

Figure S.5. Four largest input design airflows for Simulation 2.

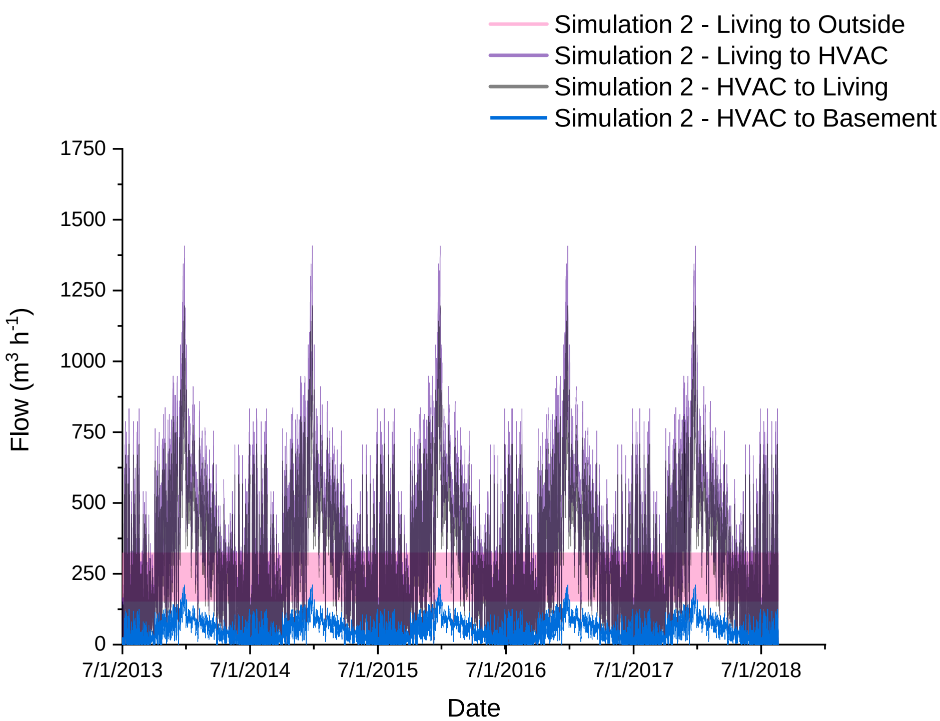

Figure S.6. Four largest input quantified airflows for Simulation 3.

S4. Comparison of predictions by Simulation 2 with different starting times

For the simulations presented in this report, the initial TCPP concentration (C_0) on July 1st, 2013 was assumed to be uniformly distributed. However, after 1.5 years of emission after SPF was sprayed, C_0 may not be uniform across the depth of the foam. Simulation 2 was run with two starting dates (2A: January 1st, 2012 and 2B: July 1st, 2013) to examine the influence of TCPP concentration distribution at the simulation starting point. The initial TCPP concentration in the SPF was set as the same value for both simulations.

For Simulation 2B the TCPP concentration in the SPF would be uniform on July 1st, 2013. In contrast, due to the TCPP emission from January 1st, 2012 to June 30th, 2013, the TCPP concentration near the surface of the SPF for Simulation 2A would be non-uniform on July 1st, 2013. Simulation 2B also had a higher initial airborne TCPP concentration due to starting during the summer, when temperature setpoints are higher, as compared to Simulation 2A with the lower winter temperature setpoints that slow mass transfer.

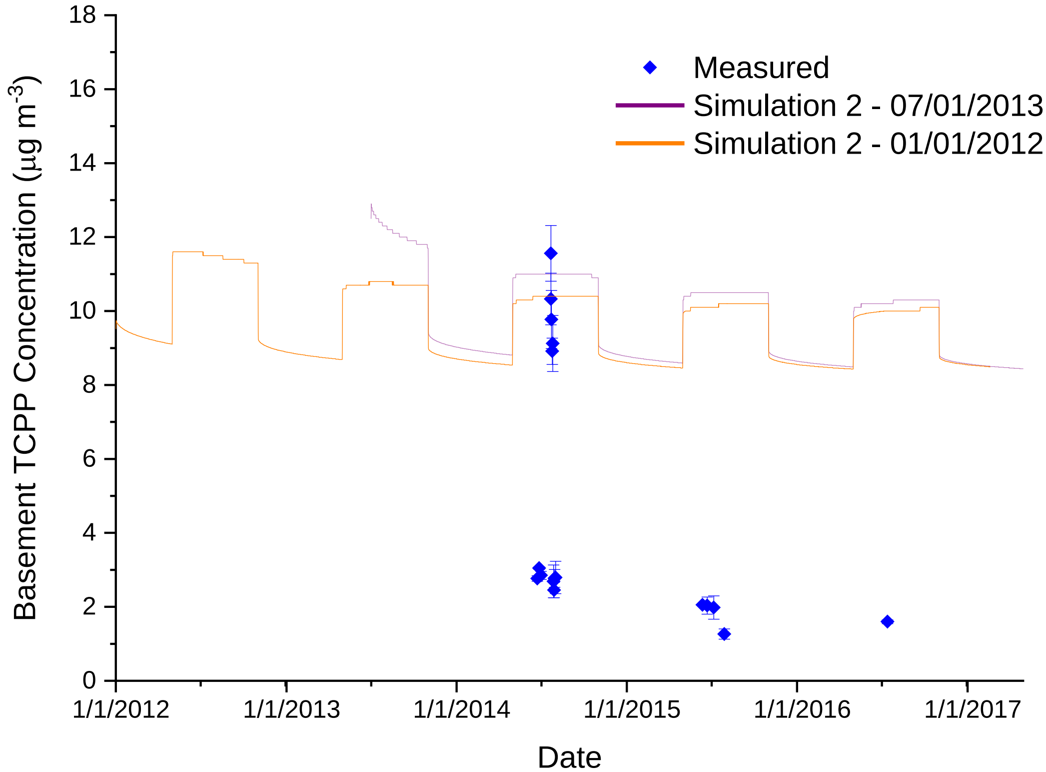

Figure S.7. Comparison of TCPP concentrations in basement from Simulation 2 with a starting date of 01/01/2012 and 7/01/2013. Error bars on triplicate measured samples represent two standard deviations. Simulation 2 did not account for the airflow and temperature perturbations that resulted in concentrations increasing from 3 µg m^{-3} to 10 µg m^{-3} in 2014.

These varying TCPP concentration profiles in the SPF explain why Simulation 2B results are roughly 1 µg m^{-3} higher than Simulation 2A during the sampling period in which measured samples were analyzed in 2014 through 2017 (Figure S.7). This indicates that starting simulations at July 1st, 2013 (Simulation 1 through Simulation 3) when building operation data recording was initiated, rather than

January 1st, 2012, when the SPF was applied may result in a roughly 1 $\mu g\ m^{-3}$ overestimate in concentrations.

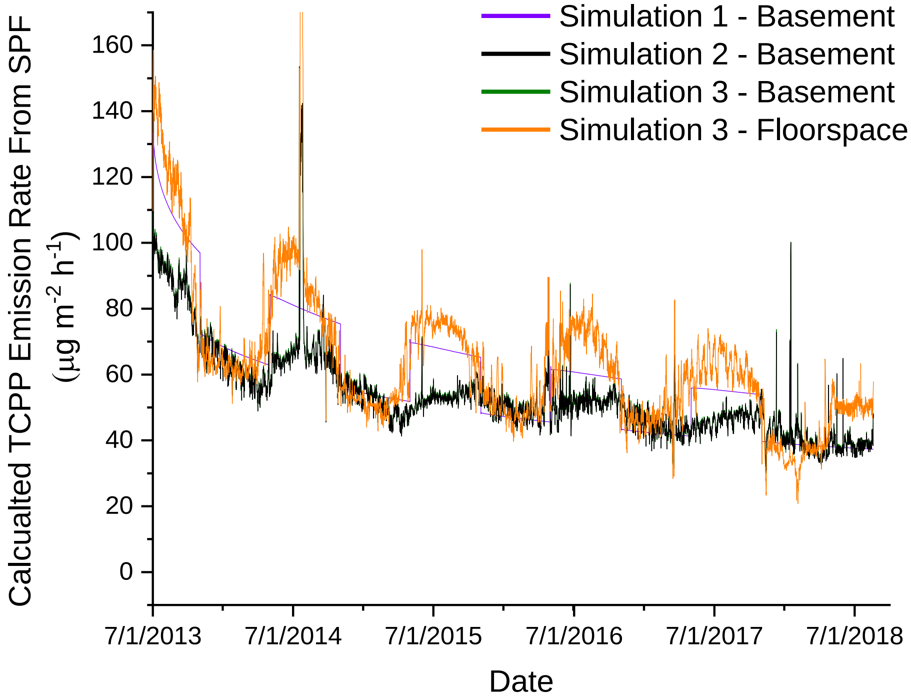

Figure S.8. Comparison of TCPP emission rates from SPF in the basement and floorspace. Simulation 3 - Basement is not identical to Simulation 2 – Basement, but the difference is not distinguishable in most of this figure.

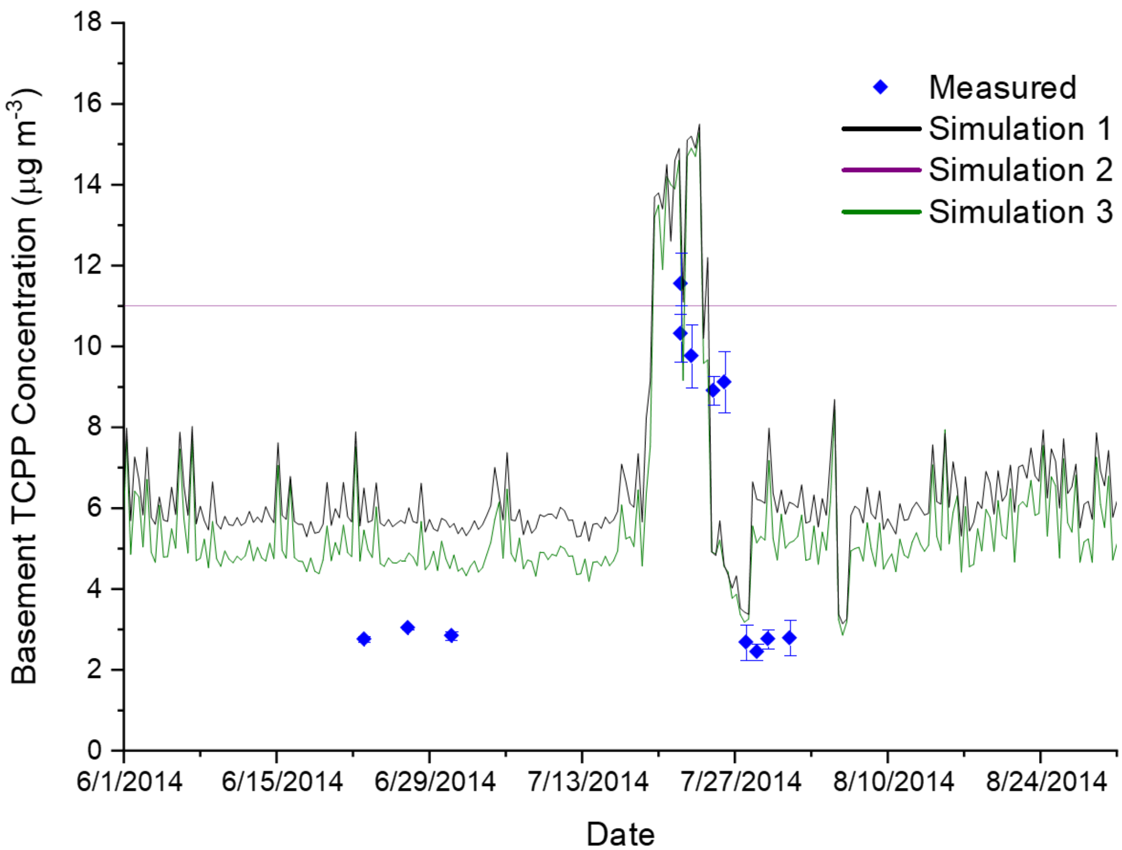

Figure S.9. Comparison of TCPP concentrations in basement simulated using quantified input (Simulation 1, Attic Configuration and Simulation 3, Floorspace Configuration) and estimated input (Simulation 2, Attic Configuration) before, during and after airflow and temperature perturbations. Error bars on triplicate measured samples represent two standard deviations.

Table S.2. Ratios of TCPP concentrations in the basement from simulations with input parameters varied and from Simulation 1 (baseline simulation). Bold values represent ratios less than 0.75 or greater than 1.25.

Parameter		Variation	Low/baseline[c]			High/baseline[d]		
			min	median	max	min	median	max
Airflows								
Fraction HVAC airflow to basement	$Q_{HVAC, B}/Q_{HVAC, L}$	0.5[a]/2[b]	**0.68**	**1.05**	**1.06**	**0.65**	**0.92**	**0.95**
Leakage Area – Exterior Walls	LA_{Wall}	0.8/1.2	**0.66**	**0.99**	**1.00**	**0.66**	**0.99**	**1.00**
Leakage Area – Basement/Living Zone	$LA_{Basement/Living}$	0.8/1.2	**0.66**	**0.99**	**1.00**	**0.66**	**0.99**	**1.00**
Leakage Area – Living/Attic Zone	$LA_{Living/Attic}$	0.8/1.2	**0.66**	**0.99**	**1.00**	**0.66**	**0.99**	**1.00**
Source - SPF								
Initial TCPP concentration	C_0	0.5/2	**0.50**	**0.50**	**0.50**	**1.99**	**2.00**	**2.00**
Partition coefficient between SPF and air	$K_{SPF/a}$	0.1/10	**1.40**	**1.58**	**8.66**	**0.10**	**0.18**	**0.21**
Diffusion coefficient - SPF	D_{SPF}	0.1/10	**0.41**	**0.45**	0.97	1.01	**1.51**	**1.68**
Convective mass transfer coefficient - SPF	$h_{m, SPF}$	0.5/2	**0.53**	**0.69**	**0.73**	1.18	**1.26**	**1.87**
Surface area - SPF	A_{SPF}	0.8/1.2	0.80	0.81	0.81	1.18	1.19	1.19
Thickness - SPF	L_{SPF}	0.8/1.2	0.99	1.00	1.00	0.99	1.00	1.00
Sink - gypsum board								
Partition coefficient between gypsum board and air	$K_{gypsum/a}$	0.1/10	1.03	**1.56**	**1.59**	**0.74**	0.83	1.00
Diffusion coefficient - gypsum	D_{gypsum}	0.1/10	1.01	**1.25**	**1.27**	0.90	0.92	1.00
Convective mass transfer coefficient - gypsum	$h_{m, gypsum}$	0.5/2	0.98	1.09	1.16	0.78	0.92	1.00
Surface area - gypsum	A_{gypsum}	0.8/1.2	1.05	1.10	1.08	0.90	0.92	0.93
Thickness - gypsum	L_{gypsum}	0.8/1.2	1.00	1.00	1.02	0.99	1.00	1.00
Sink - concrete								
Partition coefficient between concrete and air	$K_{concrete/a}$	0.1/10	1.06	**1.27**	**1.21**	**0.73**	0.82	0.99
Diffusion coefficient - concrete	$D_{concrete}$	0.1/10	1.01	**1.25**	**1.27**	0.90	0.92	1.00
Convective mass transfer coefficient - concrete	$h_{m, concrete}$	0.5/2	1.06	1.22	1.24	**0.70**	0.83	0.91
Surface area -concrete	$A_{concrete}$	0.8/1.2	1.01	1.05	1.06	0.93	0.95	0.97
Thickness - concrete	$L_{concrete}$	0.8/1.2	0.99	1.00	1.00	1.00	1.00	1.00

[a] ratio of low value and baseline value of input parameter
[b] ratio of high value and baseline value of input parameter
[c] ratio of concentrations from simulations with low value input parameter and from baseline simulation
[d] ratio of concentrations from simulations with high value input parameter and from baseline simulation

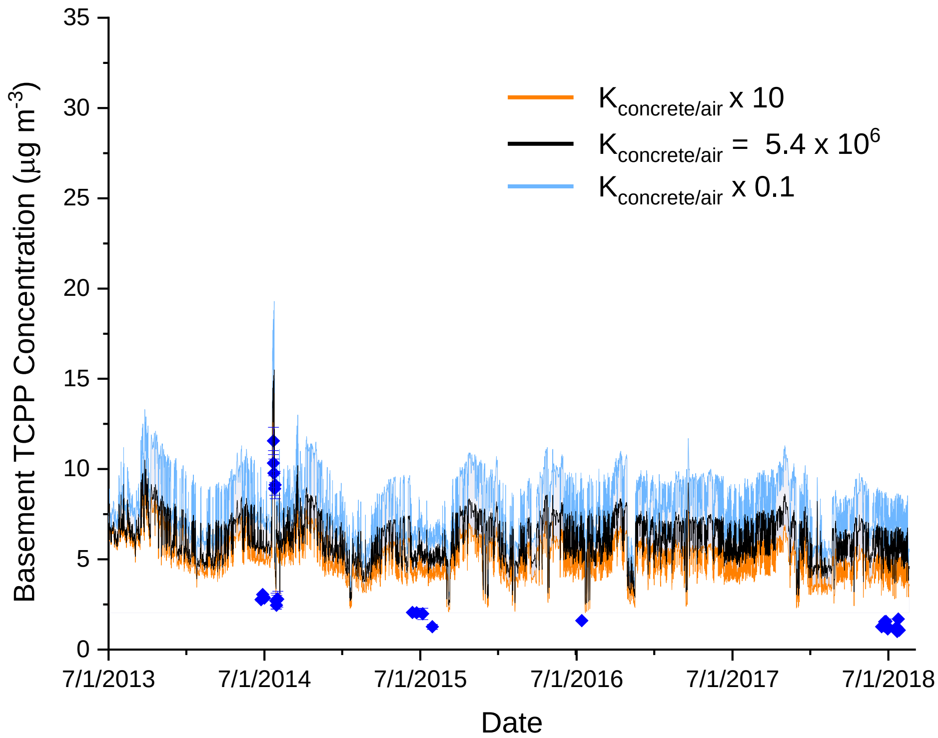

Figure S.10. TCPP basement concentration predictions for order of magnitude changes in the concrete partition coefficient. Error bars on triplicate measured samples represent two standard deviations.

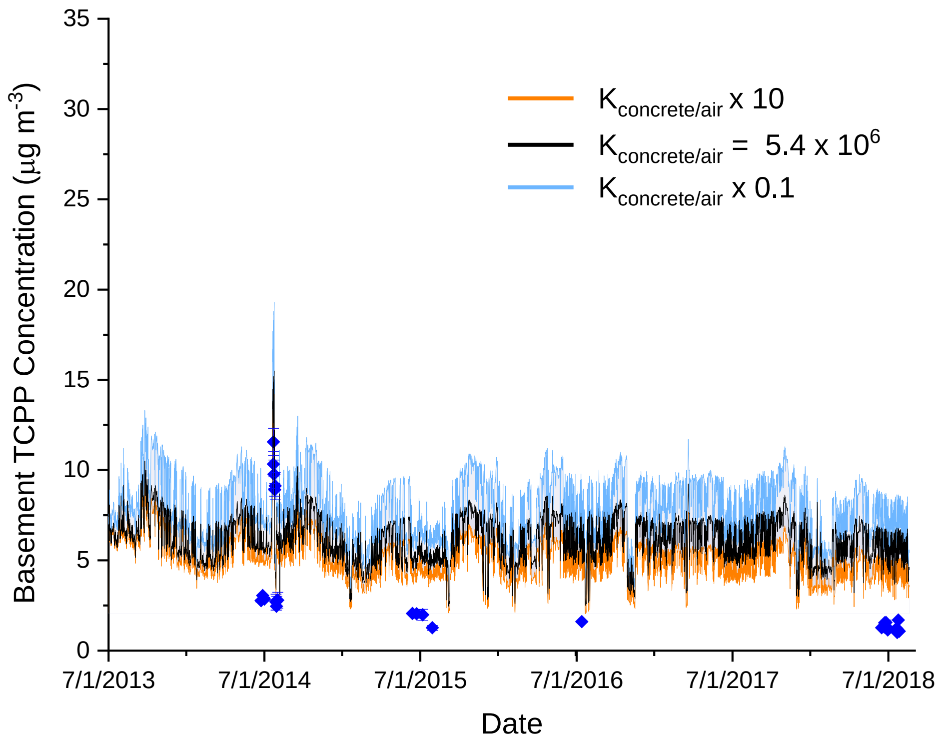

Figure S.11. TCPP basement concentration predictions for order of magnitude changes in the gypsum partition coefficient. Error bars on triplicate measured samples represent two standard deviations

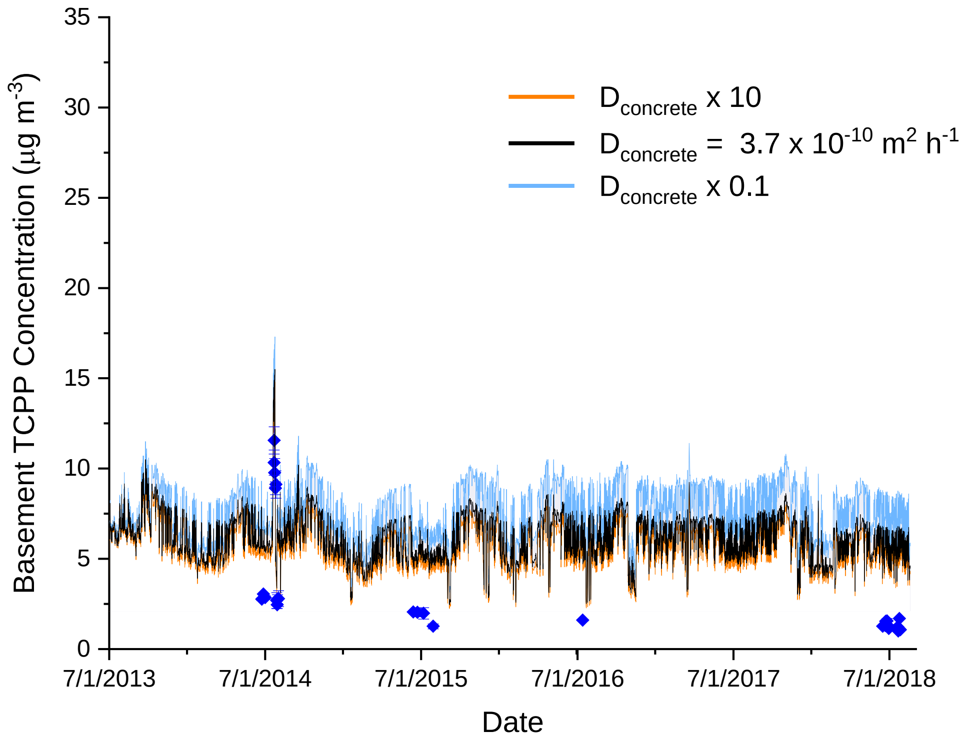

Figure S.12. TCPP basement concentration predictions for order of magnitude changes in the concrete diffusion coefficient. Error bars on triplicate measured samples represent two standard deviations

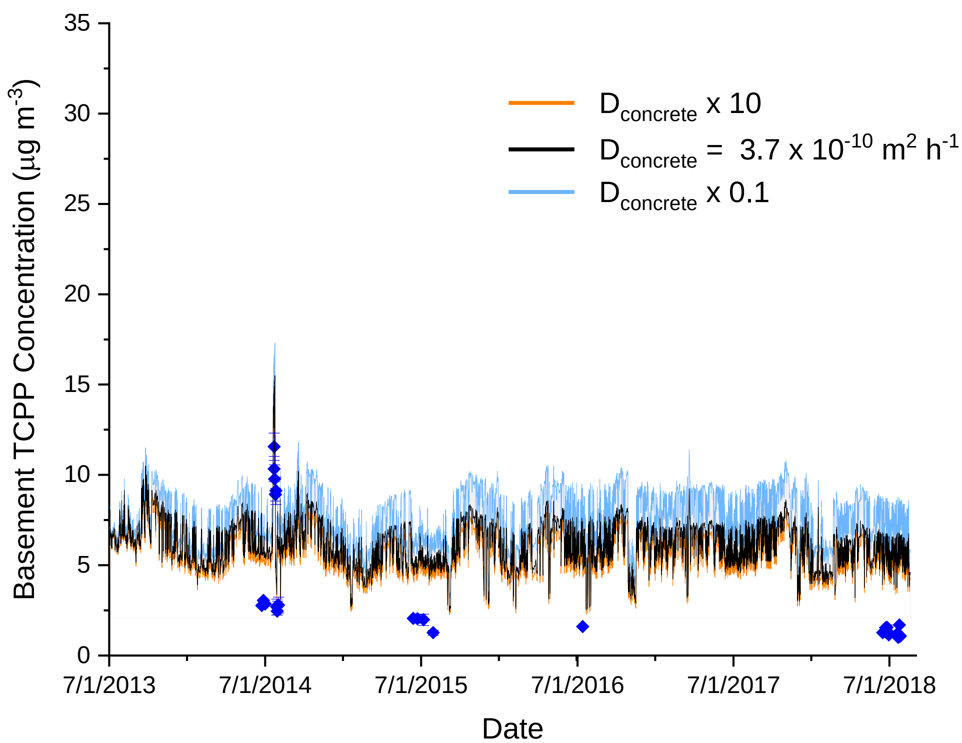

Figure S.13. TCPP basement concentration predictions for order of magnitude changes in the gypsum diffusion coefficient. Error bars on triplicate measured samples represent two standard deviations

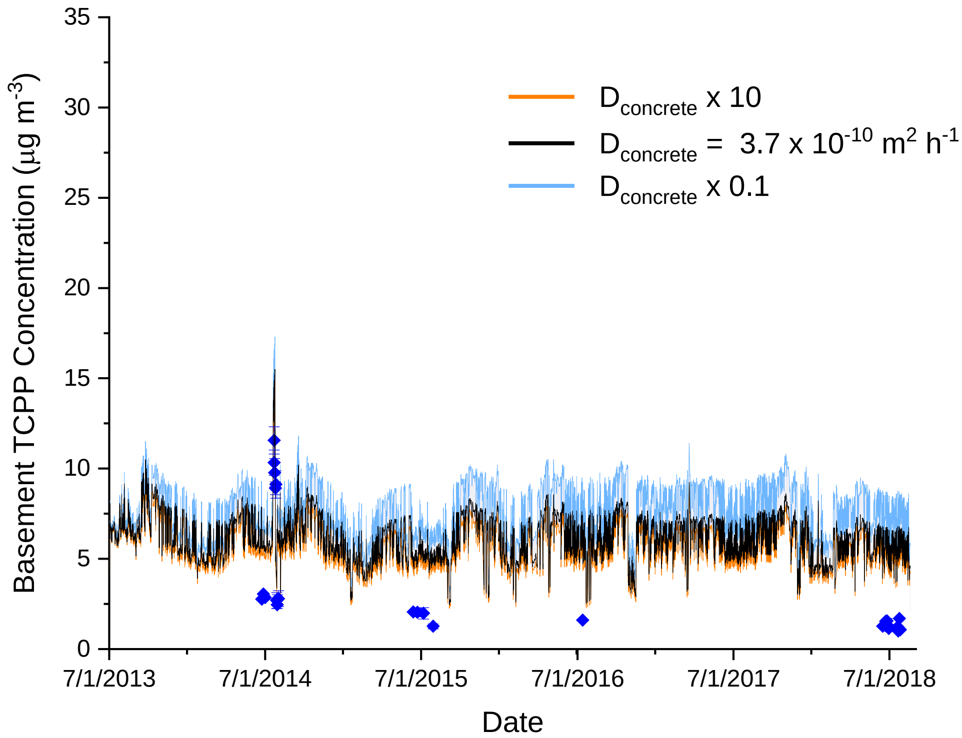

Figure S.14. TCPP basement concentration predictions for factor of two changes in the concrete mass transfer coefficient, $h_{m\ concrete}$. Error bars on triplicate measured samples represent two standard deviations.

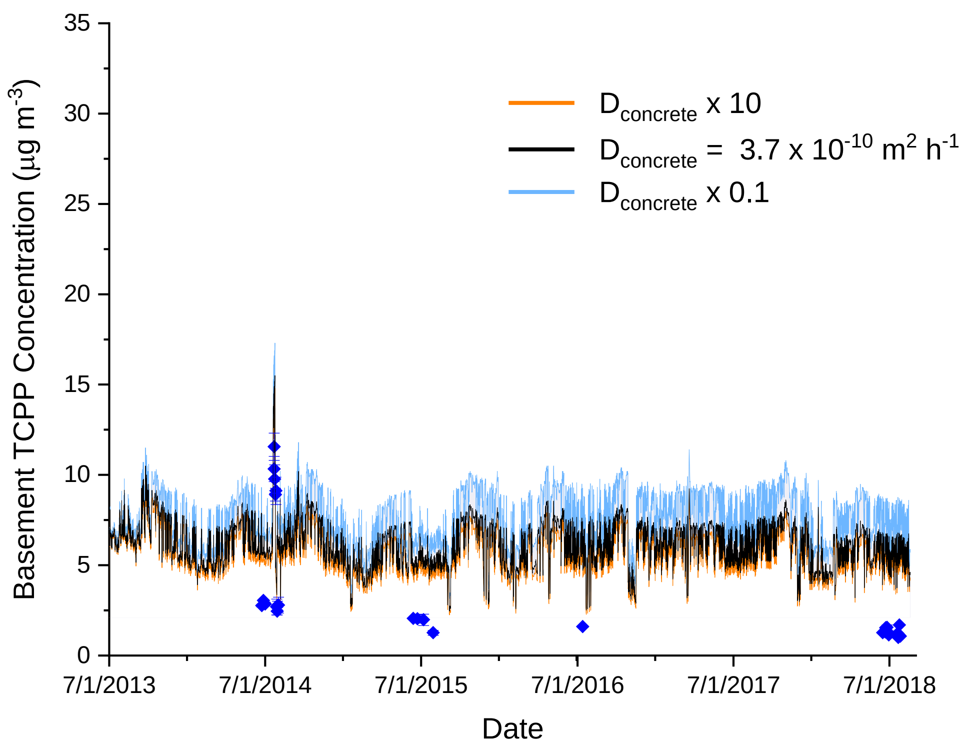

Figure S.15. TCPP basement concentration predictions for factor of two changes in the gypsum mass transfer coefficient, $h_{m\ gypsum}$. Error bars on triplicate measured samples represent two standard deviations.

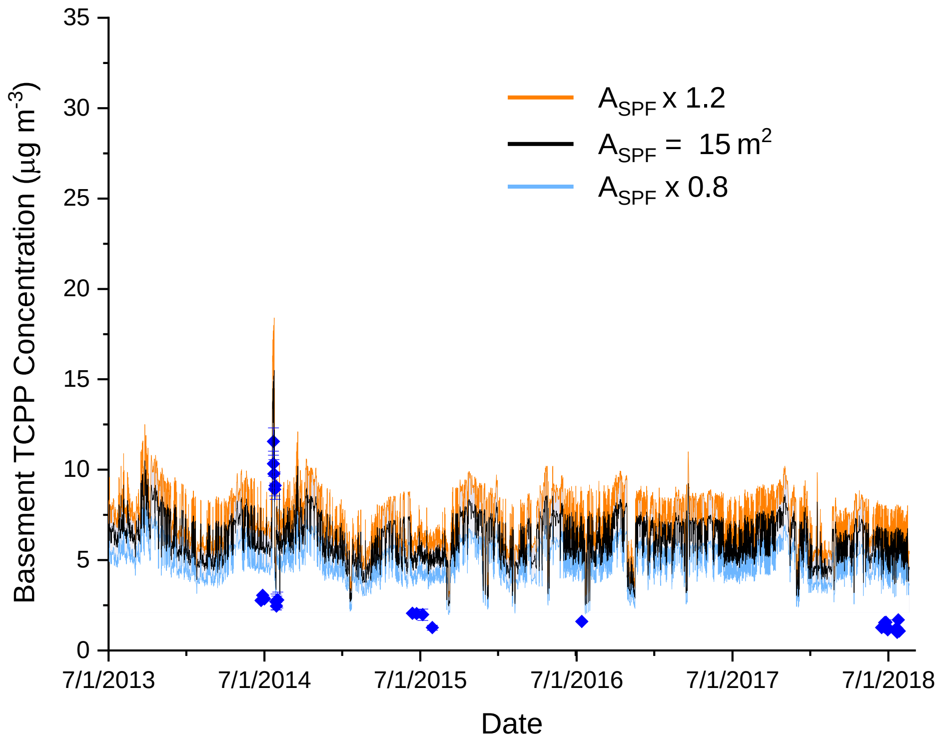

Figure S.16. TCPP basement concentration predictions for 20 % changes in the SPF area. Error bars on triplicate measured samples represent two standard deviations.

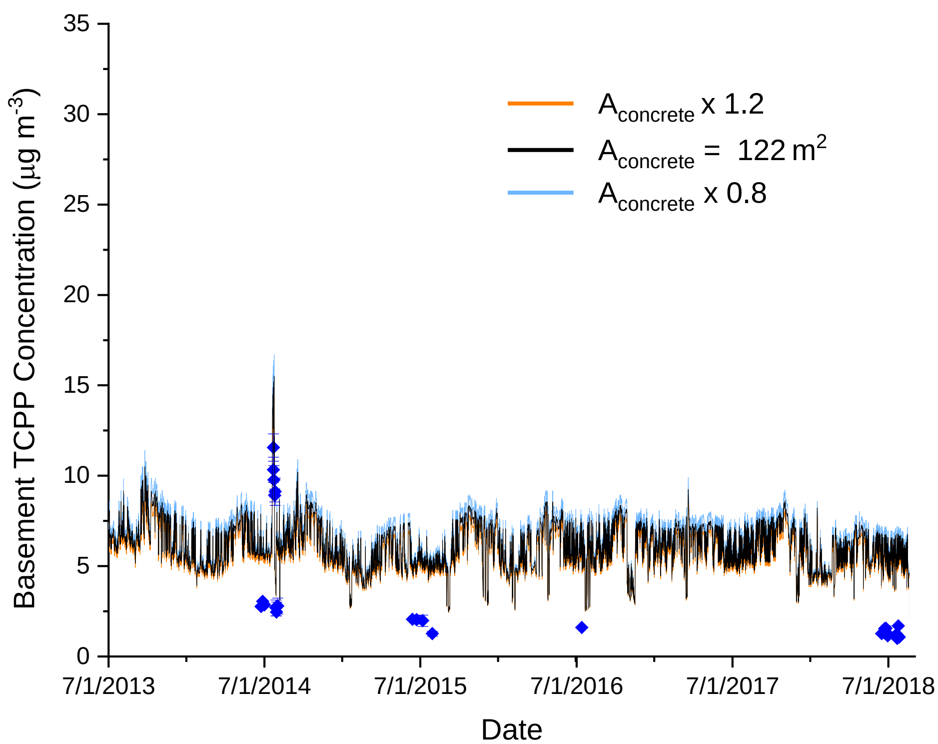

Figure S.17. TCPP basement concentration predictions for 20 % changes in the concrete area. Error bars on triplicate measured samples represent two standard deviations.

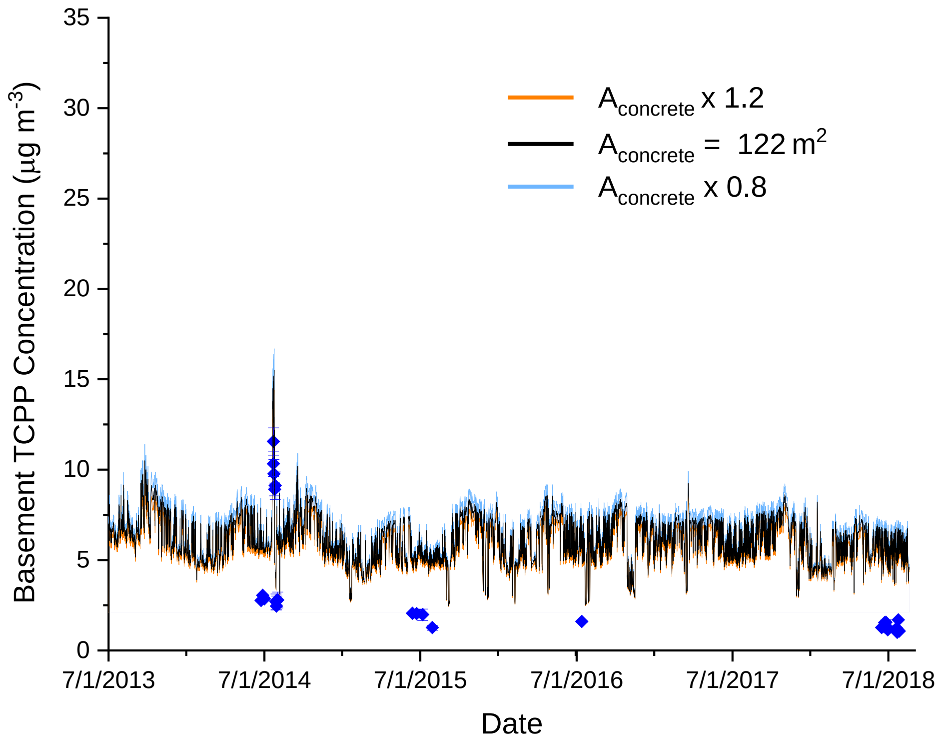

Figure S.18. TCPP basement concentration predictions for 20 % changes in the gypsum area. Error bars on triplicate measured samples represent two standard deviations.

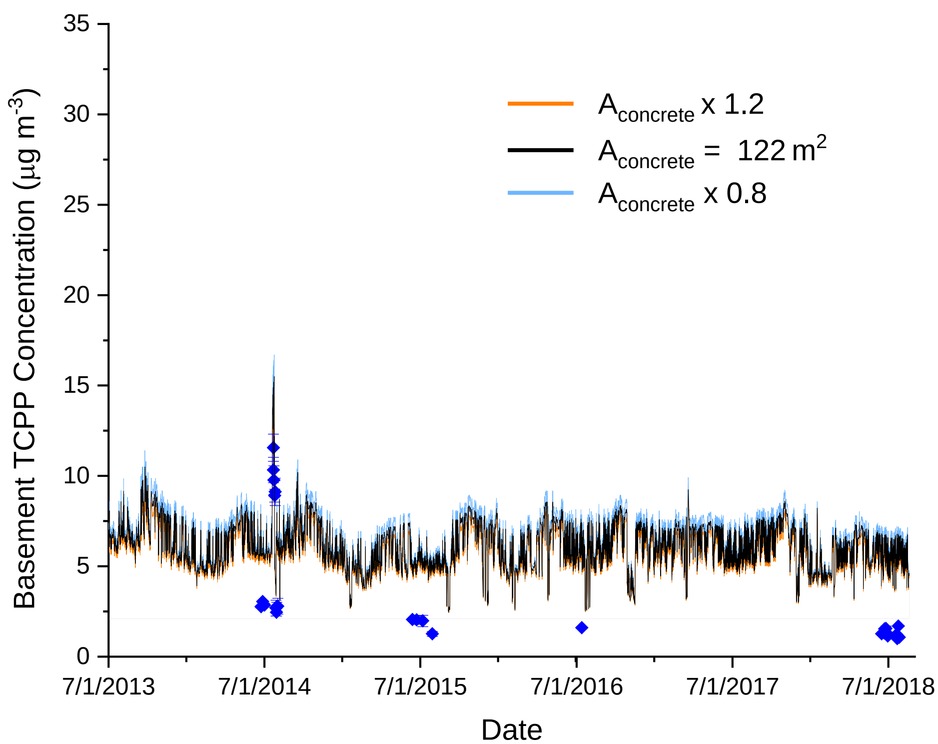

Figure S.19. TCPP basement concentration predictions for factor of two changes in the fraction of the HVAC airflow to the basement. Error bars on triplicate measured samples represent two standard deviations.

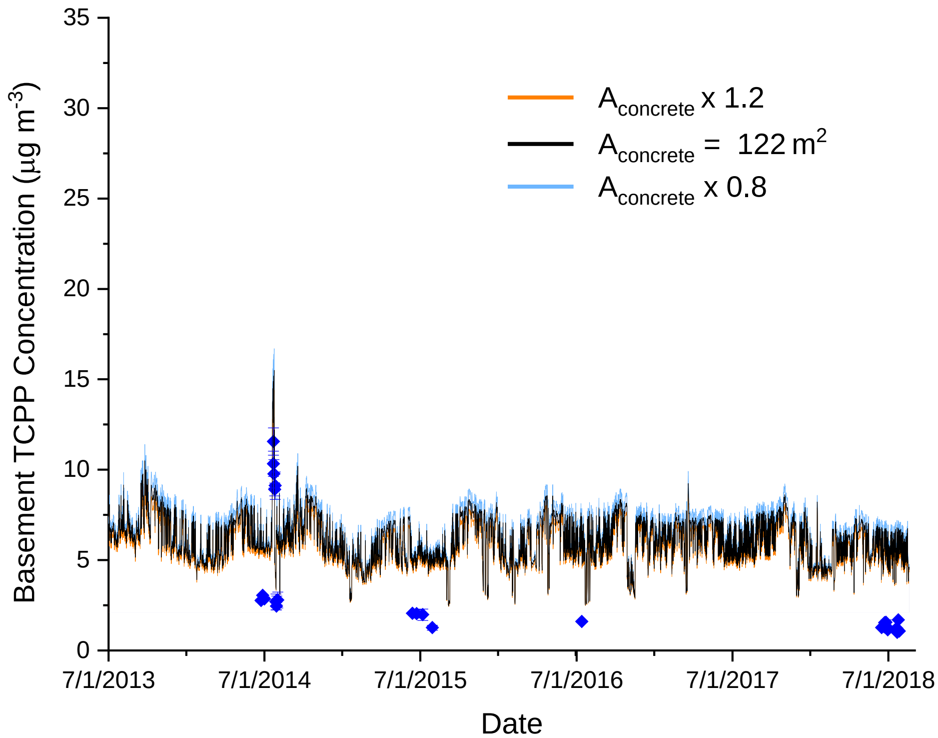

Figure S.20. TCPP basement concentration predictions for 20 % changes in the SPF thickness. Graphs for 20 % changes in thickness of gypsum wallboard, thickness of concrete, leakage area between the basement/living zones, leakage area between the attic/living zones and leakage areas of the exterior walls were identical. Error bars on triplicate measured samples represent two standard deviations.

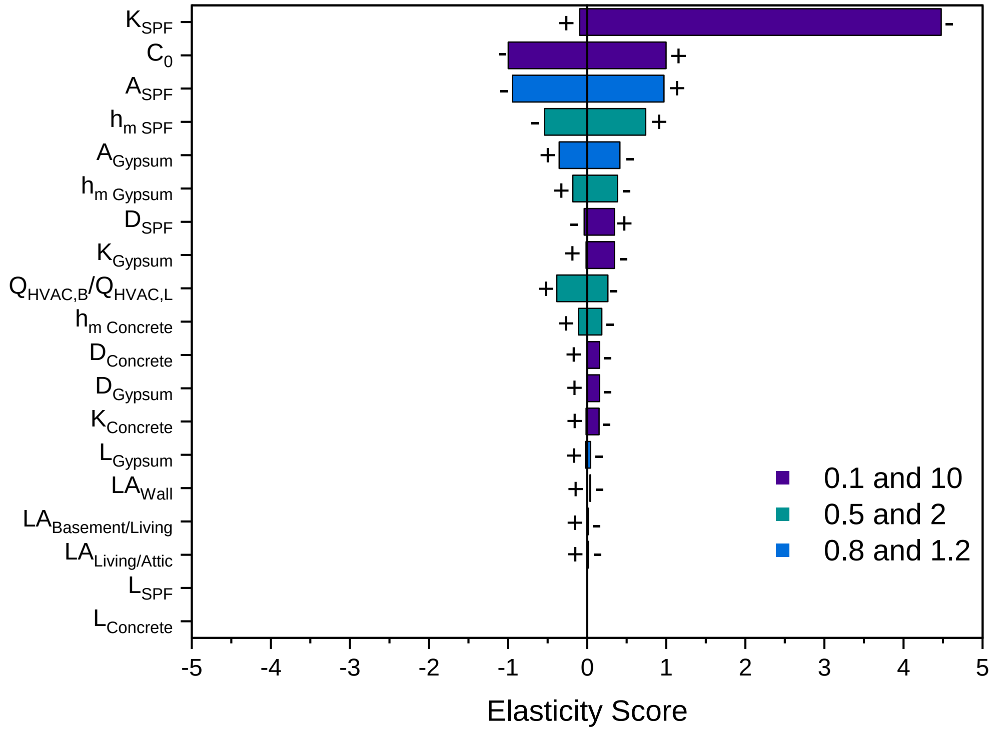

Figure S.21. Elasticity score for high and low parameter values. Positive signs indicate larger value for parameter. Legend refers to the range of values tested. Parameters defined in Table S.2

Table S.3. Model fit values for parameter variation sensitivity analysis. Bold Biot/K values show where diffusion within the SPF or concrete or gypsum is limiting process for TCPP emissions.

Parameter	**Variation**	**Biot/K**	**NMSE**	**Slope**	Intercept %	R-squared	Correlation coefficient
Baseline – Simulation 1			**0.64**	**0.58**	**122**	**0.43**	**0.66**
C_0	0.5	NA	0.56	0.29	61	0.43	0.66
	2	NA	2.26	1.15	271	0.43	0.66
$K_{SPF/a}$	0.1	**220**	1.98	1.47	49	0.57	0.76
	10	2.2	4.00	0.06	7	0.22	0.47
$K_{gypsum/a}$	0.1	8.5	1.31	0.59	114	0.31	0.55
	10	0.1	0.45	0.62	35	0.52	0.72
$K_{concrete/a}$	0.1	**230**	0.99	0.68	88	0.39	0.62
	10	2.3	0.44	0.61	41	0.52	0.72
D_{SPF}	0.1	**220**	0.50	0.35	173	0.53	0.73
	10	2.2	1.32	0.64	225	0.30	0.55
D_{gypsum}	0.1	8.5	0.91	0.55	103	0.35	0.59
	10	0.1	0.55	0.57	51	0.45	0.67
$D_{concrete}$	0.1	**230**	0.91	0.55	104	0.35	0.59
	10	2.3	0.55	0.57	51	0.45	0.67
$h_{m, SPF}$	0.5	11	0.47	0.33	34	0.34	0.58
	2	**43**	1.04	0.88	123	0.52	0.72
$h_{m, gypsum}$	0.5	0.0	0.97	0.82	84	0.46	0.68
	2	0.2	0.48	0.36	49	0.38	0.61
$h_{m, concrete}$	0.5	14	0.80	0.73	76	0.43	0.66
	2	**57**	0.52	0.42	60	0.42	0.65
$\mathbf{A_{SPF}}$	0.8	NA	0.46	0.47	42	0.43	0.66
	1.2	NA	0.87	0.69	100	0.44	0.66
$\mathbf{A_{concrete}}$	0.8	NA	0.71	0.62	79	0.42	0.65
	1.2	NA	0.56	0.54	62	0.44	0.67
$\mathbf{A_{gypsum}}$	0.8	NA	0.76	0.65	92	0.43	0.66
	1.2	NA	0.54	0.52	57	0.44	0.66
$\mathbf{L_{SPF}}$	0.8	17	0.63	0.58	57	0.43	0.66
	1.2	26	0.63	0.58	68	0.43	0.66
$\mathbf{L_{concrete}}$	0.8	23	0.63	0.58	71	0.43	0.66
	1.2	34	0.63	0.58	68	0.43	0.66
$\mathbf{L_{gypsum}}$	0.8	0.1	0.64	0.57	75	0.42	0.65
	1.2	0.1	0.62	0.58	67	0.44	0.66