SUPPLEMENTARY MATERIAL

Volatile Organic Compounds and Carbonyls Pollution in Mexico City and an Urban Industrialized Area of Central Mexico

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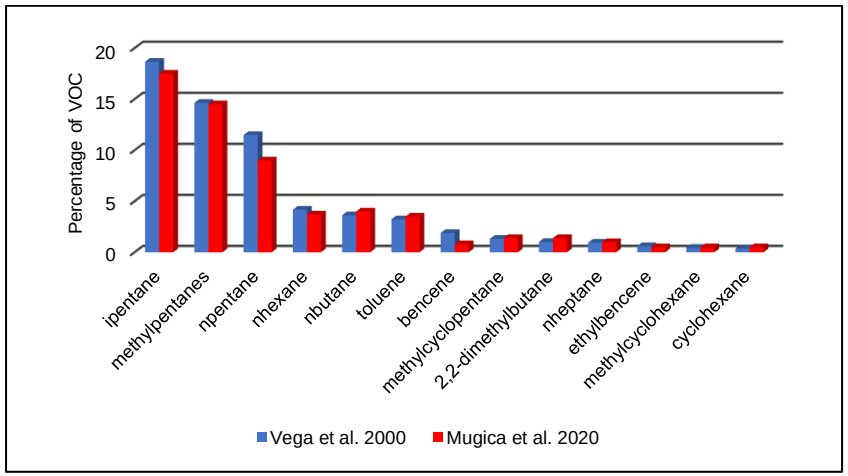

Figure S1: Comparison of VOC source profile between Mugica-Alvarez et al (2020) and Vega et al (2000).

Mugica-Alvarez, V., Martínez-Reyes, C.A., Santiago-Tello, M., Martínez-Rodríguez, I., Gutiérrez-Arzaluz, M., Figueroa-Lara, J.J., (2020). Evaporative volatile organic compounds from gasoline in Mexico City: Characterization and atmospheric reactivity. Energy Reports, 6, 825-830. doi.org/10.1016/j.egyr.2019.11.010.

Vega, E., Mugica, V., Carmona, R., Valencia, E., (2000). Hydrocarbon source apportionment in Mexico City using the chemical mass balance receptor model. Atmospheric Environment, 34, 4121-4129.

Table S1. Comparison of average carbonyl compounds (μg m^{-3}) 07:00 to 19:00 local time in the Tula industrial corridor with those reported (6:00 to 9:00 local time) in China, USA, Brazil, Greece and Mexico City.

	This study		Mexico City				Other studies			
	Industrial area		Residential 2003	Downtown 2003	Industrial 2003	Services 2003	China	USA	Brazil	Greece
Compound	JAS	TEP	Southwest	Central	Northeast	Southeast	Feng et al., 2004	Zhang et al., 1994	Gosejean et al., 2002	Bakeas et al., 2003
Formaldehyde	26.5	20.0	16.5	15.7	17.9	22.3	13.7	15.4	10.8	17.2
Acetaldehyde	14.2	13.2	7.3	7.3	7.3	10.9	8.3	4.8	10.4	15.1
Acetone	17.9	18.0	13.3	13.0	29.9	26.3	17.8	–	4.1	13.7
Propionaldehyde	1.7	1.5	9.6	7.7	10.1	11.0	1.9	3.0	1.1	2.0
Crotonaldehyde	1.1	1.4	–	–	–	–	0.15	–	0.3	1.8
2-Butanone+ Methacrolein	–	–	–	3.9	7.4	32.2	5.0	–	1.4	–
n-Butyraldehyde	–	0.2	–	–	–	–	1.4	1.5	0.5	
Benzaldehyde	–	–	–	–	–	–	1.2	1.1	1.1	1.6
Iso-Valeraldehyde	–	–	–	–	9.3	–	0.6	1.3	0.3	–
Valeraldehyde	–	–	–	–	–	–	1.0	2.8	0.3	–
o-m-p-Tolualdehyde	–	–	–	–	7.7	19.1	0.9	–	0.4	6.2
Hexaldehyde	–	0.6	–	12.5	15.4	17.9	0.4	–	0.3	3.2
∑Carbonyl compounds	61.4	54.9	46.7	60.1	105.0	139.7	52.4	29.9	31.0	60.8

Southwest, Pedregal, Residential, lightly traveled; Central, Merced, residential-commercial, heavily traveled; Northeast, Xalostoc, industrial, heavily traveled, diesel vehicles; Southeast, Iztapalapa, residential, services, heavily traveled, diesel vehicles.

Table S2. Positive Matrix Factorization (PMF) for VOCs and carbonyls at the Jasso and Tepeji sites during 2006 (07:00-19:00 LT)[a].

	F 1	%	F 2	%	F 3	%	F 4	%	F 5	%	F 6	%	F 7	%
JASSO (JAS)	Formaldehyde	6.81	Ethanol	13.42	Formaldehyde	7.29	Ethanol	10.52	Ethanol	8.43	nOctane	5.04	124TriMeBenz	10.63
	Pentane	6.80	nPentane	5.77	Acetaldehyde	6.71	Formaldehyde	4.50	Acetone	5.40	2MePentane	4.38	Isoprene	6.89
	Acetone	5.67	1Pentene	5.77	Acetone	6.23	c2Butene	4.40	Propane	5.21	iPentane	4.30	2MePentane	6.16
	Acetaldehyde	5.33	Toluene	4.94	Ethanol	5.87	Propene	4.05	Formaldehyde	5.18	nNonane	4.14	3MeHexane	6.12
	nButane	4.64	Acetone	4.45	nButane	5.05	Benzene	3.99	Acetaldehyde	4.89	nHeptane	4.05	1Bute+iButylene	5.60
	Propene	4.43	Formaldehyde	4.16	Styrene	4.80	nButane	3.97	nPentane	4.57	3MeHexane	4.00	t2Butene	4.78
	124TriMeBenz	3.84	nHexane	4.08	Toluene	3.86	Acetone	3.79	Acetylene	4.35	nHexane	3.41	Formaldehyde	4.19
	Ethane	3.75	Acetaldehyde	4.01	3MePentane	3.75	Toluene	3.75	nButane	4.18	nDecane	3.37	iPentane	4.08
	Acetylene	3.30	Propene	3.99	m/pXylene	3.66	Propane	3.61	Isoprene	4.07	Formaldehyde	3.25	nButane	3.74
	m/pXylene	3.24	iPentane	3.62	EthylBenzene	3.54	nHexane	3.54	Propene	3.40	Ethane	3.23	Toluene	3.11
	Ethylene	3.20			Propane	3.18	Acetaldehyde	3.45	Toluene	3.37	1Bute+iButylene	3.21		
	2Me2Butene	3.03					nPentane	3.32	iButane	3.00	Acetone	3.06		
											Acetaldehyde	2.97		
											m/pXylene	2.83		

SOURCE	LDV EX	OIL REF	PLAST MAN	POWER PLANT/IND SOLV	LPG/FOOD C	HDV EX	LDV EV/BIO
% contribution	13.3	15.4	14.2	13.4	18.1	19.1	6.5
Q (Robust) 343.686							
Q (true) 346.273							

TEPEJI (TEP)	iButane	7.11	Formaldehyde	6.13	c2Butene	7.29	Propene	10.44	nPentane	6.86	Ethanol	8.54	Propane	9.88
	c2Butene	6.74	Acetone	5.78	3MePentane	6.89	Propane	6.52	Ethylene	5.81	Formaldehyde	6.36	nButane	6.06
	3MePentane	6.56	nNonane	5.77	Formaldehyde	6.73	3MePentane	6.42	Ethane	4.86	Acetaldehyde	5.97	Toluene	5.55
	nButane	6.36	Acetaldehyde	4.98	Acetaldehyde	5.94	nButane	5.75	iPentane	4.75	Acetone	5.31	3MePentane	5.16
	Formaldehyde	6.31	nOctane	4.88	Acetone	5.83	Formaldehyde	5.72	nHeptane	4.29	nButane	5.06	Acetone	4.81
	Propane	5.83	Propane	4.88	c2Pentene	5.60	c2Butene	5.33	Acetaldehyde	4.06	c2Butene	4.75	Formaldehyde	4.77
	Acetone	5.70	3MePentane	4.31	Isoprene	4.81	Acetone	5.27	nHexane	4.03	Styrene	4.30	22DiMeButane	4.51
	Acetaldehyde	5.09	Crotonaldehido	4.18	iButane	4.50	Toluene	4.99	Propionaldeh	3.99	m/pXylene	4.24	c2Pentene	3.75
	Toluene	3.33	nButane	4.02	Propane	4.14	iButane	4.42	Toluene	3.74	3MePentane	3.81	Acetaldehyde	3.69
	Propene	3.23	Toluene	3.85	nButane	3.88			Acetone	3.63	iPentane	3.14	c2Butene	3.60
			Acetylene	3.71					3MePentane	3.53	nDecane	3.02	iButane	3.59
									2MePentane	3.33				

SOURCE	IND SOLV	HDV EX	LDV EV/BIO	LPG D/ IND COAT	LDV EX	PLAST MAN	LPG/FOOD C
% contribution	14.4	12.2	14.8	14.2	13.3	16.1	15.0
Q (Robust) 485.134							
Q (true) 492.211							

[a]The best solution was chosen based on the fitting criteria such as Qs values, errors, correlation coefficients between estimated and measured values, G-space, along with use of rotational tools. The physical meaning of factors is also considered. The factor profiles and contributions are derived by the PMF model minimizing the objective function Q, which is a critical parameter for PMF. The model results display two versions of Q, Q true (goodness of fit parameter calculated with all measurements), and Q robust which is calculated excluding samples not fit by the model, defined as samples for which the uncertainty-scales residuals > 4. Q robust is used as a critical parameter for choosing the optimal run from the multiple runs.

Table S3. Positive Matrix Factorization (PMF) for VOCs at the Jasso and Tepeji sites during 2006 (07:00-19:00 LT).

	F 1	%	F 2	%	F 3	%	F 4	%	F 5	%	F 6	%	F 7	%
JASSO (JAS)	124TriMeBenzene	10.30	Ethanol	26.80	Propane	8.89	Ethanol	25.90	Propane	10.64	nOctane	6.83	Ethanol	14.62
	nButane	8.09	Toluene	9.60	Ethanol	7.41	c2Butene	8.79	Ethanol	8.80	iPentane	6.13	nPentane	8.32
	iPentane	6.90	t2Butene	6.28	Toluene	5.42	iPentane	6.14	3MeHeptane	7.51	nHexane	5.37	124TriMeBenzene	5.21
	Propane	6.89	iPentane	5.61	Styrene	4.93	Benzene	4.42	Acetylene	6.75	nPentane	4.97	iPentane	4.97
	Acetylene	6.51	Propene	5.56	m/pXylene	4.45	Propene	3.92	nButane	6.52	nNonane	4.88	1Butene+iButylene	4.64
	Toluene	5.22	nHexane	5.06	iButane	4.38	nButane	3.85	2Me2Butene	6.09	nHeptane	4.84	Isoprene	3.94
	Propene	4.28			2MePentane	4.38	Toluene	3.84	Toluene	4.99	Ethane	4.67	c2Butene	3.57
	Ethane	3.78			iPentane	4.35			iButane	4.42	Propene	4.48	Toluene	3.23
	m/pXylene	3.70			3MePentane	4.11					nDecane	4.37	CycloHexane	2.99
					nButane	3.94					MeCyHexane	4.06	iButane	2.88
					3MeHexane	3.83					Ethanol	3.38		

SOURCE	LDV EX	OIL REF	PLAST MAN	IND SOLV	LPG/FOOD C	HDV EX	LDV EV/BIO
% contribution	12.6	13.9	19.9	9.3	14.7	17.3	12.3
Q (robust)288.103							
Q (true) 300.041							

TEPEJI (TEP)	c2Butene	10.31	Propane	10.95	c2Pentene	8.83	Propene	16.61	nPentane	8.39	Ethanol	12.65	Propane	9.08
	3MePentane	9.37	nNonane	7.89	Propane	8.33	Propane	9.17	Ethane	6.61	c2Butene	7.76	3MePentane	8.89
	Propene	8.94	nOctane	7.87	3MePentane	7.30	3MePentane	8.50	Ethylene	6.58	Styrene	7.43	iPentane	8.49
	iButane	8.13	c2Butene	7.28	nButane	6.34	nButane	8.28	iPentane	6.14	3MePentane	7.20	c2Butene	8.45
	nButane	6.26	iButane	4.56	Toluene	6.01	iButane	8.13	nHexane	5.55	nButane	6.32	nButane	8.27
	Propane	4.28	nButane	4.43	c2Butene	5.86	c2Butene	6.88	2MePentane	4.96	m/pXylene	5.66	Toluene	5.08
	Toluene	4.11	Acetylene	4.14	Isoprene	4.16	Toluene	5.11	nHeptane	4.92	Propene	5.60	22DiMeButane	4.54
	m/pXylene	3.96	nDecane	3.94	iPentane	3.97			Toluene	4.29			iButane	3.43
			Toluene	3.78	Ethanol	3.84			Ethanol	3.94				
									MeCyHexane	3.69				

SOURCE	IND SOLV	HDV EX	LDV EV/BIO	LPG D	LDV EX	PLAST MAN	LPG/FOOD C
% contribution	11.9	18.4	15.0	9.5	20.6	12.2	12.3
Q (robust) 370.097							
Q (true) 419.221							

Table S4. Positive Matrix Factorization (PMF) for VOCs in Mexico City at the Merced (MER) and Pedregal (PED) sites during 2006 (00:00-24:00 LT).

	F 1	%	F 2	%	F 3	%	F 4	%	F 5	%	F 6	%
MER	m-diethylbenz	18.09	C-2-butene	4.35	Propane	5.93	Octane	5.43	Propane	7.91	Propane	4.77
2006	1,2,3trimetben	12.88	1-penteno	3.99	Etylene	5.29	1,3,5-Trimetbenz	5.20	Ethylene	5.67	Propylene	3.92
	Toluene	3.31	Propylene	3.61	iPentane	5.09	Styrene	4.20	n-butane	5.33	ipropylben	3.82
	Hexane	3.28	1-Hexene	3.53	n-butane	4.56	Nonane	4.16	1-Pentene	5.03	Decane	3.78
	Propane	2.75	T-2-Butene	3.51	Toluene	4.51	o-ethyltol	4.09	iPentane	4.66	n-Butane	3.78
	1-pentene	2.62	1,2,3-Trimetbenz	3.34	Ethane	4.22	m-xylene	3.97	Propylene	4.44	1-pentene	3.60
	Propylene	2.50	Toluene	3.31	ibutane	4.20	2,3,4-trimethylpent	3.86	Toluene	4.13	C-2-butene	3.51
	n-butane	2.44	T-2-Pentene	3.30	p-xylene	3.89	Decane	3.79	iButane	4.11	Toluene	3.49
	o-xylene	2.36	Propane	3.25	Acethylene	3.67	p-xylene	3.76	Ethane	4.04	iButane	3.35
	iPentane	2.35	iButane	3.05	Propylene	3.29	Ethylbenz	3.33	Benzene	3.90	o-xylene	3.27
	2,3-dimetlbut	2.18	p-xylene	2.78	1-Pentene	3.25	Methylcyclohexa	3.15	C-2-Butene	3.42	m-ethyltol	3.25
	p-xylene	2.10	2,2,4-trimethylpent	2.71	C-2-Butene	3.12	Ethane	3.07	Acethylene	2.68	p-xylene	3.08
			1-Butene	2.65	Benzene	2.99	2-Methylhepta	3.03			Ethylbenz	2.88
			Ethylbenz	2.60			m-ethyltol	3.01			Hexane	2.71
			2,3-dimethylpent	2.44			Toluene	2.76			iPentane	2.61
			2,3-dimethylbut	2.40							Acethylene	2.56
			Hexane	2.37								
SOURCE	IND SOLV		LDV EV		LDV EX		HDV EX/ PLAST MAN		FOOD C		LPG	
% contribution	13.79		12.90		24.31		11.57		18.50		18.94	
Q (robust) 584.273												
Q (true) 655.241												
PED	1-pentene	5.01	Propane	6.69	1,2,3-trimetbenz	6.74	Propane	6.85	Propane	5.40	Propane	7.87
2006	m-diethylbenz	4.84	Propylene	5.23	1,3,5-trimetbenz	5.16	Propylene	5.57	Propylene	4.78	Toluene	7.39
	o-xylene	4.05	Toluene	5.00	iPentane	4.80	Toluene	5.30	Ethylene	4.34	Propylene	6.63
	Propane	3.97	Hexane	4.97	ipropylbenz	4.61	n-Butane	4.51	Toluene	4.07	C-2-butene	6.18
	Ethylene	3.75	iPentane	4.75	Propane	4.40	C-2-butene	4.14	Styrene	4.06	iButane	4.96
	Acethylene	3.72	1-pentene	4.42	n-propylbenz	3.64	Hexane	4.10	iButane	4.05	Acethylene	4.95
	1,2,4trimetben	3.36	iButane	4.22	1-pentene	3.61	Acethylene	3.62	C-2-butene	3.54	Ethylene	4.93
	o-ethyltol	3.31	1,3,5-trimetbenz	3.74	Ethylbenz	3.58	iButane	3.46	Benzene	3.15	Ethane	4.28
	Propylene	3.27	n-Butane	3.65	Toluene	3.15	iPentane	3.41	Ethane	3.14	Decane	3.89
	1,3,5trimetben	3.16	p-diethylbenz	3.24	o-xylene	2.80	Ethane	3.37	Hexane	3.10	p-xylene	3.72
	Toluene	3.05	1,2,3-trimetbenz	2.77	Decane	2.75	2,3-dimethylbut	3.29	Acethylene	3.04		
	p-xylene	2.90	1-Hexene	2.75	Propylene	2.74	Ethylene	3.03	1-pentene	2.98		
	ipropylbenz	2.88	Benzene	2.73	o-ethyltol	2.74	p-xylene	3.02	m-xylene	2.90		
	C-2-butene	2.82	Ipropylbenz	2.71	p-xylene	2.71	o-xylene	2.82	Ethylbenz	2.81		
SOURCE	LDV EX		IND SOLV/COAT		LDV EV		LPG/FOOD C		IND ASPH		HDV EX	
% contribution	18.91		14.88		13.99		21.43		19.69		11.09	
Q (robust) 662.772												
Q (true) 735.918												

Table S5. Positive Matrix Factorization (PMF) for VOCs in Mexico City at the Merced (MER) and Pedregal (PED) sites during 2012 (00:00-24:00 LT).

	F 1	%	F 2	%	F 3	%	F 4	%	F 5	%
MER	Propane	10.86	Propane	8.58	Propane	12.71	1,2,4-trimetilbenceno	13.76	Propane	7.54
2012	Toluene	9.25	iPentane	7.96	Propylene	10.43	o-xileno	8.01	Toluene	7.52
	n-Butane	8.46	n-Butane	7.89	n-Butane	8.07	etilbenceno	7.24	Ethylene	7.26
	Hexane	8.37	iButane	6.08	Ethylene	7.95	m-xileno	6.44	n-Butane	7.14
	iPentane	6.67	Toluene	5.95	Ethane	7.85	iButane	6.36	Propylene	6.87
	1,2,4-trimethylbenz	6.29	Ethane	5.91	iPentane	7.61	Propane	5.95	iPentane	6.70
	Propylene	6.00	Ethylene	5.61	Toluene	7.08	Toluene	5.83	Ethane	5.71
	iButane	5.64	2,3,4-trimethylpent	5.05			n-Butane	4.47	Hexane	5.54
									1-Butene	5.04
SOURCE	LPG/LDV EV		LDV EX		HDV EX		IND SOLV		FOOD C	
% contribuion	17.45		29.70		10.96		17.68		24.21	
Q (robust) 109.541										
Q (true) 106.101										
PED	Toluene	8.09	Propane	10.98	Propane	16.10	Propane	10.07	Propane	8.82
2012	Hexane	6.82	iPentane	9.16	n-Butane	10.40	n-Butane	8.39	n-Butane	7.88
	m-xylene	6.45	Toluene	8.30	Propylene	8.64	Toluene	7.41	iPentane	6.52
	2,2,4-trimethylpent	6.01	n-Butane	7.82	Ethane	8.01	Ethylene	7.15	Isoprene	6.26
	Ethylbenz	5.96	Ethane	7.28	Toluene	7.22	Ethane	6.97	Toluene	5.59
	o-xylene	5.88	Ethylene	7.12	Ethylene	6.61	Hexane	6.96	iButane	5.42
	Propane	5.88	2,2,4-trimethylpent	6.67			Propylene	6.80	T-2-butene	5.08
	n-Butane	5.59							C-2-butene	5.04
	Benzene	5.52							1,2,4-trimetbenz	4.54
SOURCE	IND SOLV		LDV EX		LPG/HDV EX		FOOD C		LDV EV/BIO	
% contribution	14.80		15.57		15.55		29.29		24.79	
Q (robust) 138.139										
Q (true) 136.244										

Table S6. Exposure concentration (EC), Lifetime Cancer Risk (LCR), and Hazard Quotient (HQ) for BTEX in different sites in Mexico.

	EC (μg/m^3)		LCR		HQ		EC (μg/m^3)		LCR		HQ	
			Tepeji (TEP) 2006						Jasso (JAS) 2006			
Element	Children	Adults	Children	Adults	Children	Adults	Children	Adults	Children	Adults	Children	Adults
Benzene	0.06	0.25	1.8E-06	7.3E-06	0.002	0.008	0.29	1.17	8.5E-06	3.4E-05	0.010	0.039
Toluene	0.21	0.83	N/A	N/A	0.000	0.000	0.06	0.25	N/A	N/A	0.000	0.000
EthylBenzene	0.05	0.21	1.3E-07	5.3E-07	0.000	0.000	0.18	0.73	4.6E-07	1.8E-06	0.000	0.001
Xylenes	0.15	0.61	N/A	N/A	0.002	0.006	0.25	1.00	N/A	N/A	0.003	0.010
			HI		0.004	0.015			HI		0.012	0.050
			Merced (MER) 2006						Pedregal (PED) 2006			
Benzene	0.52	2.09	1.5E-05	6.1E-05	0.017	0.070	0.28	1.14	8.2E-06	3.3E-05	0.009	0.038
Toluene	2.49	9.97	N/A	N/A	0.000	0.002	1.79	7.18	N/A	N/A	0.000	0.001
EthylBenzene	0.68	2.74	1.7E-06	6.8E-06	0.001	0.003	0.31	1.25	7.8E-07	3.1E-06	0.000	0.001
Xylenes	2.16	8.66	N/A	N/A	0.022	0.087	0.99	3.95	N/A	N/A	0.010	0.039
			HI		0.040	0.161			HI		0.019	0.075
			Merced (MER) 2012						Pedregal (PED) 2012			
Benzene	0.30	1.21	8.8E-06	3.5E-05	0.010	0.040	0.19	0.76	5.5E-06	2.2E-05	0.006	0.025
Toluene	2.26	9.05	N/A	N/A	0.000	0.002	0.99	3.97	N/A	N/A	0.000	0.001
EthylBenzene	0.23	0.90	5.6E-07	2.3E-06	0.000	0.001	0.12	0.47	2.9E-07	1.2E-06	0.000	0.000
Xylenes	0.64	2.55	N/A	N/A	0.006	0.025	0.23	0.90	N/A	N/A	0.002	0.009
			HI		0.017	0.069			HI		0.009	0.036