Supplement of

Evaluating the sensitivity of fine particulate matter (PM$_{2.5}$) simulations to chemical mechanism in Delhi

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35   **Table S1:** Selected atmospheric physical and chemical parameterizations

Atmospheric Process	Parameterization
Cloud Microphysics	Marrison 2-mom scheme (Marrison et al., 2009)
Short- and Long-wave radiation	Rapid Radiative Transfer Model for GCMs (Iacono et al., 2008)
Surface Layer	Monin-Obukhov (Janjic Eta)Scheme (Janjic, 1996, 2002)
Land Surface model	Unified Noah Land-surface model (Tewari et al., 2004)
Planetary Boundary Layer	BouLac TKE (Bougeault and Lacarrere, 1989)
Cumulus	Grell-Freitas ensemble scheme (Grell&Freitas, 2014)
Gas-phase Chemistry	Model for Ozone and Related Tracers (Emmons et al., 2010) and Carbon Bond 5 (CB05) (Yarwood et al., 2005)
Aerosol Processes	Goddard Global Ozone Chemistry Aerosol Radiation and Transport (GOCART) (Chin et al., 2000), Model for Simulating Aerosol Interactions and Chemistry/ Volatility Basis Set (MOSAIC) (Zaveri et al., 2008) and Modal Aerosol Dynamics Model for Europe/Secondary Organic Aerosol Model(MADE/SORGAM) (Ahmadov et al., 2012)

Table S2: Air pollution monitoring stations

State	Station name	Latitude	Longitude	Measurements
Delhi	AnandVihar	28.646835	77.316032	$PM_{2.5}$
	Aya Nagar	28.4706914	77.1099364	$PM_{2.5}$
	Burari Crossing	28.7256504	77.2011573	$PM_{2.5}$
	CRRI Mathura	28.5512005	77.2735737	$PM_{2.5}$
	DTU	28.7500499	77.1112615	$PM_{2.5}$
	IGI-Airport-T3	28.5627763	77.1180053	$PM_{2.5},$ $SO_4, NO_3,$ $NH_4,$ CL, BC,OC, O_3, NH_3, SO_2
	IHBAS-Dilshad-Garden	28.6811736	77.3025234	$PM_{2.5}$
	ITO	28.6316945	77.2494387	$PM_{2.5}$
	Lodhi Road	28.5918245	77.2273074	$PM_{2.5}$
	MandirMarg	28.636429	77.201067	$PM_{2.5}$
	North Campus DU	28.6573814	77.1585447	$PM_{2.5}$
	NSIT Dwarka	28.60909	77.0325413	$PM_{2.5}$
	Punjabi Bagh	28.563262	77.186937	$PM_{2.5}$
	Pusa IMD	28.639645	77.146263	$PM_{2.5}$
	R. K. Puram	28.674045	77.131023	$PM_{2.5}$
	Shadipur	28.6514781	77.1473105	$PM_{2.5}$
	Sirifort	28.5504249	77.2159377	$PM_{2.5}$
Punjab	Amritsar-Golden	31.62	74.876512	$PM_{2.5}$
	Ludhiana-Agricultural-University	30.9028	75.8086	$PM_{2.5}$
	Gobindgarh RIMT, Mandi	30.649961	76.331442	$PM_{2.5}$
Haryana	Sector- 16A, Faridabad	28.4088421	77.3099081	$PM_{2.5}$
	VikasSadan, Gurugram	28.4501238	77.0263051	$PM_{2.5}$
	Sector-6 Panchkula	30.7057778	76.8531805	$PM_{2.5}$
	MD University, Rohtak	28.870083	76.620500	$PM_{2.5}$
Uttar Pradesh	Sanjay Palace, Agra	27.1986583	78.0059806	$PM_{2.5}$
	Vasundhara, Ghaziabad	28.6603346	77.3572563	$PM_{2.5}$
	Nehru Nagar, Kanpur	26.4703136	80.3229863	$PM_{2.5}$
	Central School Lucknow	26.8821003	80.9302753	$PM_{2.5}$
	Lajpat Nagar, Moradabad	28.825341	78.7213009	$PM_{2.5}$
	Sector -62 Noida	28.6245479	77.3577104	$PM_{2.5}$
	Ardhali Bazar, Varanasi	25.3505986	82.9083074	$PM_{2.5}$
Rajasthan	MotiDoongri, Alwar	27.554793	76.611536	$PM_{2.5}$
	RIICO Ind., Bhiwadi	28.194909	76.862296	$PM_{2.5}$
	Adarsh Nagar, Jaipur	26.902909	75.836853	$PM_{2.5}$
	Collectorate, Jodhpur	26.268249	73.0193853	$PM_{2.5}$
	Police Commissionerate, Jaipur	26.9164092	75.7994901	$PM_{2.5}$
	Shastri Nagar, Jaipur	26.9502929	75.730943	$PM_{2.5}$
	ShrinathPuram, Kota	25.14389	75.821256	$PM_{2.5}$
	Indira Vistar, Pali	25.771061	73.340227	$PM_{2.5}$
	Ashok Nagar, Udaipur	24.5886166	73.6321397	$PM_{2.5}$

Table S3: Index of Agreement (IOA), mean bias (MB), normalized mean bias (NMB), and root mean squared error (RMSE) of hourly values of $PM_{2.5}$ for the MOZART-GOCART (MG), MOZART-MOSAIC (MM), and CB05-MADE/SORGAM(CMS) mechanisms over Delhi.

	State	Stations	MOZART-GOCART				MOZART-MOSAIC				CB05-MADE/SORGAM			
			MB	NMB (%)	RMSE	IOA	MB	NMB (%)	RMSE	IOA	MB	NMB (%)	RMSE	IOA
$PM_{2.5}$	Delhi	AnandVihar	-186.7	-65.0	231.1	0.50	-96.9	-33.7	167.9	0.65	-108.2	-37.7	175.2	0.64
		AyaNagar	-75.3	-51.5	98.2	0.51	-24.5	-16.7	79.45	0.65	-46.9	-32.1	85.1	0.62
		BurariCrossing	-42.8	-32.0	76.0	0.53	33.2	24.9	105.0	0.54	14.9	11.1	100.2	0.55
		CRRI Mathura	-85.3	-45.9	126.9	0.54	-3.6	-1.9	115.5	0.70	-13.6	-7.3	122.9	0.69
		DTU	-206.5	-72.3	256.0	0.46	-136.6	-47.9	203.0	0.52	-157.9	-55.3	216.7	0.51
		IHBAS Dilshad	-23.7	-19.3	58.8	0.62	64.1	52.3	128.2	0.46	52.3	42.6	125.3	0.46
		ITO	-97.2	-49.0	131.1	0.50	-14.6	-7.3	124.2	0.59	-24.0	-12.1	133.9	0.58
		LodhiRoad	-70.6	-41.8	113.4	0.51	8.2	4.8	123.1	0.58	-3.5	-2.1	130.5	0.56
		MandirMarg	-115.2	-56.3	147.3	0.50	-39.5	-19.3	119.8	0.62	-58.8	-28.7	125.3	0.61
		North Campus DU	-98.4	-52.5	141.1	0.51	-23.7	-12.6	122.9	0.60	-42.8	-22.8	127.1	0.59
		NSIT Dwarka	-120.6	-60.1	143.0	0.47	-58.9	-29.4	112.8	0.58	-81.9	-40.8	121.3	0.56
		Punjabi Bagh	-155.5	-64.0	193.6	0.49	-89.4	-36.8	150.3	0.62	-103.5	-42.6	160.3	0.61
		PusaIMD	-36.4	-29.2	69.4	0.60	36.3	29.2	102.9	0.57	18.1	14.5	96.6	0.58
		RKPuram	-127.3	-58.7	156.2	0.50	-50.9	-23.5	117.9	0.66	-69.3	-31.9	127.0	0.63
		Shadipur	-96.6	-52.1	142.0	0.50	-21.4	-11.5	122.0	0.63	-40.3	-21.7	125.5	0.62
		Sirifort	-124.6	-58.3	157.3	0.48	-56.7	-26.5	128.7	0.59	-75.4	-35.3	137.6	0.57
		Average	**-100.9**	**-52.9**	**146.3**	**0.50**	**-27.0**	**-14.1**	**127.3**	**0.61**	**-43.7**	**-22.9**	**133.1**	**0.59**

Table S4: Index of Agreement (IOA), mean bias (MB), normalized mean bias (NMB), and root mean squared error (RMSE) of hourly values of PM$_{2.5}$ for the MOZART-GOCART (MG), MOZART-MOSAIC (MM), and CB05-MADE/SORGAM (CMS) mechanisms over Punjab, Haryana, Uttar Pradesh, and Rajasthan.

	State	Stations	MOZART-GOCART				MOZART-MOSAIC				CB05-MADE/SORGAM			
			MB	NMB (%)	RMSE	IOA	MB	NMB (%)	RMSE	IOA	MB	NMB (%)	RMSE	IOA
PM$_{2.5}$	Punjab	Amritsar	-26.6	-30.1	54.0	0.46	19.6	22.2	56.3	0.53	4.7	5.3	47.3	0.59
		Ludhiana Agri. Uni.	-19.8	-24.4	46.0	0.39	15.7	19.4	49.7	0.44	7.6	9.4	45.5	0.47
		Gobindgarh RIMT	-31.6	-38.2	60.1	0.40	-3.9	-4.8	51.8	0.42	-14.9	-18.1	54.2	0.34
		Average	**-24.7**	**-29.4**	**52.1**	**0.42**	**13.1**	**15.5**	**52.6**	**0.48**	**1.9**	**2.2**	**48.1**	**0.51**
	Haryana	Sector- 16A	-114.3	-62.6	237.6	0.28	-61.7	-33.8	219.1	0.30	-83.2	-45.5	227.9	0.29
		VikasSadan	-82.4	-58.1	105.7	0.48	-39.7	-28.0	80.8	0.58	-57.4	-40.5	88.0	0.56
		Sector-6 Panchkula	-56.7	-62.4	68.2	0.41	-44.2	-48.7	60.5	0.41	-49.1	-54.1	62.4	0.42
		MD University	-73.1	-55.4	91.1	0.46	-29.2	-22.1	69.1	0.51	-44.2	-33.5	74.6	0.50
		Average	**-82.7**	**-59.6**	**144.7**	**0.35**	**-43.7**	**-31.5**	**128.1**	**0.41**	**-58.9**	**-42.4**	**134.2**	**0.39**
	Uttar Pradesh	Sanjay Palace	-147.1	-71.1	173.3	0.45	-90.8	-43.6	137.4	0.47	-127.8	-61.8	154.9	0.49
		Vasundhara	-195.0	-65.4	241.2	0.49	-100.0	-33.4	214.3	0.44	-106.1	-35.6	179.3	0.63
		Nehru Nagar	-176.5	-73.2	225.2	0.43	-112.1	-46.2	186.3	0.44	-158.0	-65.5	208.9	0.45
		Central School Lucknow	-95.8	-59.3	120.1	0.43	-34.1	-21.0	97.1	0.41	-79.4	-49.1	106.9	0.45
		Lajpat Nagar	-93.3	-61.4	164.1	0.40	-53.9	-35.3	142.1	0.41	-75.4	-49.6	155.3	0.37
		Sector -62 Noida	-13.6	-11.7	69.3	0.58	74.4	63. 4	157.2	0.34	71.5	61.2	150.9	0.47
		Ardhali Bazar	-134.1	-63.1	186.1	0.47	-64.1	-30.0	150.0	0.44	-101.9	-47.9	161.7	0.49
		Average	**-126.5**	**-62.2**	**180.8**	**0.45**	**-58.4**	**-28.5**	**162.3**	**0.45**	**-84.6**	**-42.3**	**162.8**	**0.52**
	Rajasthan	MotiDoongri, Alwar	-46.9	-50.2	71.2	0.46	-19.8	-21.2	59.3	0.52	-34.0	-36.4	61.4	0.51
		RIICO Ind., Bhiwadi	-124.6	-70.0	148.0	0.43	-88.4	-49.7	118.8	0.48	-107.2	-60.2	132.3	0.46
		Adarsh Nagar, Jaipur	-11.7	-19.8	29.0	0.47	20.8	35.2	45.7	0.38	1.8	3.0	27.9	0.49
		Collectorate, Jodhpur	-73.9	-63.3	90.7	0.39	-47.3	-40.6	75.7	0.39	-66.7	-57.1	85.1	0.40
		Police Commi., Jaipur	-49.8	-48.3	68.1	0.46	-9.6	-9.3	56.3	0.52	-36.8	-35.7	59.7	0.47
		Shastri Nagar, Jaipur	-42.6	-46.9	104.9	0.28	-9.0	-9.9	98.0	0.34	-29.5	-32.5	100.8	0.25
		ShrinathPuram, Kota	10.4	15.5	52.9	0.44	80.1	119.0	108.8	0.39	79.1	118.2	116.1	0.36
		Indira Vistar, Pali	-49.8	-54.5	105.1	0.29	-24.3	-26.6	97.0	0.26	-36.1	-39.5	99.0	0.26
		Ashok Nagar, Udaipur	-39.6	-48.7	66.3	0.38	-18.5	-22.8	60.2	0.35	-25.0	-30.8	60.0	0.34
		Average	**-43.1**	**-45.9**	**84.9**	**0.36**	**-7.6**	**-8.1**	**83.5**	**0.37**	**-22.3**	**-23.8**	**87.5**	**0.32**