Supplementary Material: Volatility of a Ship Emission in the Baltic Sea Using Modelling and Measurements in Real-World Conditions

Oskari Kangasniemi, Pauli Simonen, Jana Moldanová, Hilkka Timonen, Luis M. F. Barreira, Heidi Hellén, Jukka-Pekka Jalkanen, Elisa Majamäki, Barbara D'Anna, Grazia Lanzafame, Brice Temime-Roussel, Johan Mellqvist, Jorma Keskinen and Miikka Dal Maso

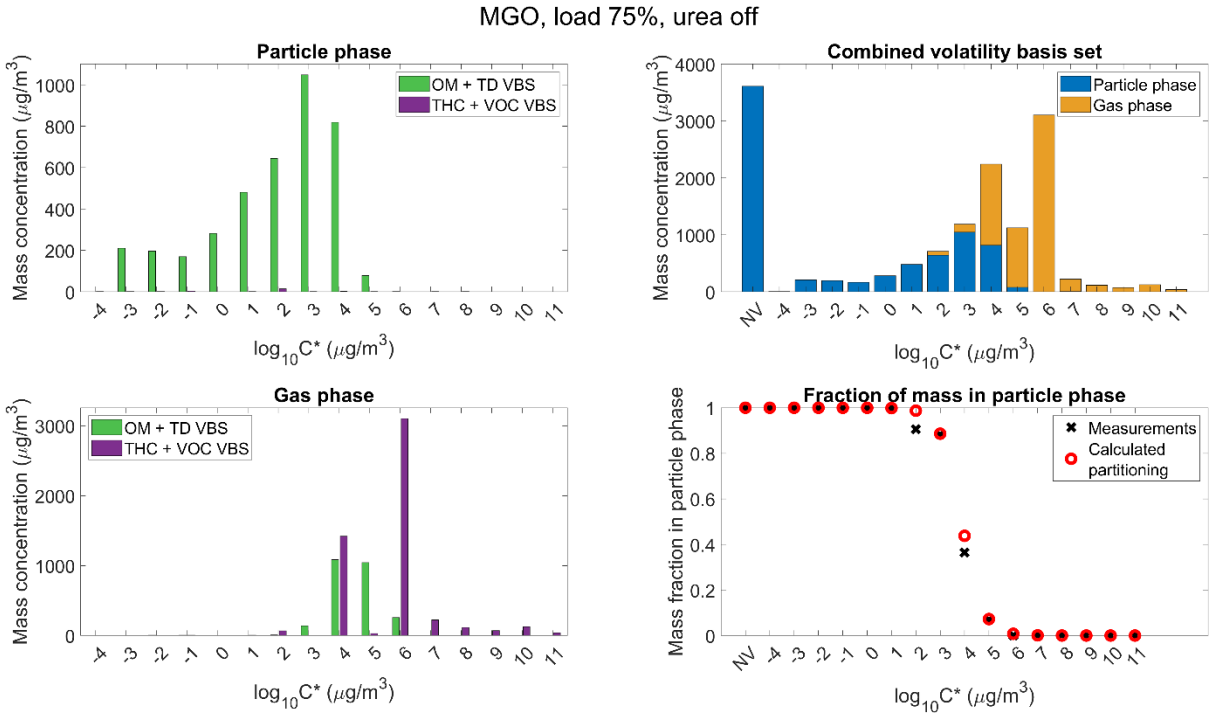

Figure S1. The gas and particle phase concentrations for marine gas oil (MGO) with 75% engine load and without urea after treatment divided in volatility bins based on organic matter (OM) concentration measurements combined with thermodenuder (TD) derived volatility distribution and total hydrocarbon (THC) concentration measurements combined with volatile organic compound (VOC) derived from STEAM emission inventory. For each bin. the higher gas or particle phase concentration is taken as the "correct" one and used in the combined volatility distribution. The mass fraction in the particle phase according to this treatment is then compared to one calculated using partitioning equation to confirm the feasibility of this approach.

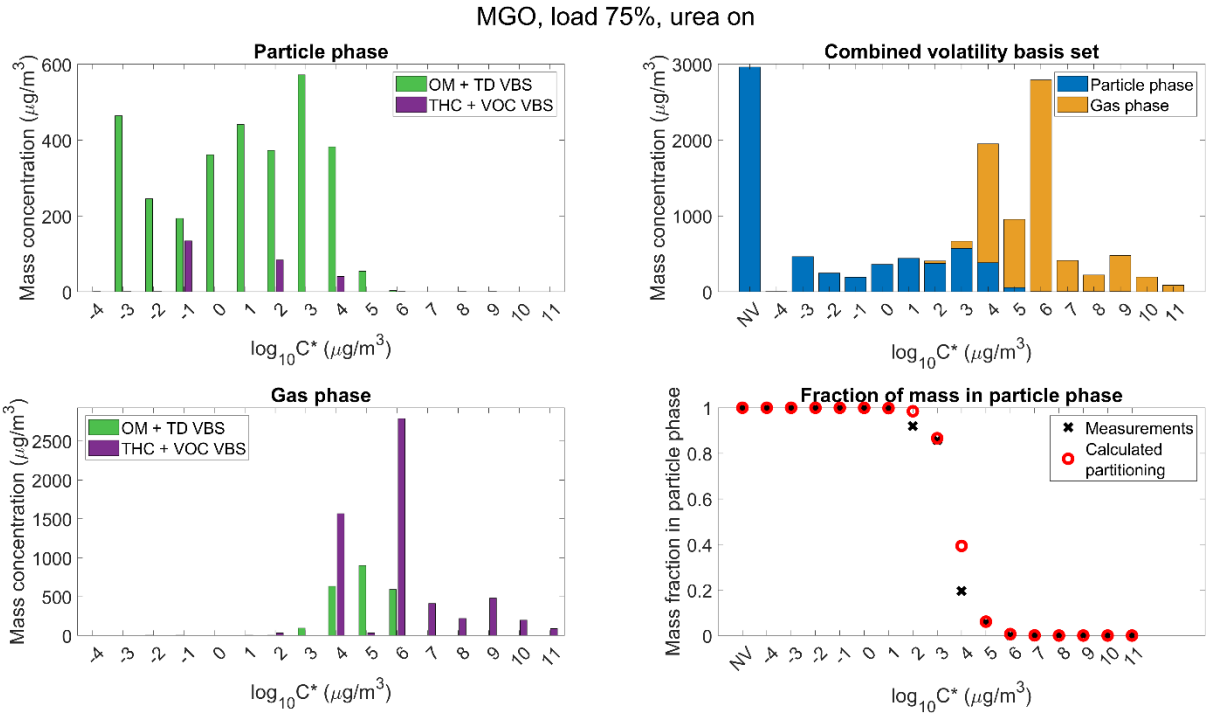

Figure S2. The gas and particle phase concentrations for marine gas oil with 75% engine load and with urea after treatment divided in volatility bins and combined to one volatility distribution as described in Figure S1.

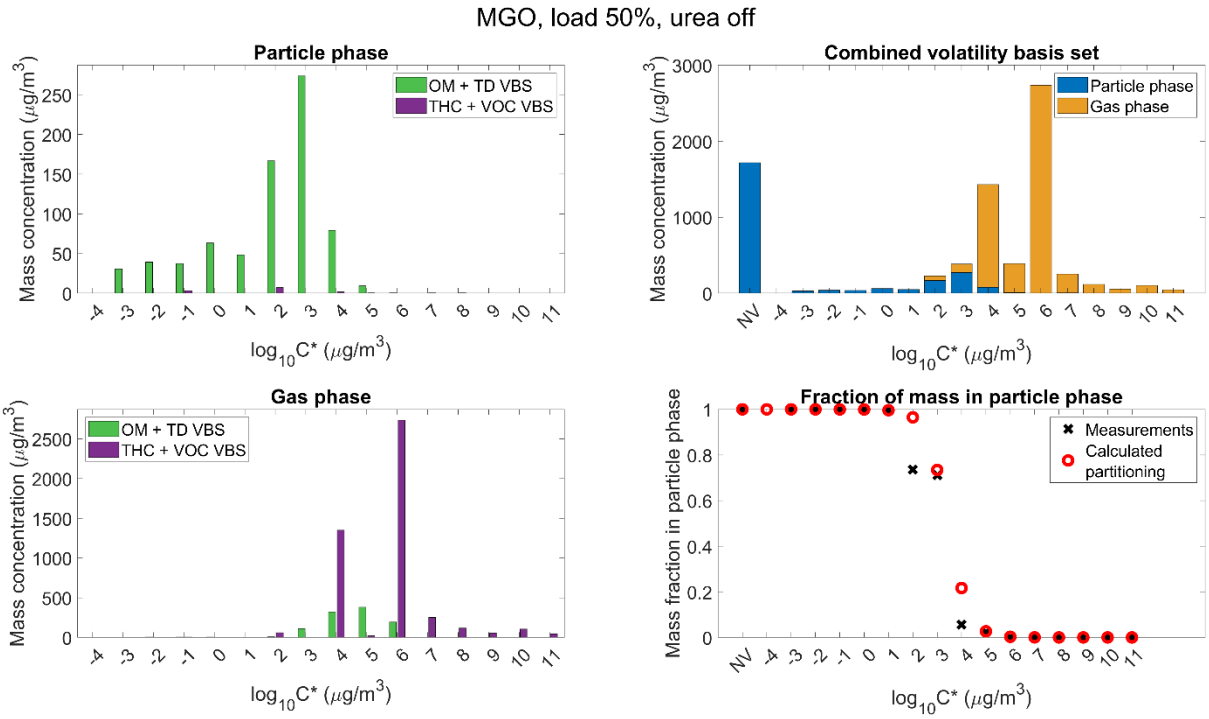

Figure S3. The gas and particle phase concentrations for marine gas oil with 50% engine load and without urea after treatment divided in volatility bins and combined to one volatility distribution as described in Figure S1.

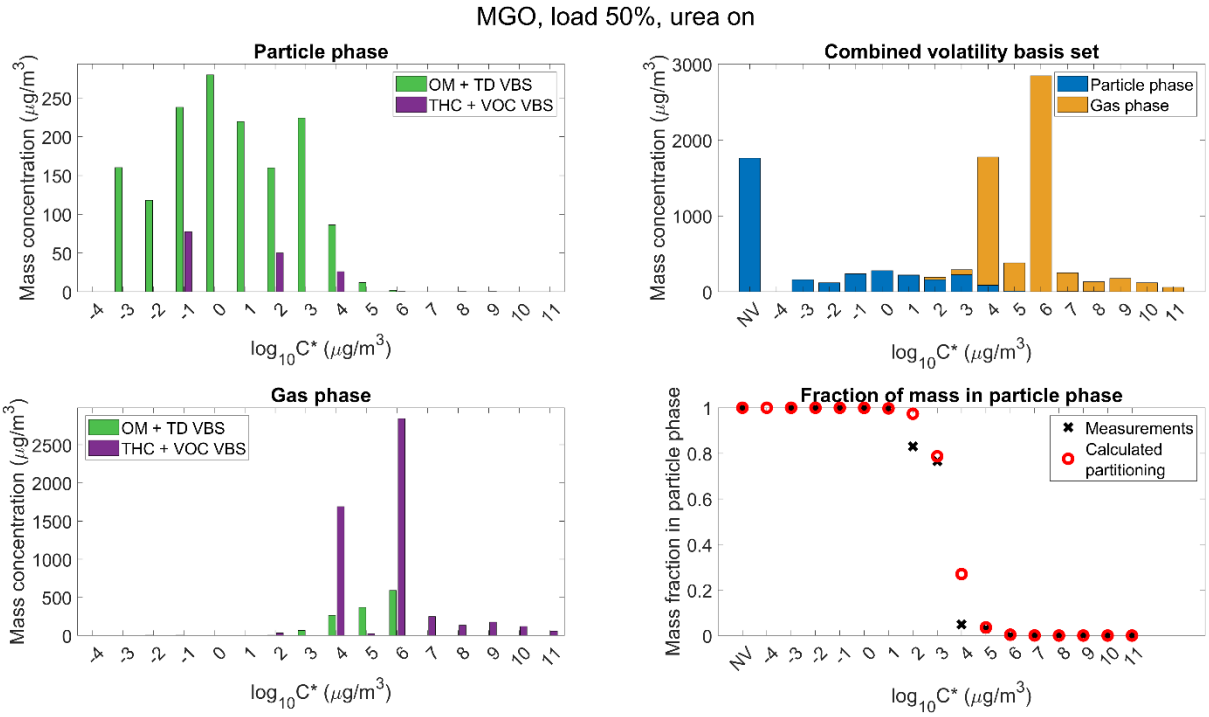

Figure S4. The gas and particle phase concentrations for marine gas oil with 50% engine load and with urea after treatment divided in volatility bins and combined to one volatility distribution as described in Figure S1.

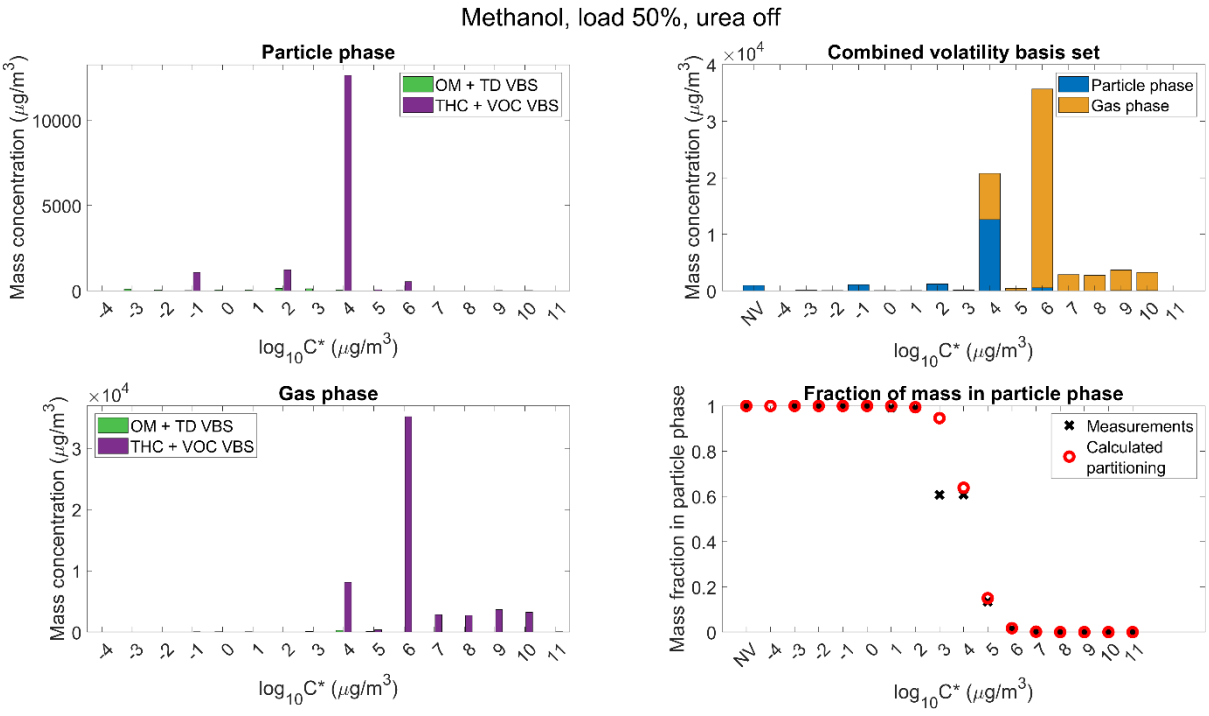

Figure S5. The gas and particle phase concentrations methanol fuel with 50% engine load and without urea after treatment divided in volatility bins and combined to one volatility distribution as described in Figure S1.

Table S1. Identified gas phase organic species, their effective saturation concentrations C*, volatility bins ($log_{10}C^*$) and their mass fraction % from the total organic mass for each five fuel, engine load and after-treatment combinations. There are pairs of species in oxygenated VOCs which could not be distinguished from each other in which case they were assumed to be divided in equal halves.

Identified species	C* (µg/m³)	Volatility bin	Mass fraction % of total organic mass				
			MGO 75% Urea on	MGO 75% Urea on	MGO 50% Urea off	MGO 50% Urea on	Methanol 50% Urea off
Polyaromatic hydrocarbons							
Naphthalene	7.01×10^{5}	6	0.013	0.013			
2-methylnaphthalene	5.98×10^{5}	6	0.018	0.025			
1-methylnaphthalene	6.97×10^{5}	6	0.010	0.015			
Biphenyl	1.11×10^{5}	5	0.005	0.005			
2.3-dimethylnaphthalene	1.23×10^{4}	4	0.007	0.009			
Acenaphthylene	5.24×10^{4}	5	0.002	0.003			
Acenaphthene	2.43×10^{4}	4	0.001	0.001			
2.3.5-trimethylnaphthalene	5.01×10^{4}	5	0.002	0.003			
Fluorene	7.33×10^{3}	4	0.002	0.002			
1-methylfluorene	4.07×10^{3}	4	0.001	0.001			
Phenanthrene	1.62×10^{3}	3	0.004	0.004			
Anthracene	8.76×10^{1}	2	0.000	0.000			
2-methylphenanthrene	9.89×10^{2}	3	0.001	0.001			
3-methylphenanthrene	9.89×10^{2}	3	0.001	0.001			
1-methylphenanthrene	2.22×10^{2}	2	0.000	0.001			
1-methylanthracene	1.32×10^{6}	6	0.000	0.001			
2-phenylnaphthalene	5.65×10^{2}	3	0.000	0.000			
Fluoranthene	1.47×10^{2}	2	0.000	0.000			
Pyrene	7.19×10^{1}	2	0.000	0.001			
1-methylfluoranthene	9.45×10^{2}	3	0.000	0.000			
Retene	5.13×10^{1}	2	0.000	0.000			
1-methylpyrene	2.80×10^{1}	1	0.000	0.000			
Benzo(a)anthracene	3.97×10^{0}	1	0.000	0.000			
Chrysene	1.19×10^{1}	1	0.000	0.000			
2-methylchrysene	5.20×10^{0}	1	0.000	0.000			
5-methylchrysene	1.12×10^{1}	1	0.000	0.000			
Benzo(b)fluoranthene	1.10×10^{1}	1	0.000	0.000			
Benzo(k)fluoranthene	2.12×10^{-2}	-2	0.000	0.000			
Benzo(e)pyrene	1.25×10^{-1}	-1	0.000	0.000			
Benzo(a)pyrene	1.20×10^{-1}	-1	0.000	0.000			
Perylene	1.15×10^{-1}	-1	0.000	0.000			
Indeno(1.2.3-c.d)pyrene	3.15×10^{-3}	-3	0.000	0.000			
Dibenzo(a.h)anthracene	2.43×10^{-2}	-2	0.000	0.000			
Benzo(g.h.i)perylene	2.52×10^{-3}	-3	0.000	0.000			
Coronene	6.24×10^{-5}	-4	0.000	0.000			

Dibenzothiophenes							
Dibenzothiophene	2.71×10^3	3	0.000	0.000			
2-methyldibenzothiophene	1.02×10^3	3	0.000	0.000			
1-methyldibenzothiophene	1.02×10^3	3	0.000	0.000			
4-methyldibenzothiophene	1.02×10^3	3	0.000	0.000			
2.8-dimethyldibenzothiophene	1.74×10^2	2	0.000	0.000			
2.4.7-trimethyldibenzothiophene	1.94×10^2	2	0.000	0.000			
Oxygenated VOCs							
(CH2O)H+ formic aldehyde*	7.01×10^9	10	0.472	0.344	0.416	0.259	2.263
(CH3OH)H+ methanol	2.44×10^8	8	0.018	0.142	0.017	0.119	1.423
(C2H4O)H+ acetaldehyde	2.21×10^9	9	0.289	0.295	0.245	0.178	0.303
(CH2O2)H+ formic acid	1.56×10^8	8	0.594	0.683	0.524	0.503	0.817
(C2H6O)H+ ethanol	1.52×10^8	8	0.006	0.001	0.007	0.001	0.004
(C3H6O)H+ acetone	7.26×10^8	9	0.032	0.068	0.025	0.031	0.055
(C2H4O2)H+ **acetic acid**/glycolaldehyde	6.30×10^7	8	1.362	2.385	1.722	1.548	1.338
(C2H4O2)H+ acetic acid/**glycolaldehyde**	1.99×10^7	7	3.184	5.242	4.250	3.387	2.703
(C4H6O)H+ **methyl ethyl ketone**. methacrolein	3.51×10^8	9	0.022	0.029	0.018	0.020	0.025
(C4H6O)H+ methyl ethyl ketone. **methacrolein**	5.85×10^8	9	0.022	0.029	0.018	0.020	0.025
(C4H2O3)H+ maleic anhydride or maleic acid frag (-H2O)	1.64×10^6	6	59.388	45.721	57.583	51.825	49.767
(C5H4O3)H+ **citraconic anhydride** or citraconic acid frag (-H2O)	6.99×10^6	7	1.023	1.386	1.006	1.088	1.244
(C5H4O3)H+ citraconic anhydride or **citraconic acid** frag (-H2O)	2.89×10^2	2	1.023	1.386	1.006	1.088	1.244
(C8H4O3)H+ phthalic anhydride or phthalic acid frag (-H2O)	4.27×10^3	4	27.292	26.425	28.439	31.268	28.913
(C9H6O3)H+ **methyl phthalic anhydride** or methyl phthalic acid frag (-H2O)	6.36×10^4	5	0.535	0.528	0.406	0.420	0.478
(C9H6O3)H+ methyl phthalic anhydride or **methyl phthalic acid** frag (-H2O)	2.67×10^2	2	0.535	0.528	0.406	0.420	0.478
Cicloalkanes/alkenes VOCs (µg/kg fuel)							
(C3H4)H+ HC fragments	1.26×10^{10}	10	0.310	0.466	0.270	0.302	0.381
(C3H6)H+ propene + HC fragments	2.11×10^{10}	10	1.209	1.813	1.239	1.234	1.569
(C4H7)H+	7.34×10^9	10	0.004	0.017	0.003	0.009	0.012
(C4H8)H+	3.92×10^9	10	0.219	0.357	0.141	0.186	0.281
(C5H8)H+	2.27×10^9	9	0.060	0.129	0.038	0.077	0.102
(C5H10)H+	1.35×10^9	9	0.074	0.140	0.061	0.092	0.117
(C6H10)H+	4.54×10^8	9	0.061	0.138	0.045	0.088	0.113
(C7H12)H+	1.21×10^8	8	0.068	0.152	0.052	0.099	0.126
(C8H14)H+	3.23×10^7	8	0.042	0.103	0.034	0.068	0.085
(C9H16)H+	1.94×10^7	7	0.014	0.035	0.011	0.023	0.029
Aromatic VOCs							
(C6H6)H+ benzene	4.60×10^8	9					0.268
(C7H8)H+ toluene	1.67×10^8	8					0.016
(C8H8)H+ styrene	4.35×10^7	8					0.004
(C8H10)H+ C8 aromatics	5.88×10^7	8	0.012	0.027	0.006	0.012	0.004
(C9H12)H+ C9 aromatics	1.99×10^7	7	0.021	0.045	0.015	0.031	0.010
(C10H8)H+ naphthalene	7.01×10^5	6			0.007	0.056	0.005

(C10H14)H+ C10 aromatics	9.73×10^{6}	7	0.013	0.042	0.008	0.022	0.007
(C12H10)H+ acenaphthene	2.35×10^{4}	4	0.005	0.017	0.003	0.007	0.003
Nitrogen VOCs							
(CHNO)H+	5.21×10^{8}	9		5.299		1.511	3.510
(CH3NO)H+	1.62×10^{5}	5					0.118
(C3H3N)H+	3.34×10^{8}	9	0.036	0.899	0.028	0.606	0.601
(C8H5NO2)H+	7.92×10^{-2}	-1	0.076	2.207	0.068	1.415	1.506
Non-Methane Hydrocarbons							
Ethane	5.35×10^{10}	11	0.075	0.044	0.083	0.035	
Ethene	8.25×10^{10}	11	0.429	1.294	0.628	0.911	
Propane	1.82×10^{10}	10	0.000	0.014	0.000	0.000	
Propene	2.11×10^{10}	10	0.167	0.226	0.126	0.184	
2-Methylpropane	8.99×10^{9}	10	0.000	0.000	0.000	0.000	
Butane	6.27×10^{9}	10	0.000	0.000	0.000	0.000	
Ethyne	5.37×10^{10}	11	0.100	0.087	0.088	0.098	
t-but-2-ene	5.32×10^{9}	10	0.027	0.004	0.016	0.000	
But-1-ene	7.48×10^{9}	10	0.000	0.000	0.000	0.005	
Cis-but-2-ene	5.32×10^{9}	10	0.000	0.000	0.000	0.000	
2-Methylbutane	3.02×10^{9}	9	0.000	0.000	0.000	0.000	
n-pentane	2.25×10^{9}	9	0.041	0.009	0.000	0.039	
1.3-butadiene	6.76×10^{9}	10	0.000	0.000	0.000	0.000	
t-pent-2-ene	2.15×10^{9}	9	0.000	0.000	0.000	0.000	
Pent-1-ene	2.70×10^{9}	9	0.000	0.000	0.000	0.000	
2-Methylpentane	1.13×10^{9}	9	0.013	0.008	0.000	0.021	
Isoprene	2.27×10^{9}	9	0.000	0.000	0.000	0.009	
Hexane	8.10×10^{8}	9	0.000	0.000	0.000	0.000	
C6-C10 alkanes							
Benzene	4.60×10^{8}	9	0.342	0.220	0.313	0.154	
Toluene	1.67×10^{8}	8	0.029	0.020	0.016	0.012	
Ethylbenzene	6.64×10^{7}	8	0.002	0.002	0.001	0.001	
p/m-xylene	5.88×10^{7}	8	0.006	0.006	0.003	0.003	
Styrene	4.35×10^{7}	8	0.012	0.004	0.003	0.003	
o-xylene	4.58×10^{7}	8	0.002	0.002	0.001	0.000	
Propylbenzene	2.75×10^{7}	7	0.004	0.003	0.001	0.002	
3-ethyltoluene	2.44×10^{7}	7	0.001	0.003	0.000	0.000	
4-ethyltoluene	2.41×10^{7}	7	0.001	0.000	0.000	0.000	
135-trimethylbenzene	1.99×10^{7}	7	0.000	0.001	0.000	0.000	
2-ethyltoluene	2.09×10^{7}	7	0.000	0.000	0.000	0.000	
124-trimethylbenzene	1.69×10^{7}	7	0.002	0.004	0.001	0.001	
123-trimethylbenzene	1.36×10^{7}	7	0.001	0.000	0.000	0.000	
Hexane	8.10×10^{8}	9	0.007	0.002	0.003	0.003	
Heptane	2.93×10^{8}	8	0.008	0.003	0.005	0.003	

Octane	1.05×10^8	8	0.016	0.009	0.011	0.012	
Nonane	3.81×10^7	8	0.019	0.010	0.014	0.009	
Decane	1.39×10^7	7	0.018	0.013	0.011	0.009	