

**Primary emissions, ozone reactivity, and byproduct emissions from
building insulation materials: Supporting Information**

Kyle Chin¹, Aurelie Laguerre¹, Pradeep Ramasubramanian¹, David Pleshakov¹, Brent Stephens², Elliott T. Gall^{1,*}

¹ Portland State University, Mechanical and Materials Engineering, Portland, OR USA

² Illinois Institute of Technology, Civil, Architectural, and Environmental Engineering, Chicago, IL USA

*Corresponding email: gall@pdx.edu

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SUPPORTING INFORMATION

Table S1. Images of prepared test material samples

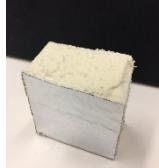
Name	Code	Material	Sample Preparation
Fiberglass	FG		
Cellulose	C		
Polyurethane	PU		
Polyisocyanurate	PI		
Stone Wool	SW		
Polystyrene with Thermal Backing	PSTB		
Polystyrene	PS		
Denim	DM		

Table S2. Summary of primary volatile organic compound source and sink behavior for eight test materials. Quantification and identification performed for five largest source fluxes for each test material and for five largest source and sink fluxes for PSTB.

Cellulose						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	flux	Reference/comment
61.028406	61.028100	0.306	C2H4O2(H+)	Acetic acid Acid fragment	24.91	
43.017800	43.016000	1.800	C2H2O(H+)	(ketene)	17.73	Keki et al. ¹
47.012756	47.012300	0.456	CH2O2(H+)	Formic acid	3.93	
33.033491	33.026280	7.211	CH4O(H+)	Methanol	2.16	Multi-peak integration to separate one oxygen-17 O2+
45.033491	45.029930	3.561	C2H4O(H+)	Acetaldehyde	1.63	Multi-peak integration, unknown interference
		Formula	# of compounds			
		CxHy	27	2.01		
		CxHyO	40	2.71		
		CxHyO2	4	2.09		
		Other	118	3.93		
					Total source	61.1
					Total sink	-0.1
Recycled denim						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	flux	Reference/comment
47.012756	47.0111	1.656	CH2O2(H+)	Formic acid	13.94	
63	63.0241	n/a	n/a	unknown	10.12	
61.028406	61.0282	0.206	C2H4O2(H+)	Acetic acid Acid fragment	8.29	
43.017800	43.0174	0.400	C2H2O(H+)	(ketene)	6.09	
45.033491	45.029930	3.561	C2H4O(H+)	Acetaldehyde	3.65	
		Formula	# of compounds			
		CxHy	19	1.76		
		CxHyO	22	1.88		
		CxHyO2	4	1.18		
		Other	66	5.75		
					Total source	52.7
					Total sink	-0.3

Polyurethane						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
47.012756	47.0111	1.656	CH2O2(H+)	Formic acid	11.5	
63	63.0244	n/a	n/a	unknown	9.00	
61.028406	61.0284	0.006	C2H4O2(H+)	Acetic acid Acid fragment	6.89	
43.017800	43.0174	0.4	C2H2O(H+)	(ketene)	5.17	
45.033491	45.029930	3.561	C2H4O(H+)	Acetaldehyde	3.38	
			Formula	# of compounds		
			CxHy	20	1.50	
			CxHyO	26	2.12	
			CxHyO2	4	0.96	
			Other	79	6.23	
			Total source	46.8		
			Total sink	-0.1		
Polyisocyanurate						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
41.038577	41.037	1.577	C3H4(H+)	Propyne Acid fragment	15.6	
43.017800	43.01641	1.39	C2H2O(H+)	(ketene)	6.08	Apparent multi-peak - required correction
42.033826	42.0436	-9.774	C2H3N(H+)	Acetonitrile	5.89	Possibly acetonitrile ² or propanal fragment
57.069877	57.0687	1.177	C4H8(H+)	2-butene	2.65	
40	40.0283	n/a	n/a	unknown	0.79	
			Formula	# of compounds		
			CxHy	13	0.51	
			CxHyO	17	1.01	
			CxHyO2	3	0.31	
			Other	28	1.09	
			Total source	33.9		
			Total sink	-0.6		

Polystyrene						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
105.0699	105.072	-2.1	C8H8(H+)	Styrene	3.52	Choczynski et al. ³
107.070271	107.074	-3.729	C4H10O3(H+)	Diethylene glycol	1.54	Solvent in building materials ⁴
63	63.0242	n/a	n/a	unknown	0.947	
79.054227	79.0564	-2.173	C6H6(H+)	Benzene	0.688	Polystyrene precursor
121.064791	121.069	-4.209	C8H8O(H+)	Acetophenone	0.519	Thermal decomposition product of polystyrene ⁵
			Formula	# of compounds		
			CxHy	7	0.22	
			CxHyO	14	0.76	
			CxHyO2	4	0.17	
			Other	50	2.74	
			Total source	11.1		
			Total sink	-0.3		
Fiberglass						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
43.017800	43.0157	2.1	C2H2O(H+)	Acid fragment (ketene)	1.21	
61.028406	61.0282	0.206	C2H4O2(H+)	Acetic acid	1.16	
47.012756	47.0112	1.556	CH2O2(H+)	Formic acid	1.11	
45.033491	45.029930	3.561	C2H4O(H+)	Acetaldehyde	0.603	
41.038577	41.0359	2.677	C3H4(H+)	Propyne	0.442	
			Formula	# of compounds		
			CxHy	10	1.06	
			CxHyO	16	1.33	
			CxHyO2	4	0.25	
			Other	51	1.26	
			Total source	8.4		
			Total sink	-0.6		

Stone wool						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
61.028	61.0283	0.106	C2H4O2(H+)	Acetic acid Acid fragment	1.64	
43.017841	43.0159	1.941	C2H2O(H+)	(ketene)	1.18	
31.017841	31.0127	5.141	CH2O(H+)	Formaldehyde	0.36	
44.01309	44.0092	3.89	CHNO(H+)	Isocyanic acid	0.16	Present in waterproofing of some building materials ⁶
60.0447	60.0444	0.3	C2H5NOH+)	Acetamide	0.11	Industrial solvent, identified elsewhere w/ PTR-MS ⁷
			Formula	# of compounds		
			CxHy	7	0.22	
			CxHyO	14	0.76	
			CxHyO2	4	0.17	
			Other	50	2.74	
			Total source	7.3		
			Total sink	-0.3		
Polystyrene with thermal backing (source)						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
41.038577	41.0365	2.077	C3H4(H+)	Propyne Acid fragment	2.54	
43.017800	43.0179	-0.1	C2H2O(H+)	(ketene)	1.46	
42.033826	42.0359	-2.074	C2H3N(H+)	Acetonitrile	0.251	Possibly propanal fragment
57.069877	57.0659	3.977	C4H8(H+)	2-butene	0.237	
105.0699	105.065	4.9	C8H8(H+)	Styrene	0.226	
			Formula	# of compounds		
			CxHy	4	0.30	
			CxHyO	2	0.25	
			CxHyO2	0	0.00	
			Other	13	0.45	
			Total source	5.7		

Polystyrene with thermal backing (sink)						
m/z exact	m/z measured	del mDa	Putative ID	Putative name	flux	Reference/comment
47.012756	47.0131	-0.344	CH2O2(H+)	Formic acid	-0.84	
45.033491	45.031	2.491	C2H4O(H+)	Acetaldehyde	-0.65	
61.028406	61.0289	-0.494	C2H4O2(H+)	Acetic acid	-0.47	
31.017841	30.997	20.841	CH2O(H+)	Formaldehyde	-0.39	
44.01309	44.0094	3.69	CHNO(H+)	Isocyanic acid	-0.38	
		Formula	# of compounds			
		CxHy	20	-0.15		
		CxHyO	35	-1.49		
		CxHyO2	6	-1.38		
		Other	82	-2.31		
				Total sink	-8.1	

Table S3. Summary of statistically significant unit masses for cellulose and polystyrene with thermal backing (PSTB) for estimation of mass emission flux.

Cellulose		Total	3.07		mg/m ² /h									
m/z	μmol/m ² /h	μg/m ² /h	m/z	μmol/m ² /h	μg/m ² /h	m/z	μmol/m ² /h	μg/m ² /h	m/z	μmol/m ² /h	μg/m ² /h	m/z	μmol/m ² /h	μg/m ² /h
61	24.23	1454.07	102	0.04	4.35	913	0.02	2.22	524	0.01	1.83	519	0.00	0.66
43	17.30	726.78	777	0.04	3.16	320	0.02	3.16	810	0.01	0.78	719	0.00	0.65
47	3.86	177.71	921	0.04	9.01	123	0.02	3.47	013	0.01	0.94	212	0.00	0.40
33	2.13	68.26	520	0.04	8.17	868	0.02	1.28	011	0.01	0.79	817	0.00	0.57
45	1.59	69.91	420	0.04	8.00	909	0.02	1.34	612	0.01	0.87	824	0.00	0.73
75	1.57	116.47	911	0.04	3.32	515	0.01	0.75	211	0.01	0.74	318	0.00	0.53
59	0.84	48.73	711	0.04	4.27	969	0.01	1.41	922	0.01	1.48	621	0.00	0.62
62	0.75	45.50	912	0.04	4.54	120	0.01	2.94	613	0.01	0.85	419	0.00	0.54
31	0.67	20.07	713	0.04	4.78	315	0.01	2.05	219	0.01	1.16	220	0.00	0.55
57	0.66	36.95	999	0.04	3.44	949	0.01	1.18	688	0.01	0.41	618	0.00	0.51
63	0.64	39.88	5819	0.03	1.99	319	0.01	2.44	321	0.01	1.27	522	0.00	0.61
41	0.53	21.33	110	0.03	3.30	116	0.01	2.03	015	0.01	0.87	615	0.00	0.38
44	0.39	16.57	914	0.03	4.85	717	0.01	2.23	423	0.01	1.36	623	0.00	0.57
89	0.31	27.42	888	0.03	2.74	6565	0.01	0.80	515	0.01	0.89	121	0.00	0.51
55	0.29	15.93	513	0.03	4.21	7272	0.01	0.87	6464	0.01	0.35	814	0.00	0.35
83	0.19	15.86	510	0.03	3.26	5353	0.01	0.57	411	0.01	0.62	624	0.00	0.58
69	0.19	12.62	316	0.03	4.92	718	0.01	2.01	117	0.01	0.91	818	0.00	0.44
73	0.18	12.76	112	0.03	3.56	521	0.01	2.30	813	0.00	0.68	722	0.00	0.52
103	0.17	17.24	3535	0.03	0.91	611	0.01	1.22	416	0.00	0.81	920	0.00	0.47
39	0.13	5.01	6712	0.03	1.74	715	0.01	1.65	8012	0.00	0.37	014	0.00	0.31
95	0.13	12.26	512	0.03	3.17	514	0.01	1.49	812	0.00	0.59	016	0.00	0.33
87	0.12	10.19	311	0.03	2.80	523	0.01	2.39	916	0.00	0.77	216	0.00	0.29
93	0.11	10.58	119	0.02	4.66	917	0.01	1.82	214	0.00	0.64	213	0.00	0.24
74	0.11	8.37	314	0.02	3.41	022	0.01	2.14	518	0.00	0.79	413	0.00	0.23
97	0.10	9.47	792	0.02	1.87	929	0.01	0.88	616	0.00	0.68	020	0.00	0.34
115	0.10	11.18	712	0.02	3.00	714	0.01	1.41	915	0.00	0.64	415	0.00	0.25
71	0.10	6.70	4949	0.02	1.10	9898	0.01	0.93	213	0.00	0.94	217	0.00	0.28
81	0.07	5.96	323	0.02	5.05	724	0.01	2.35	716	0.00	0.67	024	0.00	0.38
85	0.07	6.08	115	0.02	3.20	313	0.01	1.24	222	0.00	0.89	723	0.00	0.36
46	0.07	3.21	122	0.02	4.32	010	0.01	0.93	820	0.00	0.82	815	0.00	0.23
109	0.07	7.70	517	0.02	3.29	113	0.01	1.20	322	0.00	0.86	614	0.00	0.21
42	0.07	2.83	702	0.02	1.28	821	0.01	1.97	019	0.00	0.73	017	0.00	0.25
76	0.07	5.06	720	0.02	3.70	620	0.01	1.85	215	0.00	0.56	422	0.00	0.32
60	0.06	3.75	8410	0.02	1.43	424	0.01	0.91	324	0.00	0.88	417	0.00	0.24
123	0.06	7.35	1818	0.02	3.21	1414	0.01	1.18	1414	0.00	0.52	1616	0.00	0.23

			9		1		4		8		
111	0.05	5.51	21 7	0.02	3.65	78	0.01	0.62	17 6	0.00	0.63
107	0.05	5.17	16 5	0.02	2.65	82	0.01	0.65	11 8	0.00	0.40
48	0.04	2.11	11 9	0.02	1.90	17 3	0.01	1.35	19 9	0.00	0.67

PSTB	Total	0.29	mg/m ² /h
m/z	μmol/m ² /h	μg/m ² /h	
41	2.46	98.45	
43	1.42	59.79	
42	0.24	10.01	
57	0.23	12.93	
105	0.21	21.59	
33	0.20	6.31	
107	0.15	16.12	
79	0.12	9.71	
96	0.12	11.23	
91	0.08	7.45	
98	0.07	6.61	
59	0.06	3.26	
204	0.05	11.11	
38	0.04	1.55	
106	0.03	2.64	
121	0.02	1.94	
104	0.01	1.48	
205	0.01	2.34	
108	0.01	1.22	
78	0.01	0.80	
119	0.01	0.86	
77	0.01	0.47	
218	0.01	1.23	
80	0.00	0.38	

Uncertainty associated with assignment of transport-limited deposition velocity

We investigated the impact due to measuring only four material v_t values by assessing uncertainty on the reaction probability due to assignment of v_t from a different material. Low reactivity materials will be less affected by changes in the transport-limited deposition velocity, as the surface resistance acts as the rate-limiting step (see equation 4 in the manuscript). Higher reactivity materials will be more affected by error in the transport-limited deposition velocity term. We calculated the maximum uncertainty associated with this assignment by calculating the range of reaction probabilities that would result for materials for which we did not calculate v_t if the minimum and maximum measured v_t values were used. Results of that calculation are below:

Table S4. Estimate of uncertainty associated with assignment of transport-limited deposition velocity

Sample	v_t used	v_t value (cm/s)	γ	γ with greatest v_t	γ with lowest v_t	range of γ due max v_t error	propagated uncertainty
Polyisocyanurate	PI	0.23	2.5E-06				
PSTB	PS	0.14	1.2E-06	1.1E-06	1.2E-06	3.9E-08	9.6E-07
Polyurethane	PI	0.23	1.2E-05	9.9E-06	1.4E-05	4.0E-06	3.0E-06
Polystyrene	PS	0.14	2.9E-06				
Denim	FG	0.24	1.4E-05	1.4E-05	2.3E-05	9.1E-06	4.4E-06
Stone wool	FG	0.24	1.5E-05	1.4E-05	2.3E-05	9.4E-06	4.7E-06
Cellulose	C	0.27	3.0E-05				
Fiberglass	FG	0.24	2.8E-05				

In Table S4, the materials highlighted are those for which v_t was not directly calculated. The results show that the uncertainty associated with the maximum range of calculated v_t results in a range of uncertainty of 1-2× that of the propagated uncertainty. Note that we believe this additional uncertainty represents an extreme upper-limit, as the observation of material morphology allows us to assign v_t that are more representative for each material.

Table S5. Summary of yields for eight test materials. Quantification and identification performed for five largest source fluxes for each test material.

Polystyrene with thermal backing						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
47.012756	47.0131	-0.344	CH ₂ O ₂ (H ⁺)	Formic acid	0.158	
59.049141	59.0502	-1.059	C ₃ H ₆ O(H ⁺)	Acetone	0.103	
61.028406	61.0289	-0.494	C ₂ H ₄ O ₂ (H ⁺)	Acetic acid	0.078	
56	56.0167	n/a	n/a	unknown	0.036	
101	101.04008	n/a	n/a	unknown	0.027	possibly Acetylpropionyl
		Formula	# of compounds			
		CxHy	0		0.000	
		CxHyO	2		0.026	
		CxHyO ₂	0		0.000	
		Other	4		0.064	
				Total yield	0.492	
Polyisocyanurate						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
47.012756	47.0129	-0.144	CH ₂ O ₂ (H ⁺)	Formic acid	0.065	
83.085527	83.0804	5.127	C ₆ H ₁₀ (H ⁺)	Hexanal, fragment + parent	0.053	Pang ¹ ; Buhr et al. ⁹
59.049141	59.0485	0.641	C ₃ H ₆ O(H ⁺)	Acetone	0.051	
55.054227	55.0454	8.827	C ₄ H ₆ (H ⁺)	Butanal, hexanal, heptanal fragment	0.034	added signal at 73
61.028406	61.0292	-0.794	C ₂ H ₄ O ₂ (H ⁺)	Acetic acid	0.036	
		Formula	# of compounds			
		CxHy	2		0.009	
		CxHyO	6		0.041	
		CxHyO ₂	1		0.002	
		Other	4		0.012	
				Total yield	0.304	

Polyurethane						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
45.033491	45.0251	8.391	C2H4O(H+)	Acetaldehyde	0.104	Added contribution from 63.05, acetaldehyde water cluster
59.049141	59.0495	-0.359	C3H6O(H+)	Acetone	0.072	Possible propanal parent, given fragment at 41
41.038577	41.0357	2.877	C3H4(H+)	Propanal, pentanal, alcohol fragment	0.048	Wyche et al. ¹⁰
62.023655	62.0268	-3.145	CH3NO2(H+)	Carbamic acid	0.043	
57.0699	57.0649	5.000	C4H8(H+)	Butanol, fragment	0.039	possible butanol fragment, Maleknia ¹¹ , no signal at 75
			Formula	# of compounds		
			CxHy	7	0.084	
			CxHyO	14	0.078	
			CxHyO2	3	0.004	
			Other	17	0.054	
			Total yield		0.526	
Polystyrene						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
47.012756	47.0121	0.656	CH2O2(H+)	Formic acid	0.103	
59.049141	59.0479	1.241	C3H6O(H+)	Acetone	0.054	
61.028406	61.0286	-0.194	C2H4O2(H+)	Acetic acid	0.033	
101	101.04008	n/a	n/a	unknown	0.015	possibly Acetylpropionyl
87.044056	87.0467	-2.644	C4H6O2(H+)	unknown	0.012	
			Formula	# of compounds		
			CxHy	1	0.007	
			CxHyO	2	0.011	m/z 31 likely isotopic interference from NO at m/z 30
			CxHyO2	0	0.000	
			Other	2	0.012	
			Total yield		0.246	
signal at m/z 55 taken as water cluster b/c no signal at 73 from parent aldehyde						

Cellulose						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
59.049141	59.0488	0.341	C3H6O(H+)	Acetone	0.077	
55.054227	55.0462	8.027	C4H6(H+)	Butanal, hexanal, heptanal fragment	0.048	Fragment, Schwarz ¹² Buhr et al. ⁹ signal at 73 is added to this
45.033491	45.0259	7.591	C2H4O(H+)	Acetaldehyde	0.036	
83.085527	83.0814	4.127	C6H10(H+)	Hexanal, fragment + parent Pentanal, heptanal, octanal, nonanal fragment	0.057	Fragment, Buhr et al. ⁹ ; Schwarz ¹³ signal at 101 added
69.069877	69.0683	1.577	C5H8(H+)		0.025	Fragment, Buhr et al. ⁹ ; Schwarz ¹³ signal at 87 added
			Formula	# of compounds		
			CxHy	7	0.013	
			CxHyO	9	0.038	
			CxHyO2	4	0.015	
			Other	16	0.049	
			Total yield		0.357	
Fiberglass						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
59.049141	59.0493	-0.159	C3H6O(H+)	Acetone	0.072	
47.012756	47.0112	1.556	CH2O2(H+)	Formic acid	0.041	
55.054227	55.04695	7.277	C4H6(H+)	Butanal, hexanal, heptanal fragment	0.039	Fragment, Schwarz ¹² Buhr et al. ⁹ signal at 73 is added to this
83.085527	83.0819	3.627	C6H10(H+)	Hexanal, fragment + parent	0.046	Fragment, Buhr et al. ⁹ ; Schwarz ¹³ signal at 87 added
43.017841	43.0157	2.141	C2H2O(H+)	Acid fragment (ketene)	0.020	
			Formula	# of compounds		
			CxHy	2	0.016	
			CxHyO	7	0.057	
			CxHyO2	1	0.004	
			Other	2	0.017	
			Total yield		0.312	

Recycled denim						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
45.033491	45.0251	8.391	C2H4O(H+)	Acetaldehyde	0.170	Added contribution from 63.05, see below
59.049141	59.0493	-0.159	C3H6O(H+)	Acetone	0.094	Possible propanal parent, given fragment at 41
62.023655	62.0266	-2.945	CH3NO2(H+)	Carbamic acid	0.071	
41.038577	41.0358	2.777	C3H4(H+)	Propanal, pentanal, alcohol fragment	0.051	Wyche et al. ¹⁰
55.054227	55.04676	7.467	C4H6(H+)	Butanal, hexanal, heptanal fragment	0.044	
<i>Formula</i>						
CxHy						
8						
CxHyO						
13						
CxHyO2						
1						
Other						
21						
Total yield						
0.852						
Further notes for recycled denim						
63.05	63.05	0.000	C2H6O(H+)	Acetaldehyde, water cluster	0.032118724	Acetaldehyde, Triple peak ¹⁴
Stonewool						
m/z exact	m/z measured	del m/z (mDa)	Putative ID	Putative name	Yield	Reference/comment
59.049141	59.0496	-0.459	C3H6O(H+)	Acetone	0.130	
45.033491	45.0308	2.691	C2H4O(H+)	Acetaldehyde	0.064	Added contribution from 63.05; Herbig ¹⁴
47.012756	47.0128	-0.044	CH2O2(H+)	Formic acid	0.060	
55.054227	55.0469	7.327	C4H6(H+)	Butanal, hexanal, heptanal fragment	0.043	Fragment, Schwarz ¹² Buhr et al. ⁹ signal at 73 is added to this
83.085527	83.0817	3.827	C6H10(H+)	Hexanal, fragment + parent	0.041	Fragment, Buhr et al. ⁹ ; Schwarz ⁸ signal at 87 added
<i>Formula</i>						
CxHy						
2						
CxHyO						
3						
CxHyO2						
0						
Other						
4						
Total yield						
0.425						

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