Supplementary material

Non-polar organic compounds in aerosols in a typical city of Eastern China: Size distribution, gas-particle partitioning and tracer for $PM_{2.5}$ source apportionment

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Section S1. Tables of abbreviation, concentrations and MDRs values of NPOCs

Table S1. Abbreviation, P^{o}_{L} and ΔH_0 information for individual NPOCs

Species	Abb.	P^{o}_{L} [a]	ΔH_0 [b]	Species	Abb.	P^{o}_{L}	ΔH_0
PAHs				**n–Alkanes**			
Fluorene	FLO	1.10E–01	84.9	n–Undecane	$C_{11}H_{24}$	/	/
Phenanthrene	PHE	2.57E–02	88.9	n–Dodecane	$C_{12}H_{26}$	/	/
Anthracene	ANT	1.21E–03	99.7	n–Tridecane	$C_{13}H_{28}$	/	/
Fluoranthene	FLU	1.60E–03	98.3	n–Tetradecane	$C_{14}H_{30}$	/	/
Pyrene	PYR	7.60E–04	97.9	n–Pentadecane	$C_{15}H_{32}$	/	/
Benz[a]anthracene	BaA	3.45E–05	108	n–Hexadecane	$C_{16}H_{34}$	/	/
Chrysene	CHR	1.36E–06	118.8	n–Heptadecane	$C_{17}H_{36}$	/	/
Benzo[b]fluoranthene	BbF	1.00E–06	119.2	n–Octadecane	$C_{18}H_{38}$	/	/
Benzo[j+k]fluoranthene	BkF	4.66E–06	113	n–Nonadecane	$C_{19}H_{40}$	/	/
Benzo[a]fluoranthene	BaF	4.66E–05	113	n–Eicosane	$C_{20}H_{42}$	/	/
Benzo[e]pyrene	BeP	7.89E–07	117.9	n–Heneicosane	$C_{21}H_{44}$	/	/
Indeno[1,2,3-cd]pyrene	IcdP	1.42E–06	124	n–Docosane	$C_{22}H_{46}$	3.24E–03	115
Dibenz[a,h]+[a,c]anthracene	DahA	4.93E–09	134.1	n–Tricosane	$C_{23}H_{48}$	1.22E–03	120
Benzo[ghi]perylene	BghiP	1.01E–08	129.9	n–Tetracosane	$C_{24}H_{50}$	4.66E–04	124
Coronene	COR	3.56E–10	143.2	n–Pentacosane	$C_{25}H_{52}$	1.72E–04	129
iso–Alkane				n–Hexacosane	$C_{26}H_{54}$	6.59E–05	133
Pristane	$C_{19}H_{40}$	/ [c]	/	n–Heptacosane	$C_{27}H_{56}$	2.53E–05	137
Phytane	$C_{20}H_{42}$	/	/	n–Octacosane	$C_{28}H_{58}$	9.42E–06	142
Hopane				n–Nonacosane	$C_{29}H_{60}$	3.55E–06	146
αβ–Nnorhopane	C_{29}–αβ–NOR–H	2.74E–06	126	n–Triacontane	$C_{30}H_{62}$	1.32E–06	151
αβ–Hopane	C_{30}–αβ–H	1.01E–06	130	n–Hentriacontane	$C_{31}H_{64}$	4.96E–07	155
αβ–22R–Homohopane	C_{31}—αβ–R	3.85E–07	134	n–Dotriacontane	$C_{32}H_{66}$	1.93E–07	160
ab 22S–Homohopane	C_{31}—αβ–S	3.85E–07	134	n–Tritriacontane	$C_{33}H_{68}$	7.09E–08	164
22,29,30–Trisnorhopane	Tm	1.93E–05	117	n–Tetratriacontane	$C_{34}H_{70}$	2.63E–08	169
Sterane				n–Pentatriacontane	$C_{35}H_{72}$	1.00E–08	173
ααα–20R Cholestane	ααα–20R–C	2.03E–05	121	n–Hexatriacontane	$C_{36}H_{74}$	3.75E–09	177
αββ–20R Cholestane	αββ–20R–C	/	/	n–Hepatriacontane	$C_{37}H_{76}$	1.42E–09	182
αββ–20R24S–Methylcholestane	αββ–20R–MEC	7.60E–06	125	n–Octatriacontane	$C_{38}H_{78}$	5.37E–10	186
aaa 20R24R–Ethylcholestane	ααα–20R–EC	/	/	n–Nonatriacontane	$C_{39}H_{80}$	2.03E–10	191
αββ–20R24R–Ethylcholestane	αββ–20R–EC	2.84E–06	130	n–Tetracontane	$C_{40}H_{82}$	7.60E–11	195

[a]: pure compound vapor pressure, unit of Pa at 298 K, cited from And and Hanshaw, 2004, Xie et al., 2013;

[b]: vaporization enthalpy, unit of (KJ mol^{-1}) at 298 K, cited from Xie et al., 2013, Wang et al., 2016;

[c]: "/" means lack of related data.

Table S2. Concentrations of NPOCs of each sampling site (ng m^{-3})

	SH	XY	SL	WQ	JJ	Average
PAHs	44.1±10.5	49.7±18.9	47.6±7.6	46.4±13.3	53.7±21.6	45.3±17.6
Alkanes	134.7±56.6	109.5±33.5	93.2±31.9	96.6±31.0	130.4±74.8	112.9±55.1
Hopanes	6.7±4.7	4.4±3.0	5.2±2.5	1.9±1.1	2.8±1.8	4.2±3.0
Steranes	2.5±1.2	3.1±1.8	1.9±0.6	1.1±0.6	1.4±0.8	2.0±1.3
NPOCs	187.9±59.6	166.7±47.3	147.8±33.4	146.0±42.8	188.2±92.1	167.3±68.4
CPI	1.2±0.1	1.3±0.2	1.3±0.2	1.4±0.2	1.3±0.2	1.3±0.2
WNA%	14.6±3.0	16.0±4.5	16.8±4.4	19.3±4.1	17.2±4.7	17.0±4.4
PNA%	85.4±3.0	84.0±4.5	83.2±4.4	80.7±4.1	82.8±4.7	83.0±4.4
C_{max}	C31	C31	C31	C31	C31	C31
ACL	29.2±0.8	28.8±0.7	28.5±0.7	29.7±0.7	29.3±0.8	29.1±0.8
WAX_{cn}	20.3±11.2	16.8±5.8	15.6±6.6	18.3±6.3	20.9±10.9	17.3±9.1

Section S2. Gas-particle partitioning for NPOCs

Partition between gas and particle phases was evaluated by regression of K_p and subcooled vapor pressure P^o_L (Pa), using the following equation:

$$\log K_p = m_r \log P^o_L + b_r \qquad \text{(S1)}$$

Useful information pertaining to gas–particle partitioning can be drawn from the regressed parameter mr and br.

The calculated and Jungle-Pankow model predicted log*K*p values were depicted in fig. S1. It can be clearly that the model predicted log*K*p values were a bit lower than the empirical calculated ones, regardless of NPOCs species.

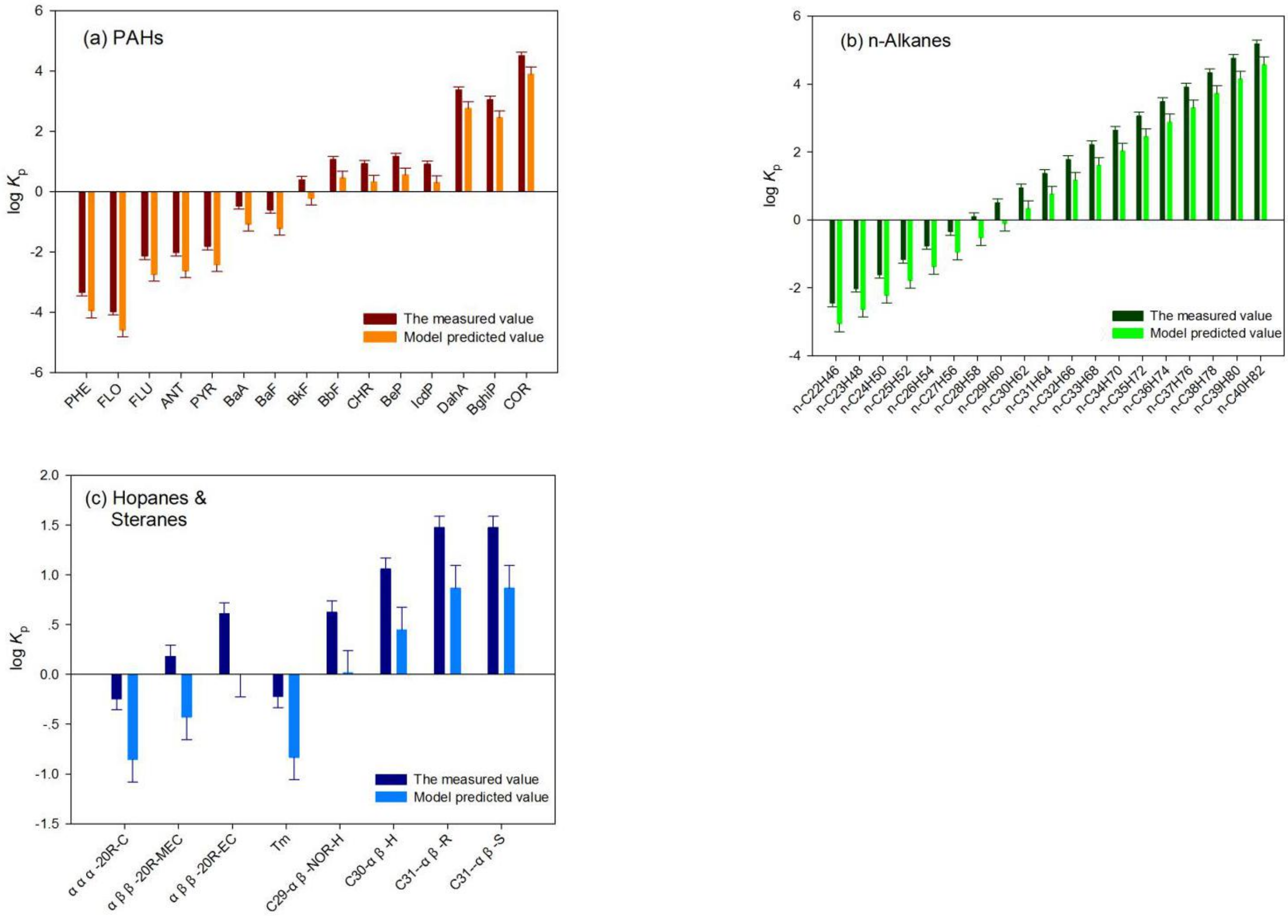

Fig. S1. Comparisons of the measured and model predicted φ values

Section S3. Source distributions extracted from single particle phase and gas-particle phases NPOCs as input data

The contributions of individual source to the total concentrations for both PMF_P and PMF_T models were compared in Fig. S2. Secondary aerosol formation was the largest contributor, occupied 24.7% and 21.8% of the single and the total concentrations in PMF_P and PMF_T, respectively. Vehicles exhaust, biomass burning, dust, industrial emission and coal combustion were major contributors, occupying of 12.5%/15.0%, 12.7%/15.7%, 8.9%/11.0%, 13.8%/11.9% and 17.5%/12.4% in PMF_P/PMF_T, respectively. For the light NPOCs source, the contributions of PMF_P and PMF_T models were 3.7% and 5.6% respectively, with a relatively high contribution for PMF_T but much smaller in the PMF_P.

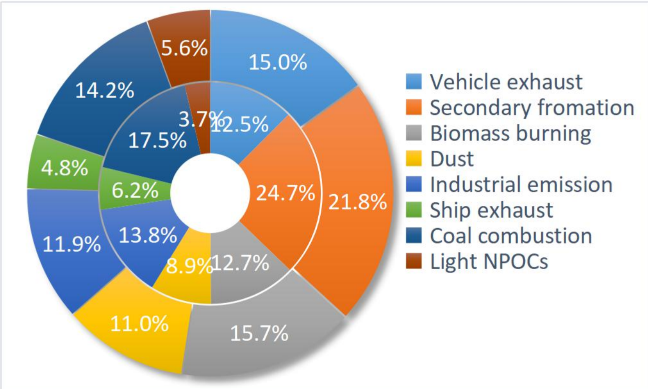

Fig. S2. Contributions of eight sources resolved by PMF (inner circular ring for single particle bound NPOCs, the outer circular ring for the total NPOCs)

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