Supplemental Information

Uncontrolled combustion of shredded tires in a landfill – Part 1: Characterization of gaseous and particulate emissions

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Calculation of mass from aerosol size distribution and assumptions of particle size and shape

PN measured by SMPS (according to electrical mobility diameter) and APS (according to aerodynamic diameter) were processed to estimate $PM_{2.5}$ mass concentrations at 10-minute time resolution. The number-to-mass conversion is based on the volume-equivalent diameter (DeCarlo et al. 2004; Khlystov et al. 2004) and accounts for the non-spherical shapes and varying densities of combustion particles (Park et al. 2003; Slowik et al. 2004). Aerosol number size distributions were processed using three sets of assumptions about particle density (ρ) and dynamic shape factor (χ). For background aerosol, spherical particles were assumed with χ=1.0 and of density 1.8 g cm^{-3}. For plume-impacted aerosol, density 1.5 g cm^{-3} and χ=1.1 was assumed, consistent with the properties of Type II soot (45% black carbon, 50% PAH, and 5% aliphatic, and fractal chain agglomerate shape) described by Slowik et al. (2004). As a sensitivity test, the physical properties of Type I soot (90% black carbon, 5% PAH, and 5% aliphatic) were also considered, with density of 1.8 g cm^{-3} and variable dynamic shape factors: particles less than 40 nm were assumed spherical (χ=1.0), particles greater than 400 nm were irregular in shape (χ=3.0), and particles 40-400 nm were parameterized by $\chi = 2\ log_{10}(d_m) - 2.204$, where d_m is the mobility diameter (nm).

The mass estimated by SMPS (M_s) was integrated across the full particle size range (14-661 nm) by the volume-equivalent diameter of each size bin, following De Carlo et al. (2004). The Cunningham slip correction was applied (TSI 2009) with the gas free mean path assumed to be 65.1 nm. APS data was integrated across aerodynamic diameters of 661-2500 nm (M_{a1}) and 542-2500nm (M_{a2}). When SMPS and APS overlapped (depending on ρ and χ), the $PM_{2.5}$ mass concentration was calculated as the sum of M_s and M_{a1}. In cases where the SMPS and APS estimated PM mass concentrations did not overlap, the un-sampled mass in the overlap region was calculated as M_u by

$$M_u = \frac{[log_{10}(a_a) - log_{10}(b_s)][f_s(a_a) + f_a(b_s)]}{2}$$

where a_a is the mobility diameter of the smallest APS channel (542nm), b_s is the mobility diameter of the highest SMPS channel (661 nm), $f_s(a_a)$ is the value of the $dN/dlogD_p$ number distribution function at a_a, and $f_a(b_s)$ is the value of the number distribution function at b_s. Un-sampled mass values, when they existed, were small (~1%) relative to the total $PM_{2.5}$. Total mass concentration was then calculated as the sum of M_s, M_u, and M_{a2}. For 10 minute periods when SMPS data were missing, M_s (and M_u, if needed) was imputed from the APS measurement and the mean SMPS:APS ratio: $M_s \cong M_{a2}\left(\overline{(M_s + M_u)/M_{a2}}\right)$ where the overbar quantity is the mean ratio of all available samples.

Type II soot assumptions (Slowik et al. 2004) were more consistent with the gravimetric and beta attenuation monitor data and were used to calculate the average $EF_{PM2.5}$ value of 5.4±5.4 g kg^{-1}. For comparison, Type I assumptions were tested and yielded an $EF_{PM2.5}$ value 53% lower than Type II assumptions, highlighting that assumptions about particle density, shape, and morphology significantly impact the estimated $EF_{PM2.5}$. Type II assumptions yielded EF_{EC} of 2.4 g kg^{-1}, whereas Type I assumptions gave 2.5 g kg^{-1}, demonstrating that EF_{EC} is insensitive to this assumption.

Works Cited

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Table S1: Summary data, including background, ambient enhancement (Δ), and emission factors (EF) for ten transects of the tire fire plume in Iowa City.

No.	Location[a]	Date in 2012	Start time[b]	End time[b]	Peak duration (h)	CO_2 background (ppm)	ΔCO_2 (ppm)	$PM_{2.5}$ background ($\mu g\ m^{-3}$)	$\Delta PM_{2.5}$ ($\mu g\ m^{-3}$)	EF $PM_{2.5}$ ($g\ kg^{-1}$)	SO_2 background (ppb)	ΔSO_2 (ppb)	EF SO2 ($g\ kg^{-1}$)	PN background ($\#\ cm^{-3}$)	DPN ($\#\ cm^{-3}$)	EF PN ($\#\ kg^{-1}$)
1	BDR	30-May	16:20	16:50	0.67	376.74	2.52	NA[c]	NA[c]	NA[c]	0.78	2.13	4.1	16,968	30,863	2.3E+16
2	BDR	30-May	19:50	20:10	0.50	373.93	1.24	6.30	0.67	NA[c]	1.24	0.63	2.4	16,932	5,533	8.2E+15
3	BDR	31-May	18:00	19:10	1.33	365.56	0.15	8.19	7.06	NA[c]	1.38	1.96	NA[c]	13,434	46,077	NA[c]
4	BDR	31-May	20:20	20:50	0.33	376.45	0.99	15.93	7.47	14.0	1.89	5.22	25.6	11,794	50,520	9.4E+16
5	IA-AMS	1-Jun	21:20	23:30	2.33	406.00	24.10	5.86	11.77	0.9	1.35	0.80	0.2	4,400	28,382	NA[c]
6	IA-AMS	2-Jun	6:40	8:20	1.83	384.20	1.72	17.28	9.01	9.6	2.54	4.12	11.5	NA[c]	NA[c]	NA[c]
7	IA-AMS	2-Jun	8:40	9:40	1.17	374.54	1.42	15.76	6.50	8.4	2.94	3.92	13.3	4,757	43,462	5.6E+16
8	IA-AMS	2-Jun	12:20	14:00	1.67	370.21	1.03	7.76	1.71	3.0	1.80	0.60	2.8	8,263	6,916	NA[c]
9	IA-AMS	3-Jun	8:50	9:10	0.33	387.21	5.51	7.38	2.14	0.7	1.63	1.14	1.0	4,966	26,633	8.9E+15
10	IA-AMS	3-Jun	13:10	14:40	1.50	374.57	2.78	3.80	1.09	0.7	1.33	1.67	2.9	6,635	27,864	1.8E+16
	Mean					378.94	4.15	9.81	5.27	5.35	1.69	2.22	7.10	9,794	29,583	3.5E+16
	Standard Deviation					11.34	7.16	5.07	3.98	5.33	0.64	1.64	8.31	5,121	15,851	3.4E+16
	Minimum					365.56	0.15	3.80	0.67	0.72	0.78	0.60	0.16	4,400	5,533	8.2E+15
	Maximum					406.00	24.10	17.28	11.77	13.97	2.94	5.22	25.57	16,968	50,520	9.4E+16

a) BDR = Black Diamond Road; b) Local; c) NA = not available;

Table S2: Heterocyclic aromatic compunds found in tire fire smoke.

Compound	Formula	Theoretical *m/z* (Da)	Observed *m/z* (Da)	Error (mDa)	t_R' (min.)
2,4-dimethylquinoline	$C_{11}H_{11}N$	157.0891	157.0899	-0.8	18.98
acridine	$C_{13}H_9N$	179.0735	179.0742	0.7	23.26
2-methyl-9,10-anthracenedione	$C_{15}H_{10}O_2$	222.0681	222.0707	2.6	26.14
benz[a]anthracene-7,12-dione	$C_{18}H_{10}O_2$	258.0681	258.0704	-2.3	30.15