
Supplementary Materials: Investigating the Complexities of VOC Sources in Mexico City in the Years 2016–2022

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2016

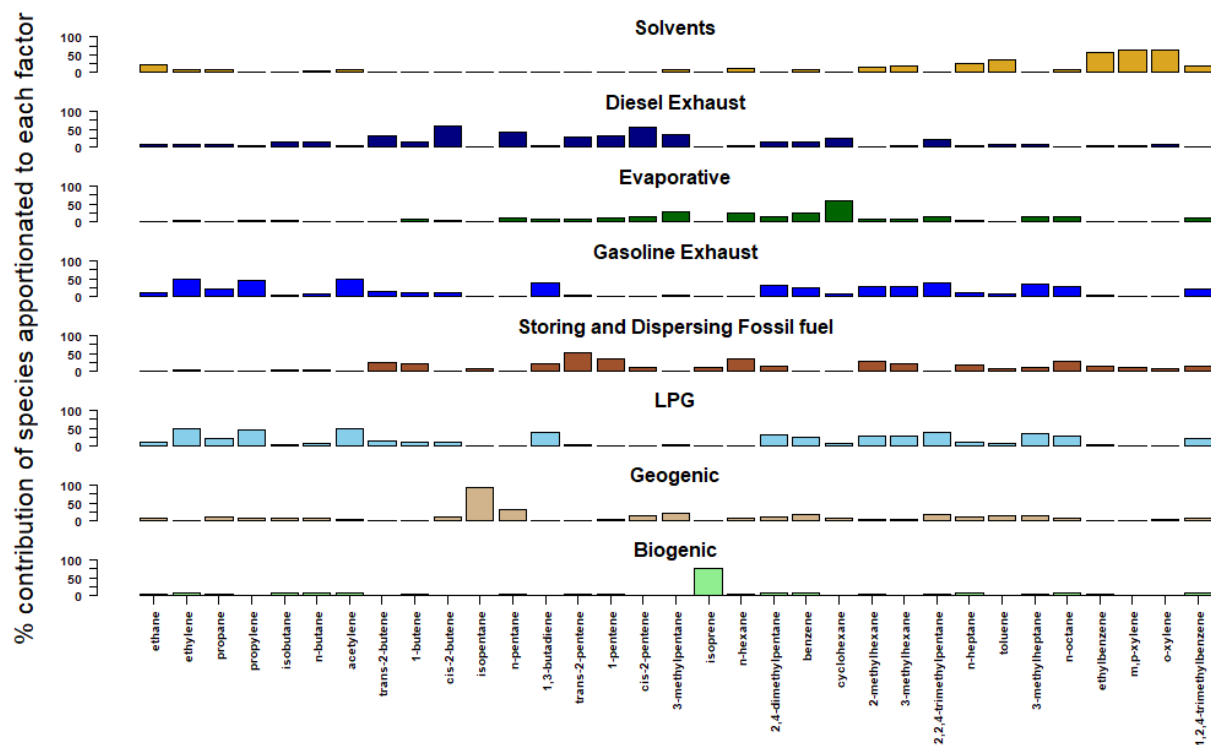


Figure S1. Profiles of source factors determined for VOCs by PMF for the month of May 2016. .

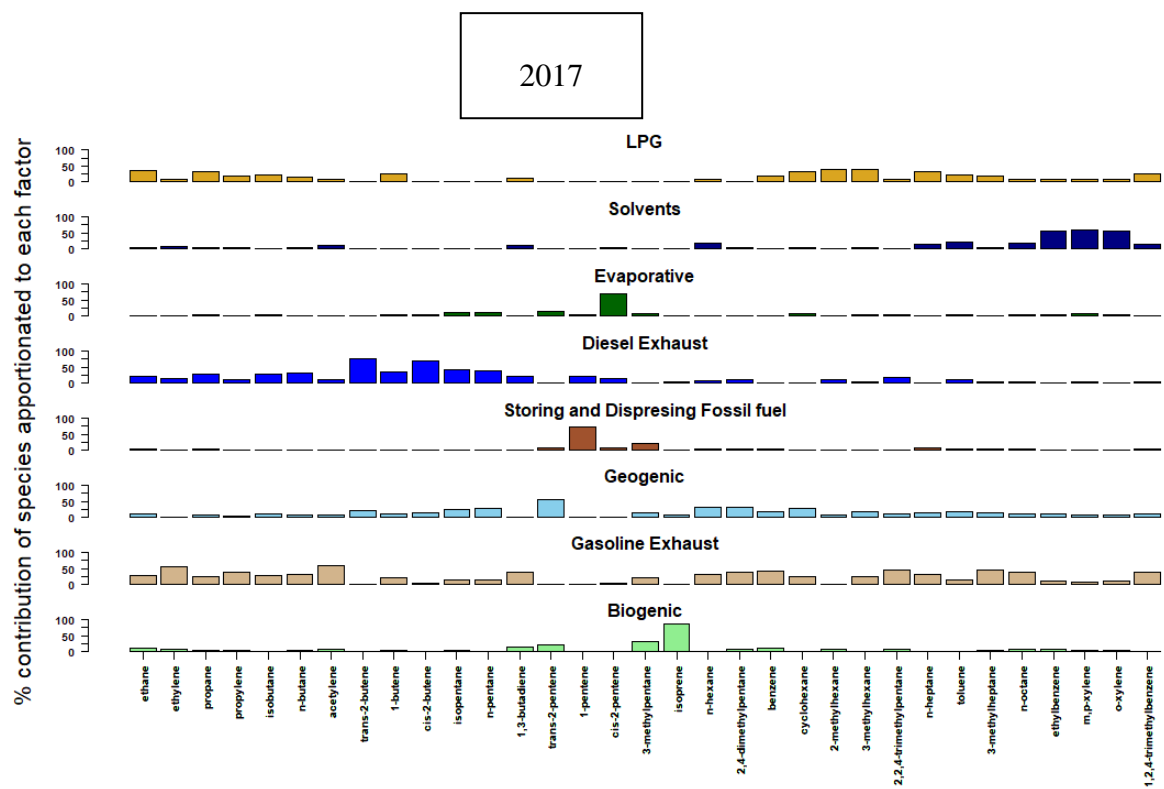


Figure S2. Profiles of source factors determined for VOCs by PMF for the month of May 2017. .

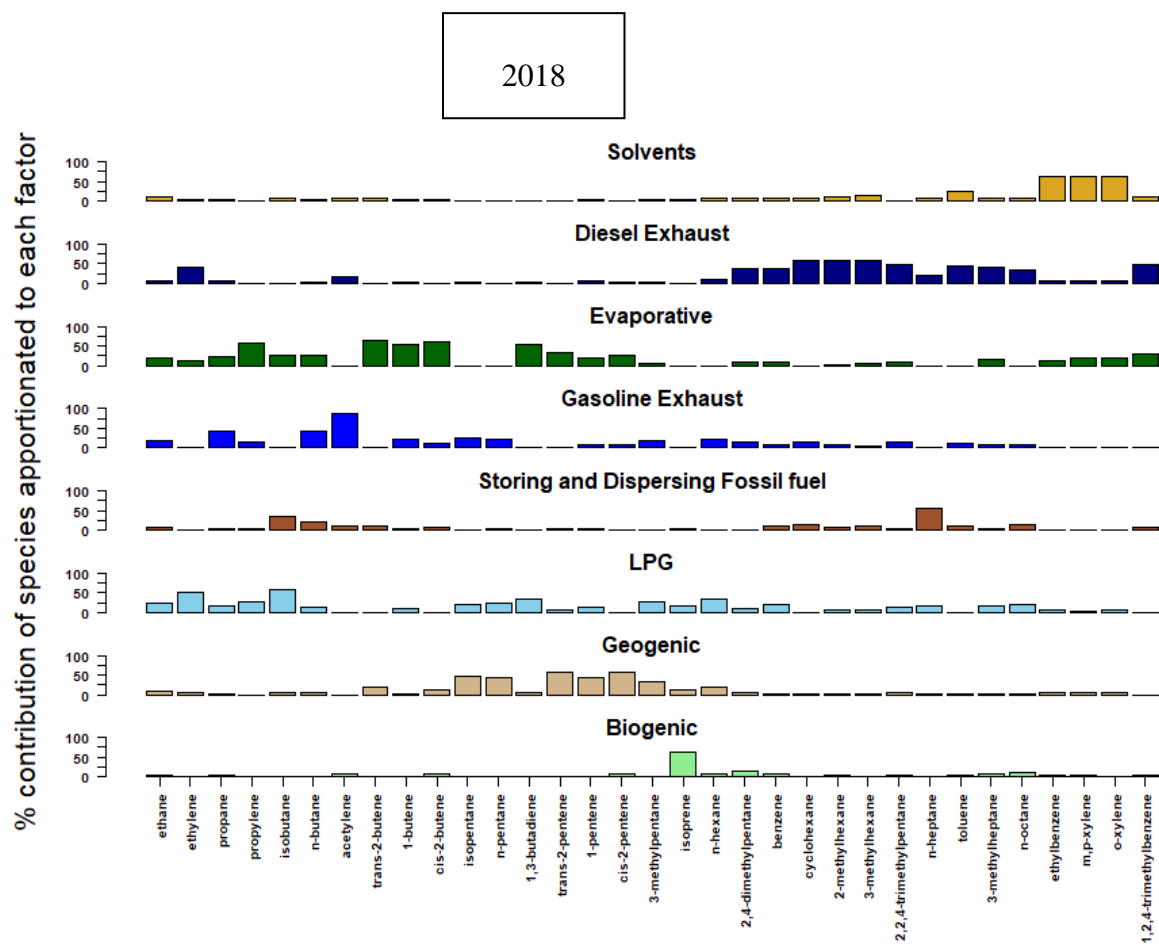


Figure S3. Profiles of source factors determined for VOCs by PMF for the month of May 2018. .

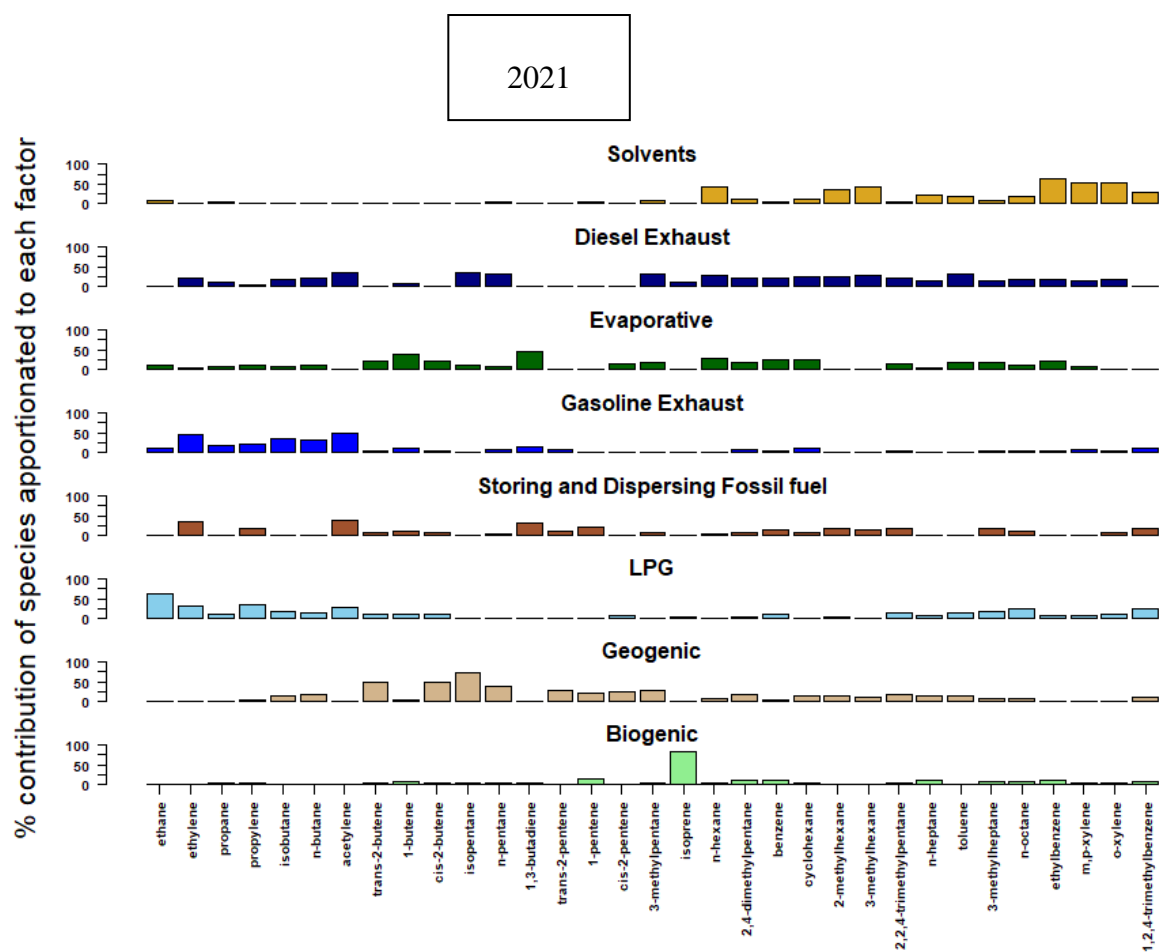


Figure S4. Profiles of source factors determined for VOCs by PMF for the month of May 2021.

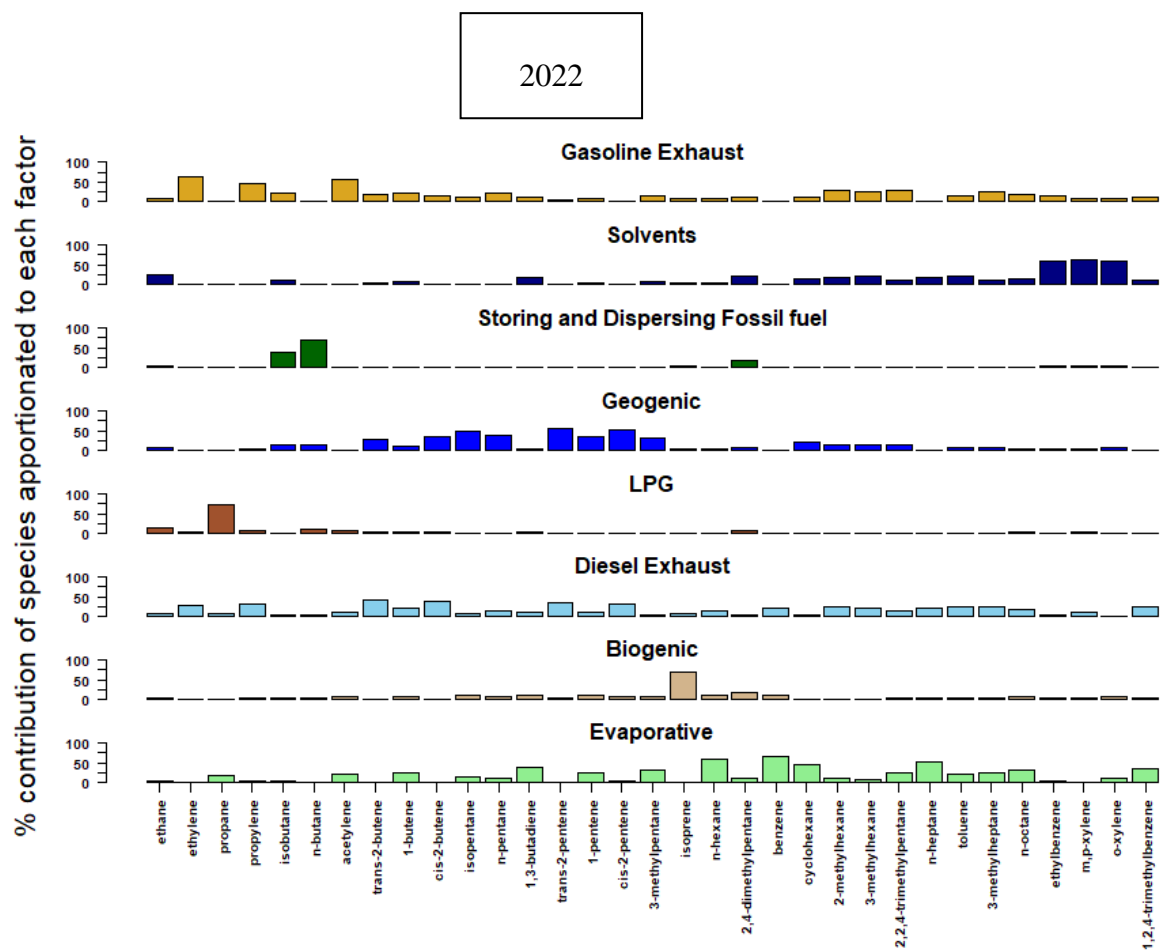


Figure S5. Profiles of source factors determined for VOCs by PMF for the month of May 2022.

Table S1. Summary of PMF runs for seven, eight, and nine-factor solutions.

Diagnostic	7 factors	8 factors	9 factors
Q_{exp}	788	716	644
Q_{rob}	82199.7	71277.7	53921.2
Q_{true}	98982.2	86238.7	62359
$Q_{\text{rob}}/Q_{\text{exp}}$	104.3	99.54	83.72
DISP % dQ	0	0	0
DISP swaps	0	0	0
BS mapping (%)	<60%	<75%	>80%
Unmapping	0	0	0

Table S2. Bootstrap analysis results for 9 factors (F) solution based on 20 bootstrap runs.

	F 1	F 2	F 3	F 4	F 5	F 6	F 7	F 8	F 9
Boot F 1	20	0	0	0	0	0	0	0	0
Boot F 2	0	20	0	0	0	0	0	0	0
Boot F 3	0	0	20	0	0	0	0	0	0
Boot F 4	0	0	0	20	0	0	0	0	0
Boot F 5	0	0	0	0	20	0	0	0	0
Boot F 6	0	0	0	0	0	20	0	0	0
Boot F 7	0	0	0	0	0	0	20	0	0
Boot F 8	0	0	0	0	0	0	0	20	0
Boot F 9	0	0	0	0	0	0	0	0	20

Table S3 Statistical parameters for VOCs, NO, NO₂, CO, and SO₂. VOCs are ordered according to their elution in the gas chromatogram. Data in ppb for VOCs, NO, NO_x, CO, SO₂ and µg/m³ for PM₁.

Index	Variable	Mean	SD	Median	Max	Min
1	ethane	5.63	4.67	3.86	30.6	1.1
2	ethylene	5.86	5.51	4.20	37.2	0.2
3	propane	52.05	52.80	33.27	322.1	3.0
4	propylene	2.31	2.38	1.45	16.1	0.1
5	isobutane	4.13	4.0	2.65	25.7	0.4
6	n-butane	8.65	8.55	5.48	53.7	0.8
7	acetylene	4.63	4.39	3.22	33.5	0.4
8	trans-2-butene	0.28	0.32	0.15	2.1	bdl
9	1-butene	0.36	0.34	0.25	2.3	bdl
10	cis-2-butene	0.25	0.31	0.13	2.1	bdl
11	isopentane	5.20	4.82	3.94	35.8	0.7
12	n-pentane	2.26	2.22	1.61	13.9	bdl
13	1,3-butadiene	0.26	0.27	0.17	2.0	bdl
14	trans-2-pentene	0.15	0.16	0.10	1.4	bdl
15	1-pentene	0.09	0.08	0.07	0.6	bdl
16	cis-2-pentene	0.07	0.08	0.04	0.6	bdl
17	3-methylpentane	0.62	0.57	0.47	3.6	bdl
18	isoprene	0.14	0.10	0.12	1.0	bdl
19	n-hexane	1.04	0.97	0.78	8.0	bdl
20	2,4-dimethylpentane	0.2	0.19	0.165	1.3	bdl
21	benzene	0.64	0.52	0.52	3.8	bdl
22	cyclohexane	0.25	0.23	0.19	1.8	bdl
23	2-methylhexane	0.38	0.34	0.28	2.5	bdl
24	3-methylhexane	0.41	0.37	0.30	2.9	bdl
25	2,2,4-trimethylpentane	0.78	0.73	0.55	5.0	bdl
26	n-heptane	0.55	0.53	0.4	4.4	bdl
27	toluene	5.44	4.94	3.91	44.3	0.3
28	3-methylheptane	0.1	0.09	0.08	0.7	bdl
29	n-octane	0.23	0.17	0.19	1.2	bdl
30	ethylbenzene	0.78	0.69	0.57	5.6	bdl
31	m,p-xylene	2.24	2.06	1.63	15.8	0.2
32	o-xylene	0.90	0.82	0.65	6.3	bdl
33	1,2,4-trimethylbenzene	0.50	0.41	0.39	3.1	bdl
34	CO	639.3	499.94	500	3610	10
35	NO	27.6	49.0	5.4	408	bdl
36	NO ₂	34.8	18.1	35.0	106	2
37	SO ₂	22.5	14.5	22.3	77	bdl
38	PM ₁	20.01	4.77	19.30	31.0	6.6

bdl = below detection limit; Nbdl: Number of samples bdl.