

Concentrations and fate of decamethylcyclopentasiloxane (D5) in the atmosphere

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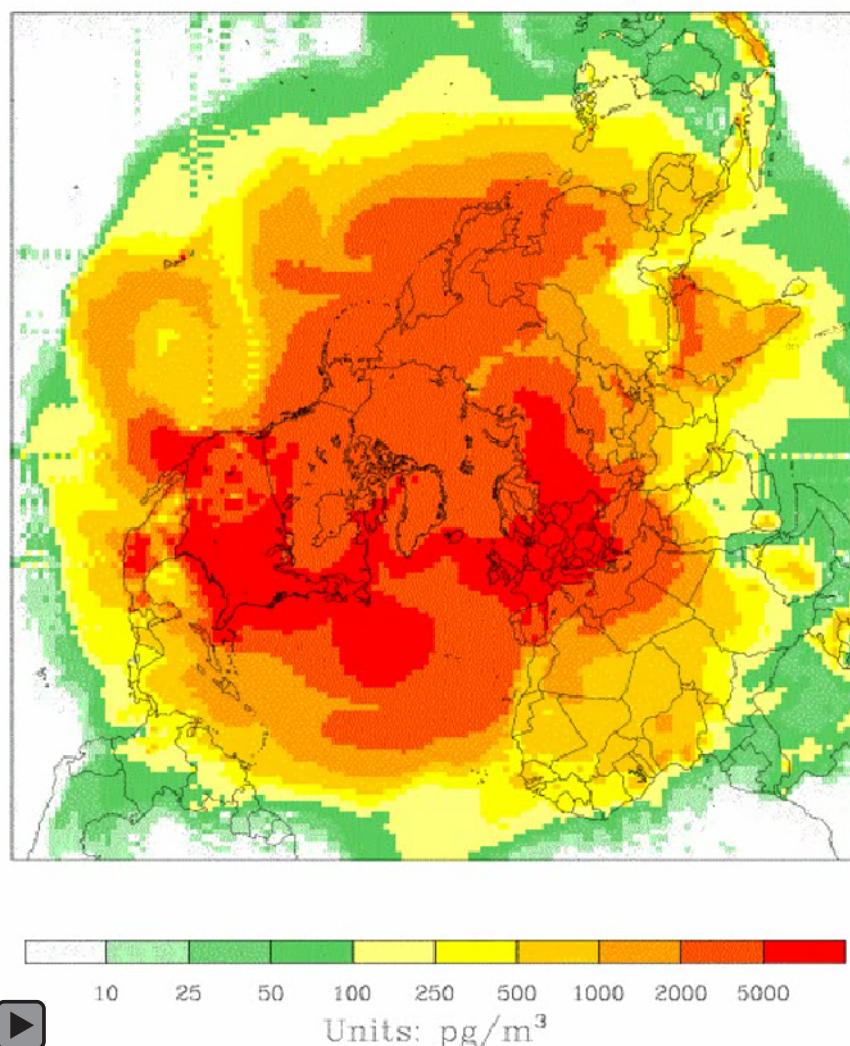
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Supporting Information

3 hourly mean D5 concentration. 03 GMT, 1 Jan, 2009



Multimedia S1: Model simulation of decamethylcyclopentasiloxane (D5) concentrations in the Northern Hemisphere during January – June 2009

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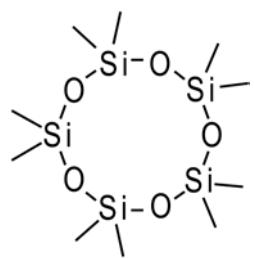


Figure S1: Molecular structure of decamethylcyclopentasiloxane (D5)



Figure S2: Picture of the sampling site

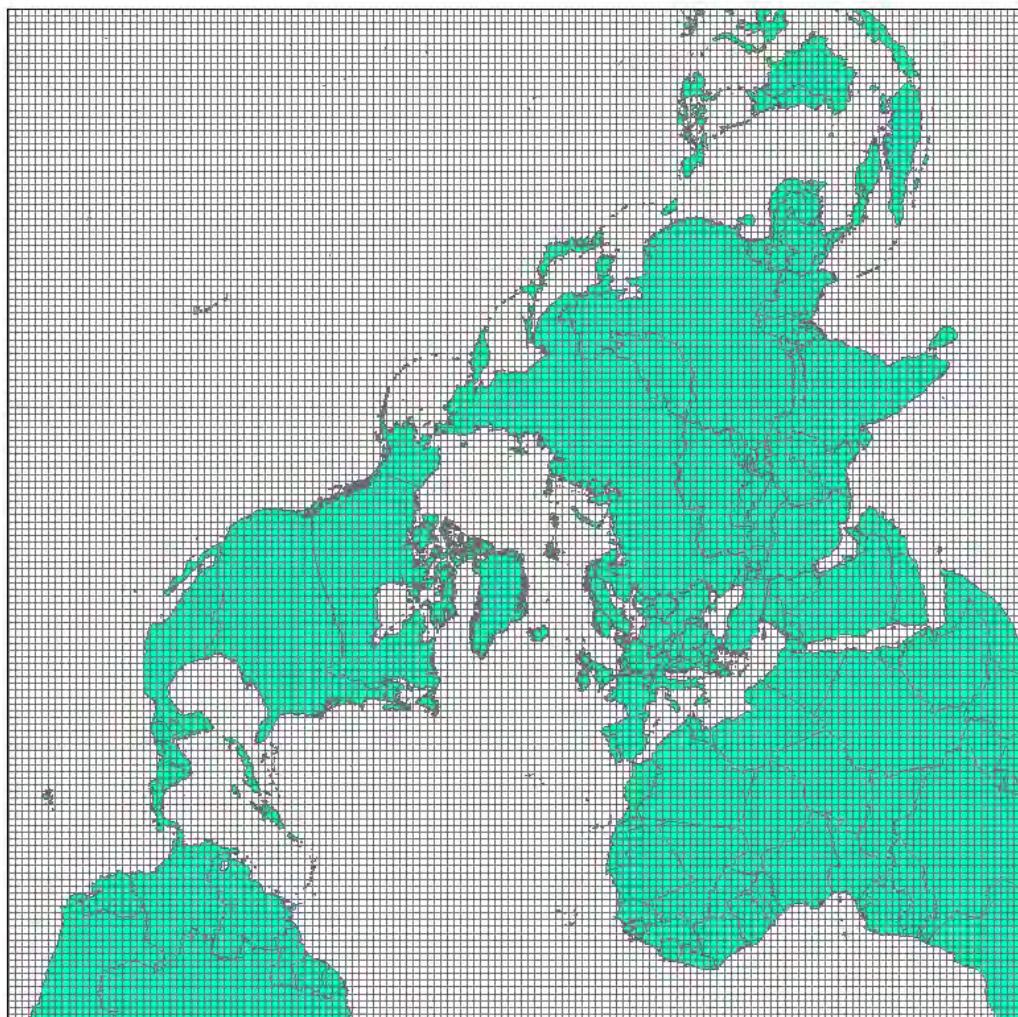


Figure S3: Domain of the DEHM model

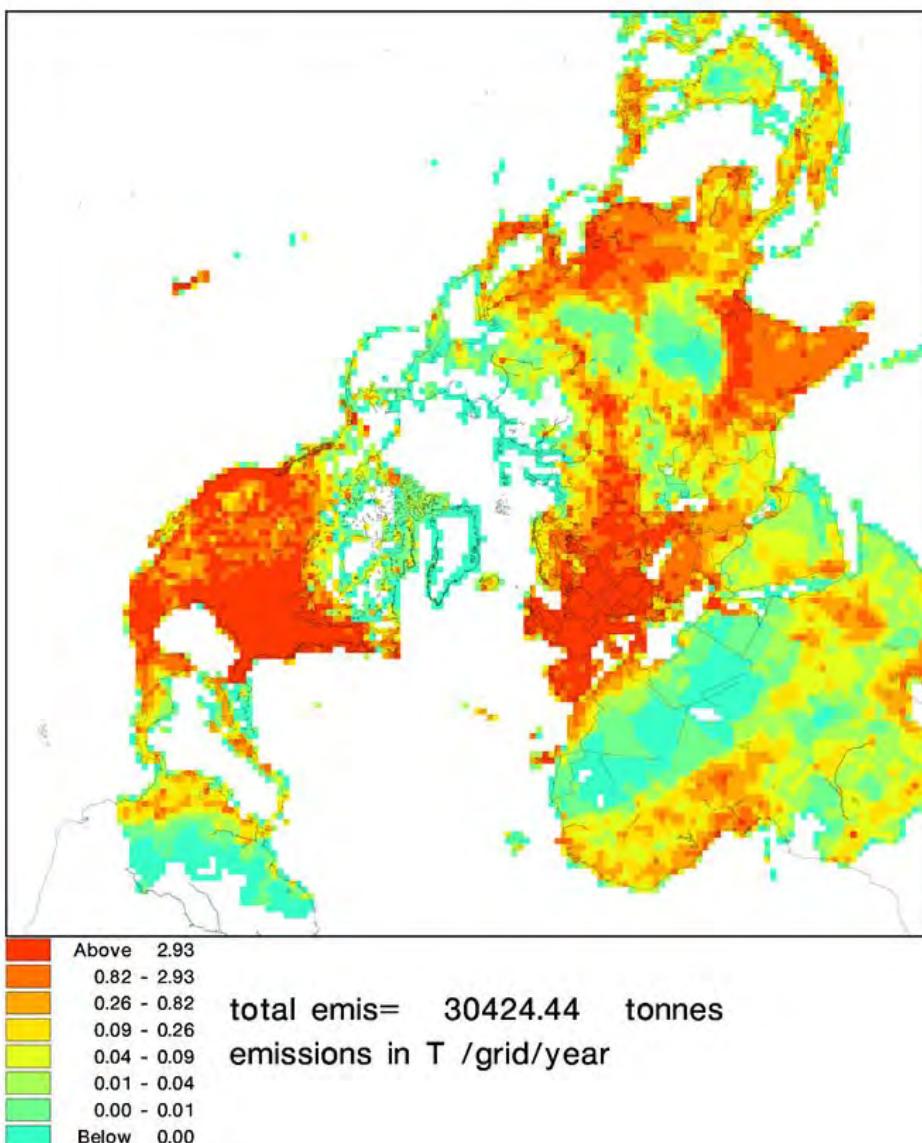


Figure S4: Map showing the emissions estimates for each grid cell in the model domain

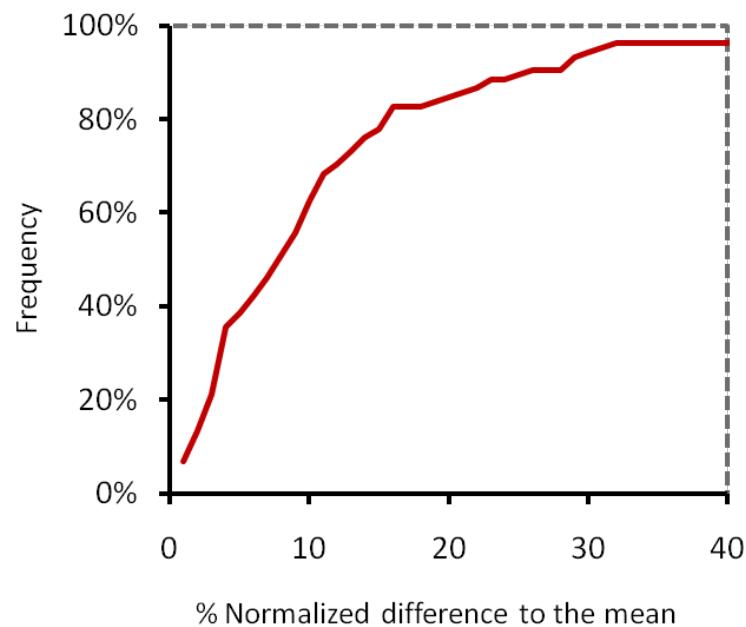


Figure S5: Repeatability of the measurement of the D₅ concentration in air illustrated with a cumulative distribution function of the % difference between the D₅ concentrations in parallel samples (normalized to the mean of the two concentrations).

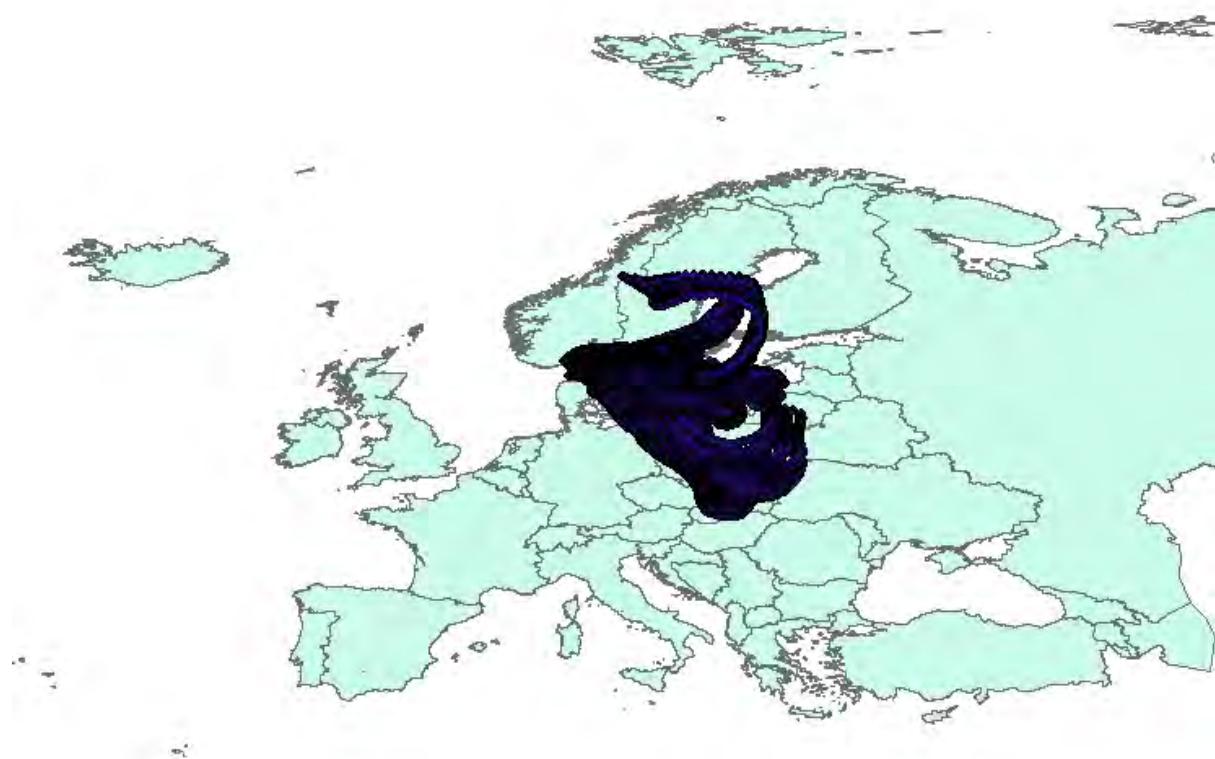


Figure S6: Three day air mass back trajectories during the period 22-30 April. The trajectories were calculated on an hourly basis using the Eta model.

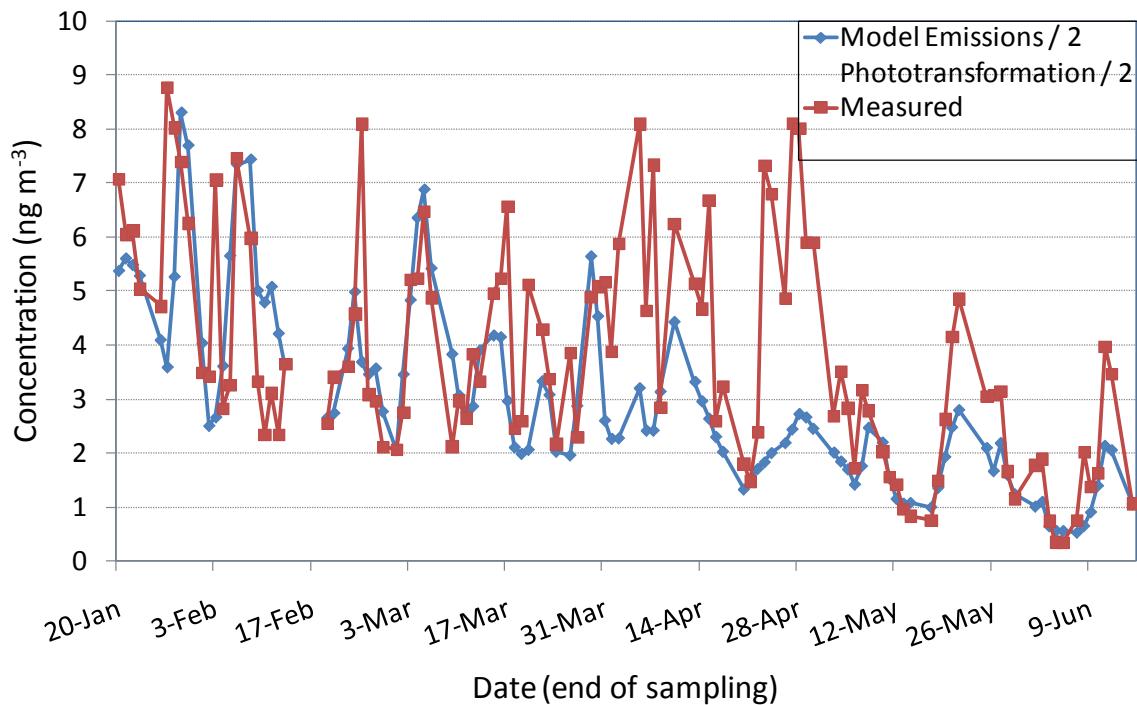


Figure S7: Comparison of modeled and measured concentrations of D5 in air when the emissions and the phototransformation rate constant are both reduced by 50% compared to the base scenario.

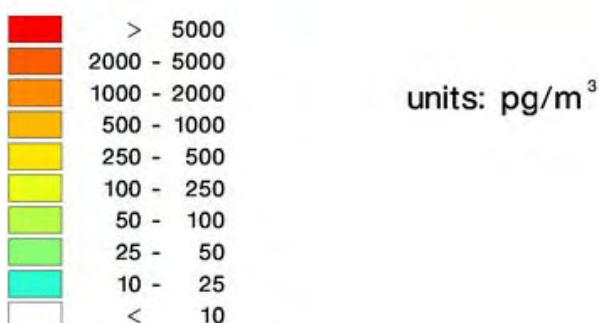
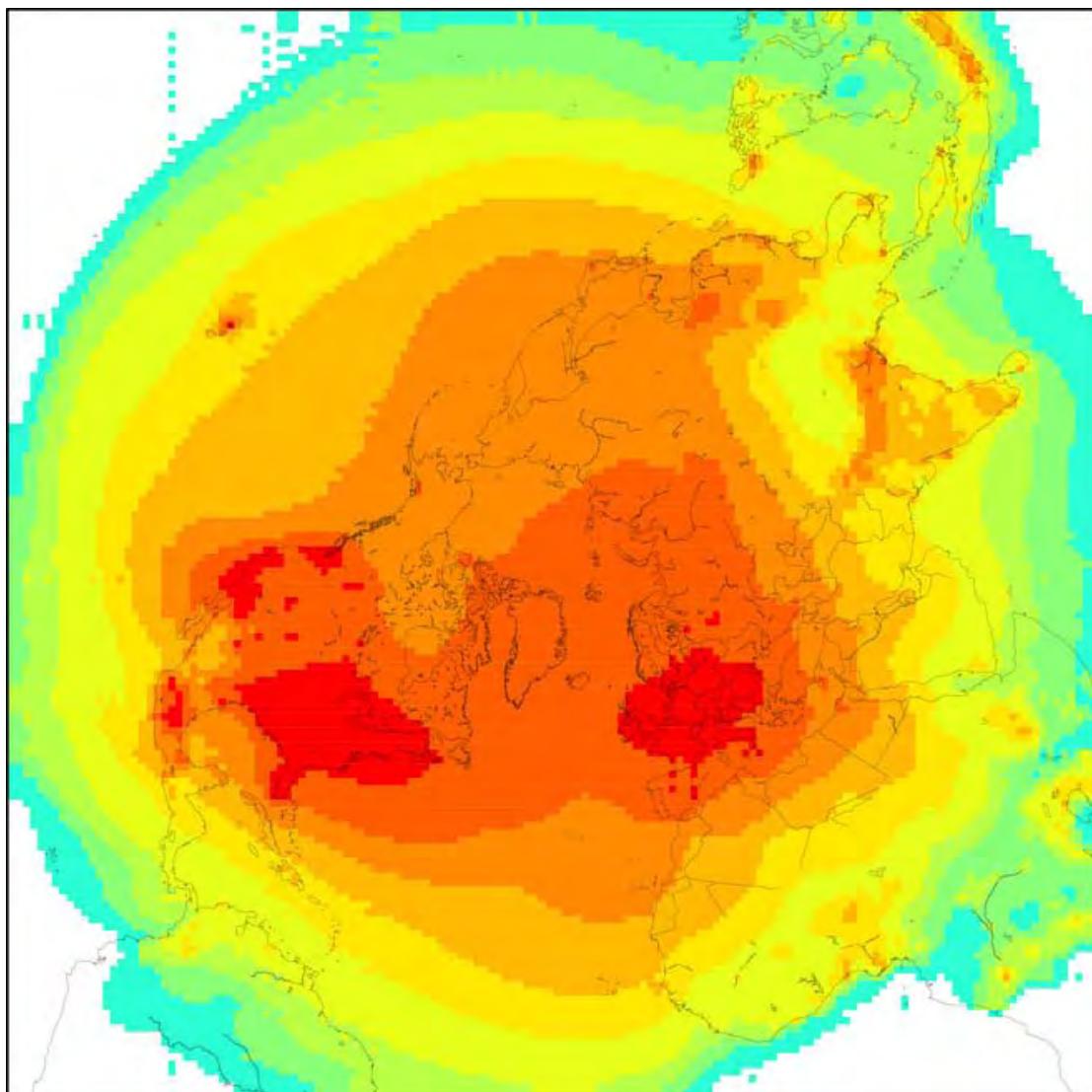
Average D5 concentration January-June 2009

Figure S8: Simulated D5 concentrations in air in the Northern Hemisphere. The average concentrations during the total simulation period (January-June 2009) are shown.

Table S1: Information on the samples collected including start time, stop time, volume sampled and the time the cartridges were stored before extraction.

Start	Stop	Sampling time		Sample volume		Storage time
				Pump A	Pump B	
		min.	hours	m ³	m ³	
2009-01-19 22:35	2009-01-20 22:35	1440	24	3.7	3.5	5.6
2009-01-20 22:35	2009-01-21 23:30	1495	25	4.0	3.8	4.5
2009-01-21 23:30	2009-01-22 23:40	1450	24	3.7	2.4	3.5
2009-01-22 23:40	2009-01-23 20:00	1220	20	3.2	2.0	2.7
2009-01-23 20:00	2009-01-26 20:00	4320	72	9.6	7.2	6.7
2009-01-26 20:00	2009-01-27 19:45	1425	24	3.2	2.4	5.7
2009-01-27 19:45	2009-01-28 21:10	1525	25	3.6	2.5	4.6
2009-01-28 21:10	2009-01-29 21:23	1453	24	3.6	3.5	3.6
2009-01-29 21:23	2009-01-30 19:40	1337	22	3.3	3.4	2.7
2009-01-30 19:40	2009-02-01 23:36	3116	52	7.6	7.7	7.5
2009-02-01 23:36	2009-02-02 20:53	1277	21	3.3	3.1	6.6
2009-02-02 20:53	2009-02-03 20:20	1407	23	3.8	3.3	5.7
2009-02-03 20:20	2009-02-04 23:34	1634	27	4.0	3.9	4.5
2009-02-04 23:34	2009-02-05 23:20	1426	24	3.6	3.7	3.5
2009-02-05 23:20	2009-02-06 20:20	1260	21	3.1	3.1	2.7
2009-02-06 20:20	2009-02-08 20:30	2890	48	5.7	4.9	7.6
2009-02-08 20:30	2009-02-09 19:43	1393	23	3.4	3.5	6.7
2009-02-09 19:43	2009-02-10 19:45	1442	24	3.5	3.4	5.7
2009-02-10 19:45	2009-02-11 20:57	1512	25	3.8	4.1	4.6
2009-02-11 20:57	2009-02-12 21:13	1456	24	3.7	3.8	3.6
2009-02-12 21:13	2009-02-13 13:30	977	16	2.4	2.3	2.4
2009-02-18 23:35	2009-02-19 18:50	1155	19	3.0	2.8	3.7
2009-02-19 18:50	2009-02-20 17:05	1335	22	2.4	3.2	2.8
2009-02-20 17:05	2009-02-22 21:25	3140	52	4.7	6.5	7.6
2009-02-22 21:25	2009-02-23 20:28	1383	23	2.7	3.8	6.6
2009-02-23 20:28	2009-02-24 18:15	1307	22	3.1	3.4	5.7
2009-02-24 18:15	2009-02-25 18:42	1467	24	3.3	3.4	4.7
2009-02-25 18:42	2009-02-26 19:31	1489	25	3.7	3.6	3.7
2009-02-26 19:31	2009-02-27 17:40	1329	22	3.3	3.5	2.8
2009-02-27 17:40	2009-03-01 23:46	3246	54	6.6	7.0	7.5
2009-03-01 23:46	2009-03-02 20:28	1242	21	3.6	3.1	6.6
2009-03-02 20:28	2009-03-03 18:31	1323	22	3.7	3.4	5.7
2009-03-03 18:31	2009-03-04 19:37	1506	25	4.1	3.7	4.7
2009-03-04 19:37	2009-03-05 18:01	1344	22	3.8	3.4	3.7
2009-03-05 18:01	2009-03-06 17:45	1424	24	4.1	3.4	2.8
2009-03-06 17:45	2009-03-09 19:50	4445	74	12	12	6.7
2009-03-09 19:50	2009-03-10 19:50	1440	24	5.1	5.5	5.7
2009-03-10 19:50	2009-03-11 17:50	1320	22	4.9	5.9	4.8
2009-03-11 17:50	2009-03-12 17:50	1440	24	5.0	5.5	3.8
2009-03-12 17:50	2009-03-13 17:47	1437	24	5.2	6.0	2.8
2009-03-13 17:47	2009-03-15 23:59	3252	54	9.0	9.6	7.5
2009-03-15 23:59	2009-03-16 18:30	1111	19	4.0	4.6	6.7

2009-03-16 18:30	2009-03-17 17:35	1385	23	5.3	5.7	5.8
2009-03-17 17:35	2009-03-18 18:55	1520	25	5.7	6.8	4.7
2009-03-18 18:55	2009-03-19 17:50	1375	23	5.3	6.0	3.8
2009-03-19 17:50	2009-03-20 19:05	1515	25	5.6	6.4	2.7
2009-03-20 19:05	2009-03-22 23:20	3135	52	7.2	7.9	7.5
2009-03-22 23:20	2009-03-23 18:57	1177	20	4.4	4.6	6.7
2009-03-23 18:57	2009-03-24 17:18	1341	22	5.0	5.2	5.8
2009-03-24 17:18	2009-03-26 19:24	3006	50	11	12	3.7
2009-03-26 19:24	2009-03-27 17:13	1309	22	4.9	5.2	2.8
2009-03-27 17:13	2009-03-29 20:35	3082	51	8.4	8.3	4.6
2009-03-29 20:35	2009-03-30 17:21	1246	21	4.7	5.1	3.8
2009-03-30 17:21	2009-03-31 18:27	1506	25	5.3	5.7	2.7
2009-03-31 18:27	2009-04-01 18:56	1469	24	5.0	5.6	1.7
2009-04-01 18:56	2009-04-02 17:33	1357	23	4.8	5.4	0.8
2009-04-02 17:33	2009-04-05 20:20	4487	75	11	11	8.7
2009-04-05 20:20	2009-04-06 19:21	1381	23	4.1	4.4	7.7
2009-04-06 19:21	2009-04-07 18:54	1413	24	4.1	4.8	6.7
2009-04-07 18:54	2009-04-08 21:02	1568	26	4.8	5.2	5.6
2009-04-08 21:02	2009-04-10 07:43	2081	35	6.3	6.4	4.2
2009-04-10 07:43	2009-04-13 23:16	5253	88	13	12	9.5
2009-04-13 23:16	2009-04-14 18:26	1150	19	3.1	3.5	8.7
2009-04-14 18:26	2009-04-15 19:15	1489	25	4.8	4.5	7.7
2009-04-15 19:15	2009-04-16 19:26	1451	24	4.3	5.1	6.7
2009-04-16 19:26	2009-04-17 18:45	1399	23	1.4	2.9	5.7
2009-04-17 18:45	2009-04-20 19:17	4352	73	3.7	7.8	6.7
2009-04-20 19:17	2009-04-21 20:00	1483	25	1.4	3.0	5.7
2009-04-21 20:00	2009-04-22 19:42	1422	24	1.4	2.7	4.7
2009-04-22 19:42	2009-04-23 18:17	1355	23	1.3	2.6	3.7
2009-04-23 18:17	2009-04-24 18:03	1426	24	1.4	2.8	2.7
2009-04-24 18:03	2009-04-26 21:51	3108	52	2.8	4.9	7.6
2009-04-26 21:51	2009-04-27 19:18	1287	21	1.3	2.4	6.7
2009-04-27 19:18	2009-04-28 19:50	1472	25	3.5	2.8	5.7
2009-04-28 19:50	2009-04-29 19:52	1442	24	3.1	4.5	4.7
2009-04-29 19:52	2009-04-30 16:56	1264	21	2.6	4.1	3.8
2009-04-30 16:56	2009-05-03 23:28	4712	79	7.6	10.9	7.5
2009-05-03 23:28	2009-05-04 19:58	1230	20	2.6	4.0	6.7
2009-05-04 19:58	2009-05-05 20:30	1472	25	2.9	4.9	5.6
2009-05-05 20:30	2009-05-06 19:36	1386	23	2.9	4.6	4.7
2009-05-06 19:36	2009-05-07 22:43	1627	27	3.1	5.3	3.6
2009-05-07 22:43	2009-05-08 21:31	1368	23	3.2	3.7	2.6
2009-05-08 21:31	2009-05-10 23:06	2975	50	6.3	6.8	7.5
2009-05-10 23:06	2009-05-11 18:02	1136	19	3.3	4.1	6.7
2009-05-11 18:02	2009-05-12 17:52	1430	24	5.2	4.7	5.8
2009-05-12 17:52	2009-05-13 17:36	1424	24	4.1	4.8	4.8
2009-05-13 17:36	2009-05-14 19:37	1561	26	4.5	5.6	3.7
2009-05-14 19:37	2009-05-17 23:51	4574	76	9.4	10.0	7.5
2009-05-17 23:51	2009-05-18 19:47	1196	20	3.4	4.0	6.7

2009-05-18 19:47	2009-05-19 19:18	1411	24	4.3	4.7	5.7
2009-05-19 19:18	2009-05-20 19:06	1428	24	4.4	4.6	4.7
2009-05-20 19:06	2009-05-21 12:50	1064	18	3.4	3.6	4.0
2009-05-21 12:50	2009-05-25 19:31	6161	103	12	12	6.7
2009-05-25 19:31	2009-05-26 19:09	1418	24	4.4	4.6	5.7
2009-05-26 19:09	2009-05-27 17:37	1348	22	4.2	4.4	4.8
2009-05-27 17:37	2009-05-28 19:13	1536	26	4.4	5.0	3.7
2009-05-28 19:13	2009-05-29 06:03	650	11	1.8	2.0	3.2
2009-05-29 06:03	2009-06-01 18:18	5055	84	11	11	6.7
2009-06-01 18:18	2009-06-02 19:40	1522	25	4.5	5.1	5.7
2009-06-02 19:40	2009-06-03 20:33	1493	25	4.3	4.6	4.6
2009-06-03 20:33	2009-06-04 18:56	1343	22	3.9	4.2	3.7
2009-06-04 18:56	2009-06-05 19:00	1444	24	4.2	4.6	2.7
2009-06-05 19:00	2009-06-07 23:02	3122	52	6.4	7.1	8.5
2009-06-07 23:02	2009-06-08 19:52	1250	21	3.7	4.0	7.7
2009-06-08 19:52	2009-06-09 17:10	1278	21	3.5	4.3	6.8
2009-06-09 17:10	2009-06-10 19:16	1566	26	4.6	4.8	5.7
2009-06-10 19:16	2009-06-11 19:59	1483	25	4.1	4.5	4.7
2009-06-11 19:59	2009-06-12 19:33	1414	24	4.7	4.5	3.7
2009-06-12 19:33	2009-06-15 18:46	4273	71	9.3	8.7	4.7

Table S2: Physical chemical properties of D5 used in the model simulations

Property	Value	Units	Source
Log air/water partition coefficient ($\log K_{AW}$)	2.96	$m^3 m^{-3}$	Brooke et al. (2009)
Log octanol/water partition coefficient ($\log K_{OW}$) (25°C)	8.03	$m^3 m^{-3}$	Brooke et al. (2009)
Log octanol/air partition coefficient ($\log K_{OA}$) (25°C)	5.07	$m^3 m^{-3}$	Brooke et al. (2009)
Heat of phase change between air and water (ΔU_{AW}) (25°C)	92.7	$kJ mol^{-1}$	Xu (2009)
Heat of phase change between octanol and water (ΔU_{OW})	40.0	$kJ mol^{-1}$	Xu (2009)
Heat of phase change between octanol and air (ΔU_{OA})	-47.9	$kJ mol^{-1}$	Xu (2009)
Rate constant for phototransformation (24°C)	1.55×10^{-12}	$cm^3 mol^{-1} s^{-1}$	Atkinson (1991)
Activation energy for phototransformation	0.648*	$kJ mol^{-1}$	Jiménez et al. (2005)

*based on 2-butanone due to the absence of a measured value for D5.

Table S3: D5 quantities in the field blanks, back-up cartridges, and samples, as well as the concentrations in the samples.

Sampling stop time	Sample cartridge		Field blanks		D5 concentration		Mean
	A	B	A	B	A	B	Conc.
	ng	ng	ng	ng	ng/m ³	ng/m ³	ng/m ³
2009-01-20 22:35	26	25	0.74	0.16	7.2	7.2	7.2
2009-01-21 23:30	24		0.18		6.1		6.1
2009-01-22 23:40	19	17	0.13	0.15	5.3	7.0	6.2
2009-01-23 20:00	17	9.7	0.17	0.13	5.3	4.9	5.1
2009-01-26 20:00	36	41	0.69	0.09	3.8	5.7	4.7
2009-01-27 19:45	29	21	1.0	1.6	8.8	8.7	8.8
2009-01-28 21:10	28	21	4.5	2.3	7.7	8.3	8.0
2009-01-29 21:23	27	26	1.7	1.3	7.6	7.2	7.4
2009-01-30 19:40	21	20	0.36	3.0	6.5	6.0	6.3
2009-02-01 23:36	32	21	3.4	2.2	4.3	2.7	3.5
2009-02-02 20:53	11	11	1.6	1.4	3.3	3.6	3.4
2009-02-03 20:20	25	25	1.3	1.5	6.6	7.6	7.1
2009-02-04 23:34	11	11	1.2	2.9	2.9	2.8	2.8
2009-02-05 23:20	13	11	1.5	0.56	3.5	3.0	3.3
2009-02-06 20:20	24	21	0.51	0.99	7.9	7.0	7.5
2009-02-08 20:30	31	32	0.84	2.8	5.5	6.4	5.9
2009-02-09 19:43	13	9.7	0.59	0.83	3.8	2.8	3.3
2009-02-10 19:45	5.7	10	0.45	1.0	1.6	3.0	2.3
2009-02-11 20:57	11	13	0.61	0.62	3.0	3.2	3.1
2009-02-12 21:13	8.5	9.0	2.8	0.74	2.3	2.4	2.3
2009-02-13 13:30	8.3	8.7	0.62	0.47	3.5	3.8	3.6
2009-02-19 18:50	7.8	6.9	1.1	1.8	2.6	2.4	2.5
2009-02-20 17:05	8.1	11	0.51	0.58	3.4	3.4	3.4
2009-02-22 21:25	16	24	0.09	0.09	3.5	3.7	3.6
2009-02-23 20:28	12	17	0.14	0.16	4.6	4.6	4.6
2009-02-24 18:15	25	28	0.12	0.10	8.0	8.2	8.1
2009-02-25 18:42	8.7	12	0.69	0.47	2.6	3.5	3.1
2009-02-26 19:31	10	11	0.57	0.91	2.8	3.1	3.0
2009-02-27 17:40	6.8	7.4	1.6	0.09	2.1	2.1	2.1
2009-03-01 23:46	12	16	0.12	0.12	1.8	2.3	2.1
2009-03-02 20:28	9.3	9.0	0.16	0.19	2.6	2.9	2.7
2009-03-03 18:31	22	15	0.13	0.09	6.0	4.5	5.2
2009-03-04 19:37	23	18	0.06	0.06	5.7	4.7	5.2
2009-03-05 18:01	24	22	0.05	0.05	6.4	6.6	6.5
2009-03-06 17:45	20	16	0.06	0.06	4.8	4.7	4.8
2009-03-09 19:50	25	26	0.25	0.10	2.1	2.2	2.1
2009-03-10 19:50		16		0.06		3.0	3.0
2009-03-11 17:50		15		0.10		2.6	2.6
2009-03-12 17:50		21		0.10		3.8	3.8
2009-03-13 17:47		20		0.10		3.3	3.3
2009-03-15 23:59	43	50	0.18	0.17	4.8	5.2	5.0

2009-03-16 18:30	22	23	0.20	0.11	5.5	5.0	5.2
2009-03-17 17:35	40	32	0.19	0.14	7.6	5.5	6.6
2009-03-18 18:55	15	15	0.18	0.07	2.6	2.3	2.5
2009-03-19 17:50	14	16	0.12	0.05	2.6	2.6	2.6
2009-03-20 19:05	32	30	0.11	0.22	5.6	4.7	5.1
2009-03-22 23:20	29	36	0.08	0.10	4.1	4.5	4.3
2009-03-23 18:57	13	17	0.56	0.67	3.0	3.8	3.4
2009-03-24 17:18	11	10	0.12	0.41	2.3	2.0	2.2
2009-03-26 19:24	41	47	0.06	0.20	3.8	3.9	3.8
2009-03-27 17:13	11	12	0.11	0.19	2.3	2.2	2.3
2009-03-29 20:35	46	35	0.19	0.35	5.5	4.3	4.9
2009-03-30 17:21	22	28	0.10	0.11	4.8	5.4	5.1
2009-03-31 18:27	29	28	0.15	0.10	5.4	4.9	5.2
2009-04-01 18:56	19	22	0.21	0.07	3.8	3.9	3.9
2009-04-02 17:33	28	32	0.05	0.04	5.8	5.9	5.9
2009-04-05 20:20	88	95	0.34	0.18	7.9	8.3	8.1
2009-04-06 19:21	19	20	0.23	0.28	4.6	4.7	4.6
2009-04-07 18:54	31	35	0.39	0.44	7.5	7.2	7.3
2009-04-08 21:02	13	15	0.28	0.20	2.8	2.9	2.8
2009-04-10 07:43	37	42	0.47	0.35	6.0	6.5	6.3
2009-04-13 23:16	66	63	0.31	0.35	4.9	5.4	5.1
2009-04-14 18:26	15	16	0.33	0.56	4.9	4.5	4.7
2009-04-15 19:15	35	28	0.46	0.21	7.2	6.2	6.7
2009-04-16 19:26	11	13	0.26	1.2	2.6	2.6	2.6
2009-04-17 18:45	4.6	9.0	0.23	0.17	3.3	3.2	3.2
2009-04-20 19:17	6.8	14	0.20	0.27	1.8	1.8	1.8
2009-04-21 20:00	1.9	4.8	0.32	0.47	1.4	1.6	1.5
2009-04-22 19:42	3.4	6.2	0.47	0.49	2.4	2.3	2.4
2009-04-23 18:17	9.1	20	0.11	0.28	7.1	7.6	7.3
2009-04-24 18:03	9.0	20	0.19	0.16	6.5	7.1	6.8
2009-04-26 21:51	13	24	0.20	0.10	4.8	4.9	4.9
2009-04-27 19:18	9.8	21	0.25	0.30	7.7	8.5	8.1
2009-04-28 19:50	28	23	0.23	0.50	7.9	8.1	8.0
2009-04-29 19:52	17	28	0.46	1.05	5.5	6.2	5.9
2009-04-30 16:56	15	24	0.12	0.59	5.9	5.9	5.9
2009-05-03 23:28	20	30	0.11	0.12	2.6	2.7	2.7
2009-05-04 19:58	8.7	15	0.26	0.19	3.3	3.7	3.5
2009-05-05 20:30	7.3	15	0.20	0.39	2.5	3.2	2.8
2009-05-06 19:36	4.9	8.1	0.43	0.22	1.7	1.7	1.7
2009-05-07 22:43	9.1	18	0.26	0.19	2.9	3.4	3.2
2009-05-08 21:31	8.8	10	0.13	0.14	2.7	2.8	2.8
2009-05-10 23:06	11	16	0.29	0.13	1.7	2.3	2.0
2009-05-11 18:02	5.2	6.2	0.13	0.42	1.6	1.5	1.6
2009-05-12 17:52	4.4	9.3	0.60	0.45	0.9	2.0	1.4
2009-05-13 17:36	3.9	4.5	0.56	0.18	1.0	0.9	1.0
2009-05-14 19:37	3.6	4.7	0.12	0.14	0.8	0.9	0.8
2009-05-17 23:51	7.2	7.2	0.17	0.19	0.8	0.7	0.7

2009-05-18 19:47	5.4	5.4	2.1	0.65	1.6	1.4	1.5
2009-05-19 19:18	11	12	0.64	0.20	2.7	2.6	2.6
2009-05-20 19:06	18	19	1.4	0.17	4.2	4.1	4.1
2009-05-21 12:50	17	17	0.61	0.17	5.0	4.7	4.9
2009-05-25 19:31	40	33	0.10	0.10	3.4	2.7	3.0
2009-05-26 19:09	14	13	0.32	0.45	3.3	2.9	3.1
2009-05-27 17:37	13	14	0.16	0.25	3.2	3.1	3.1
2009-05-28 19:13	7.1	8.5	0.19	0.25	1.6	1.7	1.7
2009-05-29 06:03	2.1	2.3	0.28	0.26	1.2	1.1	1.1
2009-06-01 18:18	19	20	0.52	0.22	1.7	1.8	1.8
2009-06-02 19:40	8.5	9.7	0.11	0.11	1.9	1.9	1.9
2009-06-03 20:33	3.2	3.6	0.24	0.15	0.7	0.8	0.8
2009-06-04 18:56	1.3	1.6	0.07	0.18	0.3	0.4	0.4
2009-06-05 19:00	1.4	1.4	0.11	0.21	0.3	0.3	0.3
2009-06-07 23:02	4.5	5.5	0.11	0.21	0.7	0.8	0.7
2009-06-08 19:52	7.8	7.7	0.28	0.20	2.1	1.9	2.0
2009-06-09 17:10	4.5	6.2	1.2	1.1	1.3	1.4	1.4
2009-06-10 19:16	6.9	8.4	0.09	1.8	1.5	1.7	1.6
2009-06-11 19:59	17	17	0.06	0.30	4.1	3.9	4.0
2009-06-12 19:33	18	14	0.05	0.60	3.9	3.1	3.5
2009-06-15 18:46	9.9	9.1	0.07	0.22	1.1	1.0	1.1

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