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*Supplement of*

## **A new method to determine the aerosol optical properties from multiple-wavelength $O_4$ absorptions by MAX-DOAS observation**

**Chengzhi Xing et al.**

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**Table S1. Discussion of break points based on  $\sigma_{sca}$** 

Date	Breakpoint	$v_{sca}$	$a_{sca}$	$a'_{sca}$
2016/11/01	09:00	-113.22	-2076.08	-28172.69
	12:00	-45.88	841.84	36474.01
	14:00	251.89	2836.27	31514.06
	16:00	-200.00	-5648.61	-106060.96
2016/11/02	10:00	-3.25	2459.38	101349.83
	16:00	5.33	95.37	-26266.72
2016/11/03	12:00	11.67	-1012.04	-24508.74
	14:00	469.75	5841.20	73018.74
2016/11/04	11:00	35.89	-4820.68	-118465.30
	14:00	-12.88	-609.55	52639.13
	16:00	233.25	3003.13	37469.62
2016/11/05	10:00	-138.25	-4643.75	-95585.94
	12:00	16.33	1717.59	70681.58
2016/11/06	10:00	24.50	102.08	-20193.87
	12:00	27.00	-1148.61	-30649.40
	16:00	-224.50	-2718.75	-28671.88
2016/11/07	09:00	-65.33	1768.52	49858.54
2016/11/08	09:00	247.00	3015.63	26588.54
	11:00	60.67	-2070.37	-56511.06
	14:00	138.25	1753.13	21601.56
2016/11/09	10:00	-124.67	-2921.30	-51938.01
2016/11/10	11:00	-9.63	1438.02	54491.46
	14:00	-52.89	1333.18	22417.27
2016/11/11	12:00	166.75	2400.00	33650.17
	14:00	-189.33	-3956.48	-70627.57
	15:00	-34.38	1936.98	73668.26
2016/11/12	09:00	-9.25	314.06	-20286.46
	12:00	208.75	2770.31	35963.54
	14:00	-192.67	-4460.19	-80338.86
2016/11/13	09:00	-15.25	2217.71	83473.67
	10:00	-10.00	65.63	-26901.04
2016/11/14	09:00	338.38	4449.13	64797.21
	13:00	-31.25	-4620.31	-113368.06
	15:00	9.11	448.46	56319.66
2016/11/15	10:00	-944.22	-10617.75	-118634.69
	12:00	1064.38	25107.47	446565.15
	15:00	-6.88	-13390.63	-481226.13
2016/11/16	11:00	-6.22	7.25	148865.31
	13:00	-139.89	-2458.49	-38427.64
2016/11/17	13:00	-109.38	381.42	35498.89
	14:00	15.56	2127.01	32869.51
2016/11/18	10:00	53.75	477.43	-20619.70
2016/11/19	10:00	-121.50	-3965.97	-72686.15
	12:00	-69.00	687.50	20243.06
	13:00	-149.25	-2110.94	-40234.38

	15:00	-141.78	83.02	24377.36
2016/11/20	09:00	-4.50	1300.00	26883.68
2016/11/21	09:00	28.00	-1298.61	-25331.79
	11:00	-17.67	1073.15	20691.23
	12:00	-22.13	1034.55	24235.87
2016/11/23	10:00	157.50	1959.38	23697.92
	12:00	60.56	-1077.16	-33739.28
	15:00	39.50	1345.14	25406.06
	16:00	18.13	-267.19	-20154.08
2016/11/24	09:00	31.38	-1387.50	-33513.45
2016/11/25	10:00	244.38	2992.19	33999.57
	12:00	5.78	-2651.08	-62702.97
	13:00	7.25	18.40	33368.54
	15:00	84.56	3935.34	70635.72
2016/11/26	12:00	-23.25	-1347.57	-66036.36
	14:00	-170.50	-2007.81	-24943.58
2016/11/27	10:00	-6.22	1825.31	42590.23
	12:00	-23.00	788.89	20918.21
	16:00	-37.33	728.24	21754.76
2016/12/05	09:00	-53.25	-4481.25	-84058.16
	11:00	-57.44	-46.60	49273.83
	13:00	188.63	2240.63	28174.91
2016/12/06	10:00	35.67	-1699.54	-43779.58
	12:00	796.00	9351.39	108539.74
	15:00	204.88	-7389.06	-209255.64
2016/12/07	10:00	154.11	-564.04	75833.55
	15:00	50.63	1598.44	20852.86
2016/12/08	11:00	-15.89	-739.04	-25972.01
	12:00	5.63	-1411.63	-22097.56
	15:00	-6.00	-2081.94	-29608.41
2016/12/10	10:00	-5.50	6.25	26102.43
	13:00	48.89	-819.29	-25127.53
	15:00	54.44	-1581.17	-31700.53
2016/12/11	10:00	-33.13	1348.44	32706.16
	14:00	-142.25	604.69	29583.33
2016/12/17	11:00	812.88	10113.64	126417.88
	14:00	-30.56	-9371.45	-216501.02
	15:00	-26.00	56.94	117854.94
2016/12/18	12:00	21.33	1373.15	29146.09
	13:00	45.00	-931.25	-28819.44
	15:00	455.13	5102.95	58767.60
2016/12/19	11:00	-12.89	-33.49	26850.14
	14:00	25.00	1231.94	24191.74
	15:00	-9.38	-1620.31	-36994.36
2016/12/20	13:00	17.11	294.29	21273.36
	15:00	-39.78	741.36	22612.31
2016/12/21	11:00	8.88	1195.31	26499.57

2016/12/22	10:00	46.38	2667.19	41325.95
	12:00	48.75	29.69	-32968.75
	15:00	31.13	918.23	23104.02
2016/12/23	10:00	-74.38	-1942.19	-36048.18
	12:00	5.63	1000.00	36777.34
2016/12/24	10:00	171.38	2067.19	29572.48
	12:00	-17.25	-2357.81	-55312.50
2016/12/30	09:00	17.67	387.96	30508.62
	10:00	27.13	-1229.69	-26265.19
	16:00	-143.50	-1822.92	-21617.48
2016/12/31	12:00	19.75	2040.63	48294.27
2017/01/01	11:00	-35.67	-615.74	-29515.17
2017/01/02	09:00	-276.50	-3384.38	-46979.17
	10:00	102.22	4208.02	84360.00
	12:00	25.50	-959.03	-64588.16
	15:00	-31.50	-2521.88	-47673.61
2017/01/03	09:00	-8.11	259.88	30908.35
	13:00	27.50	-1125.69	-20762.92
	15:00	-263.13	-4725.17	-73129.10
2017/01/04	11:00	-66.00	2464.06	89865.45
	16:00	239.63	2785.59	34173.66
2017/01/05	11:00	59.50	-2251.56	-62964.41
	14:00	-794.56	-9489.51	-80421.60
2017/01/06	09:00	-3052.13	-28219.62	-234126.40
	11:00	1424.25	55954.69	1052178.82
	14:00	2286.56	9581.17	-515261.27
2017/01/07	11:00	-36.00	-29031.94	-482663.97
2017/01/08	10:00	-15.50	256.25	366102.43
	12:00	205.89	2154.32	27200.79
	13:00	75.25	-1632.99	-47341.34
	15:00	13.11	-1868.21	-35410.67
2017/01/09	13:00	3.38	-121.70	21831.36
	15:00	80.50	1760.94	27539.06
2017/01/11	09:00	31.56	-543.83	-25608.50
	10:00	-125.75	-3064.93	-54310.86
	12:00	-31.38	4570.31	67771.27
2017/01/12	10:00	105.63	1712.50	-35722.66
	12:00	-158.88	-1903.99	-21708.86
	15:00	-23.75	1689.06	44913.19
2017/01/14	09:00	-18.13	1330.38	31759.02
2017/01/15	09:00	-82.25	-1462.85	-23063.75
	11:00	-20.88	767.19	27875.43
	14:00	-12.50	-656.25	-26831.60
2017/01/16	09:00	42.13	1640.63	21516.93
	11:00	10.56	-350.77	-22126.63
	14:00	219.88	2616.49	37090.81
2017/01/17	09:00	-137.63	-4468.75	-88565.54

	14:00	-5.33	1469.91	65985.08
2017/01/18	11:00	52.13	723.44	24229.60
	14:00	6.13	-2284.38	-45305.99
	16:00	-529.89	-5955.71	-40792.61
2017/01/19	10:00	-349.25	2257.99	102671.20
	12:00	-277.89	-1073.77	-35264.06
	16:00	-86.00	2398.61	43404.71
2017/01/20	10:00	-85.00	12.50	-29826.39
	12:00	-292.56	-2306.17	-25763.03
	15:00	-98.50	2425.69	59148.34
2017/01/21	10:00	-41.13	717.19	-21356.34
	12:00	-220.75	-2500.00	-30056.42
	15:00	-139.78	899.69	37774.35
2017/01/22	11:00	-464.00	-4052.78	-61905.86
	16:00	-593.25	-1615.63	30464.41
2017/01/23	11:00	-333.11	2890.43	50067.30
	14:00	-870.63	-6718.92	-120116.95
	16:00	-716.63	1925.00	108049.05
2017/01/24	11:00	-117.56	6656.33	52570.30
	14:00	-50.13	842.88	-72668.07
2017/01/25	11:00	-173.75	-1806.25	-20629.34
2017/01/26	11:00	-83.33	1004.63	31232.00
	14:00	-135.25	-648.96	-20669.85
	16:00	-215.78	678.86	27213.01
2017/01/27	10:00	-63.88	571.01	20825.86
	13:00	-56.63	714.06	21161.02
	15:00	10.38	581.08	20386.53
	16:00	199.67	2154.63	24582.69
2017/01/28	11:00	2796.38	32458.85	378802.81
	13:00	1290.25	-18826.56	-641067.71
2017/01/29	09:00	506.44	-8708.95	112417.91
	11:00	159.13	-4341.49	54593.22
	14:00	149.00	-126.56	52686.63
2017/01/31	13:00	-930.38	-11457.81	-140588.11
	15:00	-2374.11	-16041.51	-50930.00
2017/02/01	16:00	-1244.63	14118.58	377001.11
2017/02/02	11:00	-1079.00	2070.31	-150603.30
	14:00	-471.78	6746.91	51962.23
2017/02/03	10:00	-239.63	2901.91	-48062.55
	11:00	-138.88	1259.38	-20531.68
	13:00	1431.00	17842.75	223004.05
	15:00	56.44	-15272.84	-367951.05
2017/02/04	10:00	88.38	399.13	195899.64
2017/02/07	10:00	25.67	-993.98	-24863.68
	12:00	-253.88	-2596.88	-21243.49
	13:00	-143.67	1224.54	42460.13
	15:00	202.50	2732.81	31436.63

2017/02/08	13:00	100.22	-1136.42	-42991.47
	15:00	-64.50	1193.75	34782.99
2017/02/11	10:00	-43.25	-2039.06	-37656.25
	12:00	-5.11	423.77	27364.75
	13:00	230.00	2148.61	21998.46
	15:00	252.38	279.69	-23361.55
2017/02/12	10:00	31.78	-3048.30	-41335.31
	12:00	26.75	-62.85	37318.19
	13:00	12.25	-2205.21	-47345.20
	15:00	53.38	514.06	33990.89
2017/02/13	11:00	115.88	-958.51	-31311.97
	14:00	203.50	2022.92	31426.50
2017/02/14	09:00	105.50	-1225.00	-40598.96
	14:00	390.25	4260.07	61036.36
2017/02/15	11:00	88.88	-3767.19	-100340.71
2017/02/16	09:00	206.44	1306.33	56372.39
	11:00	71.25	-1679.69	-20868.06
	14:00	185.00	1743.06	25356.87
2017/02/17	11:00	30.25	-1934.38	-45967.88
2017/02/18	10:00	20.78	-105.25	20323.65
	12:00	-76.44	1357.56	34806.24
	16:00	-232.00	-2292.19	-32999.13
2017/02/19	09:00	-100.38	2682.81	45062.93
	10:00	-37.50	785.94	-23710.94
	12:00	246.00	2719.44	35268.13
2017/02/21	09:00	164.75	-1015.63	32688.37
	12:00	-539.88	-6135.94	-85501.30
2017/02/22	09:00	39.88	0.00	-29199.22
	12:00	241.75	3262.15	29748.75
	16:00	-1115.38	-12094.97	-131513.07

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## Radiative Transfer Model Simulation of O<sub>4</sub> DSCDs

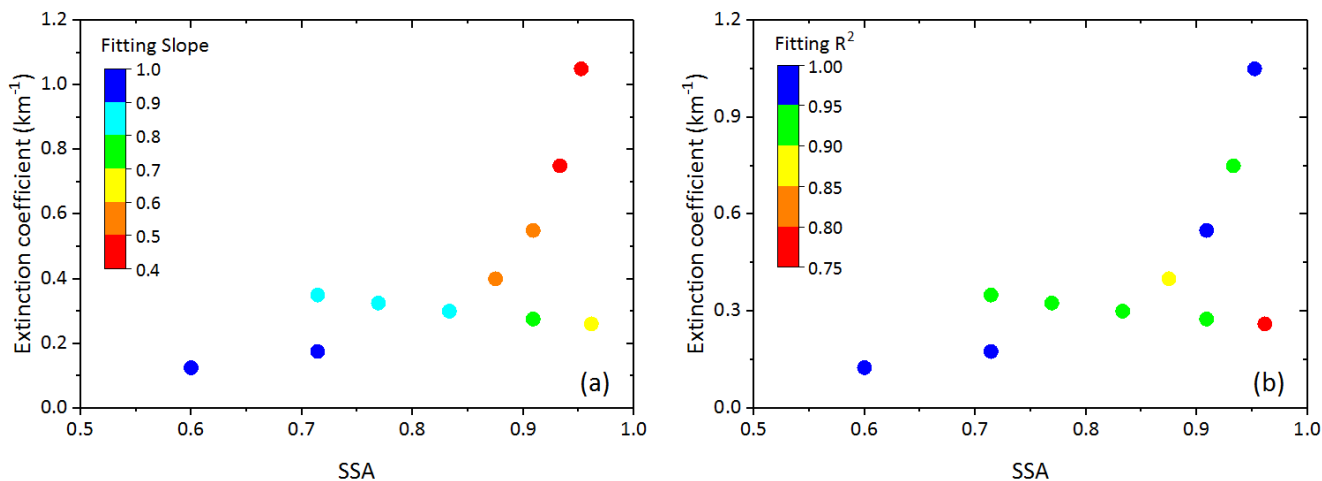
45 In order to illustrate the variations on the O<sub>4</sub> absorptions due to the aerosol loadings, we used radiative transfer model of  
 SCIATRAN to simulate O<sub>4</sub> DSCDs in UV and Visible bands under conditions with different aerosol optical properties. As  
 listed in Table S2, 11 different aerosol scenarios were simulated in total, in which case 1 is the default case to represent haze  
 condition. Case 1 to 7 describe the aerosol scenarios of gradually increase of scattering properties with a fixed  $\sigma_{abs}$  of 0.050  
 km<sup>-1</sup>, which cause the growths in both extinction and SSA. Case 8 to 11 present another process of the gradually increase of  
 50 haze with more absorbing aerosols under the condition that  $\sigma_{sca}$  are fixed on 0.250 km<sup>-1</sup>, consequently resulting in an  
 increase extinction but decrease of SSA. The simulation of different aerosol scenarios were carried out with the same  
 observation geometry series of elevation angle, solar zenith angle and relative azimuth angle. Therefore, the simulated  
 results were only impacted by the input of absorption and scattering vertical profiles.

55 **Table S2. Simulation-based correlation information between O<sub>4</sub> DSCDs at 360.8 and 477.1 nm under conditions with different aerosol optical properties.**

No.	Aerosol information				Slope	R <sup>2</sup>	Intercept
	$\sigma_{abs}$	$\sigma_{sca}$	$\sigma_{ext}$	SSA			
1	0.050	0.075	0.125	0.6000	0.9560	0.9968	0.5516
2	0.050	0.125	0.175	0.7143	0.9117	0.9859	0.3178
3	0.050	0.250	0.300	0.8333	0.8089	0.9087	0.1438
4	0.050	0.350	0.400	0.8750	0.5672	0.8842	0.3861
5	0.050	0.500	0.550	0.9091	0.5649	0.9800	0.2305
6	0.050	0.700	0.750	0.9333	0.4519	0.9447	0.2603
7	0.050	1.000	1.050	0.9524	0.4875	0.9979	0.1654
8	0.010	0.250	0.260	0.9615	0.6754	0.7963	0.3948
9	0.025	0.250	0.275	0.9091	0.7682	0.9138	0.2353
10	0.075	0.250	0.325	0.7692	0.8051	0.9007	0.1407
11	0.100	0.250	0.350	0.7143	0.8446	0.9063	0.1011

Afterward, we did the linear-regression analysis for the simulated UV and Visible O<sub>4</sub> DSCDs under different aerosol conditions. As shown in Figure S2, the slope and R<sup>2</sup> between UV and Visible O<sub>4</sub> DSCDs demonstrate that:

- 60 (1) Case 1-7 show an exponential trend in Figure S1. The fitting slope decrease accompanied with the increase of extinction coefficients and SSA if the condition of absorption coefficients are determined.
- (2) Case 8-11 show a linear trend in Figure S1. The fitting slope will decrease together with the decrease of extinction coefficients and the increase of SSA when the condition of absorption coefficients are determined.
- (3) The correlation coefficients are high (R<sup>2</sup> are mainly greater than 0.90) for all the simulation results.



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**Figure S1. Correlation information (fitting slope and R<sup>2</sup>) of the linear regression analysis between the simulated O<sub>4</sub> DCSDs at 360.8 and 477.1 nm under conditions of different aerosol optical properties in the simulation sensitivity studies.**

70 The forward RTM simulation results indicate that the O<sub>4</sub> absorptions information, including the value of UV and Visible O<sub>4</sub> DSCDs, the corresponding linear-regression slope and R<sup>2</sup> between them, could greatly reflect the variation of aerosol optical properties, which present the theoretical evidences to some extent and enhance the principle basis of the proposed method. Moreover, the simulation results are consistent with the conclusions in the manuscript. The more detailed simulations in the future could provide the better quantitative relationship to the aerosol properties even more.

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