Supplementary Information:

Regulation and Reformulation: How the EU Paints Directive Shaped Volatile Organic Compound Emissions from UK Decorative Paints

Lidia Kristia Alfanti *[a], Amber May Yeoman [a,b], Andrew Robert Rickard [a,b], David Shaw [b,c], Martyn William Ward [a,b], Sarah Julia Moller [a,b], and Alastair Charles Lewis [a,b]

[a] *Wolfson Atmospheric Chemistry Laboratories, University of York, York, YO10 5DD, UK*
[b] *National Centre for Atmospheric Science, University of York, York, YO10 5DD, UK*
[c] *Department of Environment and Geography, University of York, York, YO10 5DD, UK*

S1. Estimation of photochemical ozone creation potential ($POCP_E$)

The equation for $POCP_E$ in Eq. (1) includes γs, R, and S, which are the core parameters used for all VOCs. γs is obtained with the following equation:

$$\gamma s = (n_B/6) \times (28.05/M) \quad \text{(i)}$$

n_B is the number of oxidizable bonds of the VOC, and M is the molecular mass. 6 and 28.05 are the number of oxidizable bonds and molecular mass of ethene as the reference VOC, as POCP values are relative to ethene = 100. R is a reactivity element that is also related to the OH reactivity of the VOC, as follows:

$$R = 1 - (B \bullet \gamma_R + 1)^{-1} \quad \text{(ii)}$$

$$\gamma_R = (k_{OH}/k_{OH}{}^{o}) \times (6/n_B) \quad \text{(iii)}$$

k_{OH} is the rate coefficient for the reaction of the VOC with OH under standard conditions (298 K, 1 atm) and $k_{OH}{}^{o}$ for the reference VOC, ethene. B is a numerical constant, which multi-day north-west European conditions is used in this study. The parameter S is related to the size of the VOC, and is given by:

$$S = (1 - \alpha) \times exp(-C \bullet n_C{}^{\beta}) + \alpha \quad \text{(iv)}$$

n_C is the carbon number of the VOC. The values of α, C, and β may be adjusted and optimised to represent the dependence of POCP on VOC size across varying timescales. The value for the parameters used in this study is based on Jenkin et al. (2017) [1] as follows:

Table S1. Parameters for the calculation of $POCP_E$ values

Parameter	VOC class	North-west European conditions
A	aliphatics	100
	aromatics with 0 alkyl substituents	66
	aromatics with 1 alkyl substituents	130
	aromatics with 2 alkyl substituents	173
	aromatics with 3 alkyl substituents	206
B	all	4
α	all	0.56
C	all	0.0038
β	all	2.7
F	all	1
	t-Butanol	0.7
P	all	0
R_{O3}	all	0
	Limonene	54
Q	all	0

S2. Comparative VOC profiling of wall paints

Figure S1 supports Section 3.2. of the main text. The figure illustrates how the paint samples were grouped by functional type to assess similarities in their chemical profiles. This grouping did not reveal consistent patterns in VOC composition; therefore, in Figure 3 the samples are instead categorised by manufacturer.

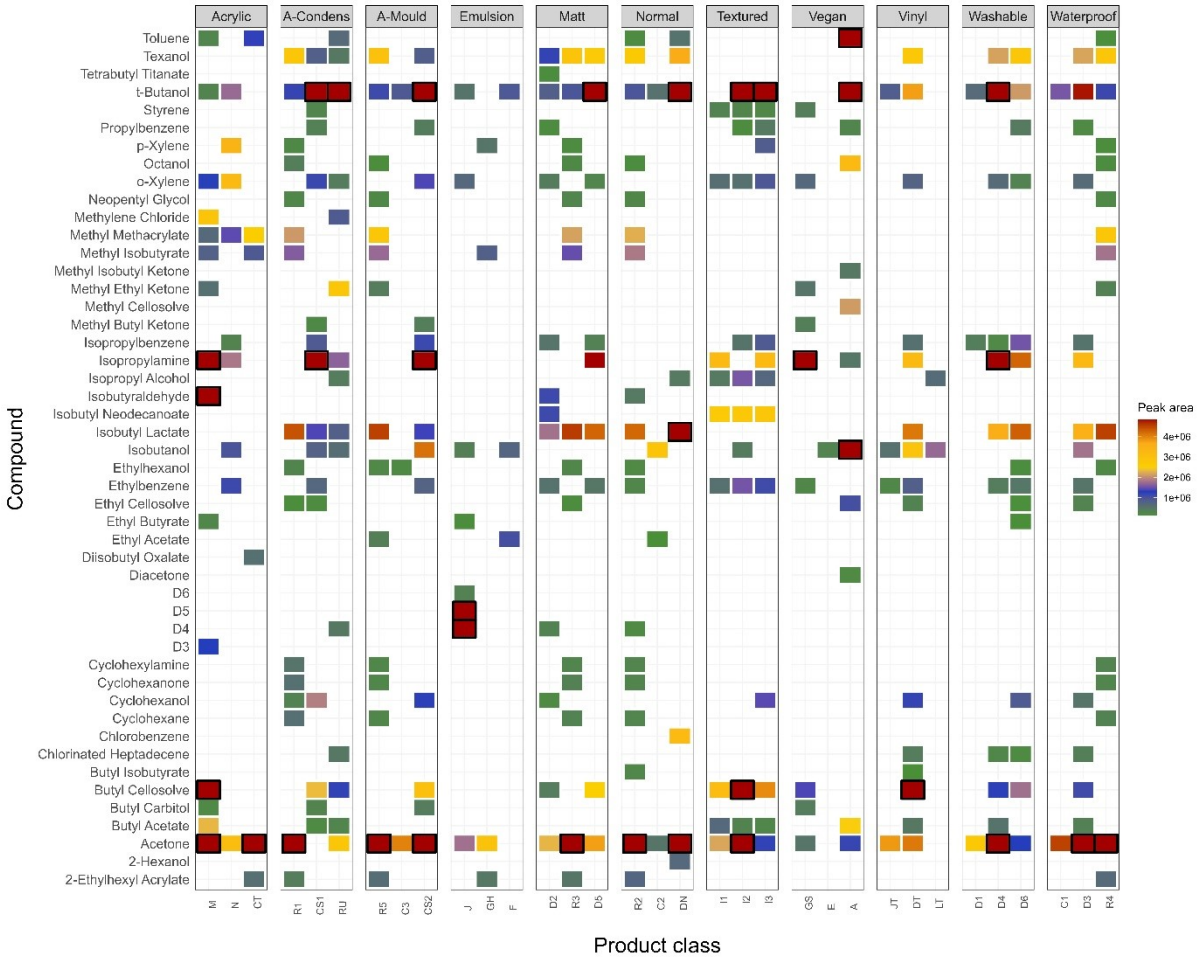

Figure S1. VOC speciation profiles of 33 decorative wall paints based on 2024 formulation data, grouped by functional type and VOC classification.

S3. Atmospheric modelling settings

Table S2 supports section 3.5. of the main text. The table summarises the key input parameters used in the INCHEM-Py atmospheric model simulations. Simulations were run for decane ($NC_{10}H_{22}$) and t-butanol (TBUTOL) separately, each representing a dominant solvent in the 1990 and 2024 paint formulations respectively.

Table S2. INCHEM-Py input parameters

Parameter	Value
MCM version	v3.3.1 [2]
Temperature	293 K
Relative humidity	50%
Light type	Off (no indoor or outdoor light)
Surface deposition	None
Air change rate	0 h^{-1}
OH (constant)	1.00×10^{6} molecules cm^{-3}
O_3 (constant)	1.00×10^{12} molecules cm^{-3}
NO_3 (constant)	1.00×10^{8} molecules cm^{-3}
Initial concentration – decane ($NC_{10}H_{22}$)	4.92×10^{10} molecules cm^{-3}
Initial concentration – t-butanol (TBUTOL)	9.45×10^{10} molecules cm^{-3}
Simulation duration	7 days
Output timestep	3600 s (1 hour)

S4. INCHEM-Py simulation output data

The following data were extracted from the INCHEM-Py model output for decane and t-butanol simulations, providing hourly concentrations of key species over seven days.

Table S3. INCHEM-Py output data

Time (h)	Concentration (molecules $cm^{-3} \times 10^{10}$)			
	decane	HCHO	t-butanol	HCHO
0	4.920	0.000	9.450	0.000
1	4.727	0.000	9.414	0.035
2	4.542	0.000	9.378	0.068
3	4.363	0.002	9.343	0.101
4	4.192	0.004	9.307	0.133
5	4.028	0.007	9.272	0.163
6	3.870	0.013	9.236	0.192
7	3.718	0.020	9.201	0.221
8	3.572	0.029	9.166	0.248
9	3.432	0.040	9.131	0.275
10	3.298	0.054	9.097	0.301
11	3.168	0.070	9.062	0.325
12	3.044	0.089	9.028	0.349
13	2.925	0.111	8.993	0.372
14	2.810	0.135	8.959	0.395
15	2.700	0.162	8.925	0.416
16	2.594	0.192	8.891	0.437
17	2.492	0.226	8.857	0.457
18	2.394	0.262	8.823	0.477
19	2.300	0.301	8.790	0.495
20	2.210	0.342	8.756	0.513
21	2.123	0.387	8.723	0.531
22	2.040	0.435	8.690	0.548
23	1.960	0.485	8.657	0.564
24	1.883	0.538	8.624	0.580
25	1.809	0.594	8.591	0.595
26	1.738	0.652	8.558	0.609
27	1.670	0.713	8.526	0.623
28	1.605	0.776	8.493	0.637
29	1.542	0.841	8.461	0.650
30	1.481	0.909	8.429	0.662
31	1.423	0.978	8.397	0.674
32	1.367	1.049	8.365	0.686
33	1.314	1.122	8.333	0.697
34	1.262	1.197	8.301	0.708
35	1.213	1.273	8.270	0.718
36	1.165	1.350	8.238	0.728
37	1.119	1.429	8.207	0.738
38	1.076	1.508	8.176	0.747
39	1.033	1.589	8.145	0.756
40	0.993	1.670	8.114	0.764
41	0.954	1.752	8.083	0.772
42	0.916	1.834	8.052	0.780
43	0.881	1.917	8.022	0.788
44	0.846	1.999	7.991	0.795
45	0.813	2.082	7.961	0.802
46	0.781	2.165	7.930	0.808
47	0.750	2.247	7.900	0.815
48	0.721	2.329	7.870	0.821
49	0.693	2.411	7.840	0.827
50	0.665	2.492	7.810	0.832
51	0.639	2.572	7.781	0.837
52	0.614	2.651	7.751	0.843
53	0.590	2.730	7.722	0.847
54	0.567	2.807	7.692	0.852
55	0.545	2.884	7.663	0.856
56	0.523	2.959	7.634	0.861
57	0.503	3.033	7.605	0.865
58	0.483	3.105	7.576	0.868
59	0.464	3.176	7.547	0.872
60	0.446	3.246	7.518	0.875
61	0.429	3.314	7.490	0.879
62	0.412	3.380	7.461	0.882
63	0.396	3.444	7.433	0.885
64	0.380	3.507	7.405	0.887
65	0.365	3.568	7.376	0.890
66	0.351	3.627	7.348	0.892
67	0.337	3.684	7.320	0.895
68	0.324	3.739	7.293	0.897
69	0.311	3.792	7.265	0.899
70	0.299	3.843	7.237	0.901
71	0.287	3.892	7.210	0.902
72	0.276	3.939	7.182	0.904
73	0.265	3.984	7.155	0.905
74	0.255	4.027	7.128	0.907
75	0.245	4.067	7.101	0.908
76	0.235	4.106	7.074	0.909
77	0.226	4.142	7.047	0.910
78	0.217	4.177	7.020	0.911
79	0.209	4.209	6.993	0.912
80	0.200	4.240	6.966	0.913
81	0.192	4.268	6.940	0.914
82	0.185	4.294	6.914	0.914
83	0.178	4.318	6.887	0.915
84	0.171	4.340	6.861	0.915

Time (h)	Concentration (molecules $cm^{-3} \times 10^{10}$)			
	decane	HCHO	t-butanol	HCHO
85	0.164	4.360	6.835	0.915
86	0.158	4.378	6.809	0.916
87	0.151	4.395	6.783	0.916
88	0.145	4.409	6.757	0.916
89	0.140	4.421	6.732	0.916
90	0.134	4.432	6.706	0.916
91	0.129	4.440	6.680	0.916
92	0.124	4.447	6.655	0.916
93	0.119	4.452	6.630	0.916
94	0.114	4.455	6.605	0.915
95	0.110	4.457	6.579	0.915
96	0.106	4.457	6.554	0.915
97	0.101	4.455	6.529	0.914
98	0.098	4.451	6.505	0.914
99	0.094	4.446	6.480	0.913
100	0.090	4.440	6.455	0.913
101	0.086	4.432	6.431	0.912
102	0.083	4.423	6.406	0.911
103	0.080	4.412	6.382	0.911
104	0.077	4.400	6.358	0.910
105	0.074	4.386	6.333	0.909
106	0.071	4.371	6.309	0.908
107	0.068	4.355	6.285	0.907
108	0.065	4.338	6.261	0.906
109	0.063	4.320	6.238	0.905
110	0.060	4.300	6.214	0.904
111	0.058	4.280	6.190	0.903
112	0.056	4.258	6.167	0.902

Time (h)	Concentration (molecules $cm^{-3} \times 10^{10}$)			
	decane	HCHO	t-butanol	HCHO
113	0.054	4.235	6.143	0.901
114	0.051	4.212	6.120	0.900
115	0.049	4.187	6.097	0.899
116	0.047	4.162	6.073	0.898
117	0.046	4.135	6.050	0.897
118	0.044	4.108	6.027	0.896
119	0.042	4.080	6.004	0.894
120	0.040	4.052	5.981	0.893
121	0.039	4.022	5.959	0.892
122	0.037	3.992	5.936	0.891
123	0.036	3.961	5.913	0.889
124	0.034	3.930	5.891	0.888
125	0.033	3.898	5.869	0.887
126	0.032	3.866	5.846	0.885
127	0.031	3.833	5.824	0.884
128	0.029	3.800	5.802	0.882
129	0.028	3.766	5.780	0.881
130	0.027	3.731	5.758	0.880
131	0.026	3.697	5.736	0.878
132	0.025	3.662	5.714	0.877
133	0.024	3.626	5.692	0.875
134	0.023	3.591	5.671	0.874
135	0.022	3.555	5.649	0.872
136	0.021	3.519	5.628	0.871
137	0.020	3.482	5.606	0.869
138	0.020	3.446	5.585	0.868
139	0.019	3.409	5.564	0.866
140	0.018	3.372	5.542	0.865

Time (h)	Concentration (molecules $cm^{-3} \times 10^{10}$)			
	decane	HCHO	t-butanol	HCHO
141	0.017	3.335	5.521	0.863
142	0.017	3.298	5.500	0.862
143	0.016	3.261	5.479	0.860
144	0.015	3.224	5.459	0.858
145	0.015	3.186	5.438	0.857
146	0.014	3.149	5.417	0.855
147	0.014	3.111	5.397	0.854
148	0.013	3.074	5.376	0.852
149	0.013	3.037	5.356	0.850
150	0.012	2.999	5.335	0.849
151	0.012	2.962	5.315	0.847
152	0.011	2.925	5.295	0.846
153	0.011	2.888	5.275	0.844
154	0.010	2.851	5.254	0.842
155	0.010	2.814	5.234	0.841
156	0.010	2.778	5.215	0.839
157	0.009	2.741	5.195	0.838
158	0.009	2.705	5.175	0.836
159	0.008	2.668	5.155	0.834
160	0.008	2.632	5.136	0.833
161	0.008	2.596	5.116	0.831
162	0.008	2.561	5.097	0.829
163	0.007	2.525	5.077	0.828
164	0.007	2.490	5.058	0.826
165	0.007	2.455	5.039	0.824
166	0.006	2.420	5.020	0.823
167	0.006	2.386	5.000	0.821
168	0.006	2.352	4.981	0.819

References

1. M. E. Jenkin, R. G. Derwent and T. J. Wallington, Photochemical ozone creation potentials for volatile organic compounds: Rationalization and estimation, *Atmospheric Environment*, 2017, **163**, 128-137.
2. Master Chemical Mechanism v3.3.1, www.mcm.york.ac.uk.