Electronic Supplementary Material to: Evaluation and Evolution of MAX-DOAS-observed Vertical NO_2 Profiles in Urban Beijing*

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Text S1 Detailed processing after observation

After the observations, we adopted the spectral analysis software QDOAS developed by the Belgian Institute of High-altitude Atmospheric Physics (BIRA-IASB) to perform wavelength calibration, spectral simulation of the MAX-DOAS-observed spectrum with high-resolution solar spectra (SAO2010 solar spectra) (Chance and Kurucz, 2010), and inversion of the trace gas slant column concentration via DOAS data fitting with the QDOAS software by the least-square method (Stutz and Platt, 1996). Detailed information on the DOAS fitting approach is provided in Table S1.

Text S2 Specific settings for the retrieval

For this retrieval, we divided the 0–4 km tropospheric atmosphere into 40 layers with 100 m each. Both aerosol and trace gas profiles chose an exponential decreasing a priori with a scale height of 1 km. The a priori surface aerosol extinction was set to 0.2 km^{-1}, and the a priori surface concentration of NO_2 was set to 5 ppb. A priori uncertainties of aerosol and trace gas were all set to 100%, and the correlation height was set to 0.5 km. Moreover, fixed aerosol optical properties (asymmetry = 0.69, single scattering albedo = 0.9, and surface albedo = 0.05) were used during the retrieval (Xing et al., 2020).

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Table S1. DOAS spectrum analysis settings of O_4 and NO_2..

	Data source	Fitting interval	
		O_4	NO_2
		338–370 nm	338–370 nm
NO_2	298 K, I_0^* correction (SCD of 10^{17} molecules cm^{-2}); Vandaele et al., 1998	√	√
NO_2	220 K, I_0 correction (SCD of 10^{17} molecules cm^{-2}), pre-orthogonalized; Vandaele et al., 1998	√	√
O_3	223 K,I_0 correction (SCD of 10^{20} molecules cm^{-2}), Serdyuchenko et al., 2014	√	√
O_3	243 K,I_0 correction (SCD of 10^{20} molecules cm^{-2}), pre-orthogonalized; Serdyuchenko et al., 2014	√	√
O_4	293 K; Thalman and Volkamer, 2013	√	√
HCHO	297 K; Meller and Moortgat, 2000	√	√
BrO	223 K; Fleischmann et al., 2004	√	√
H_2O	296 K, HITEMP; Rothman et al., 2010	×	×
Ring	Calculated with QDOAS according to Chance and Spurr, 1997	√	√
Polynomial degree		Order 3	Order 3
Intensity offset		Constant	Constant

*Solar I_0 correction; Aliwell et al., 2002.

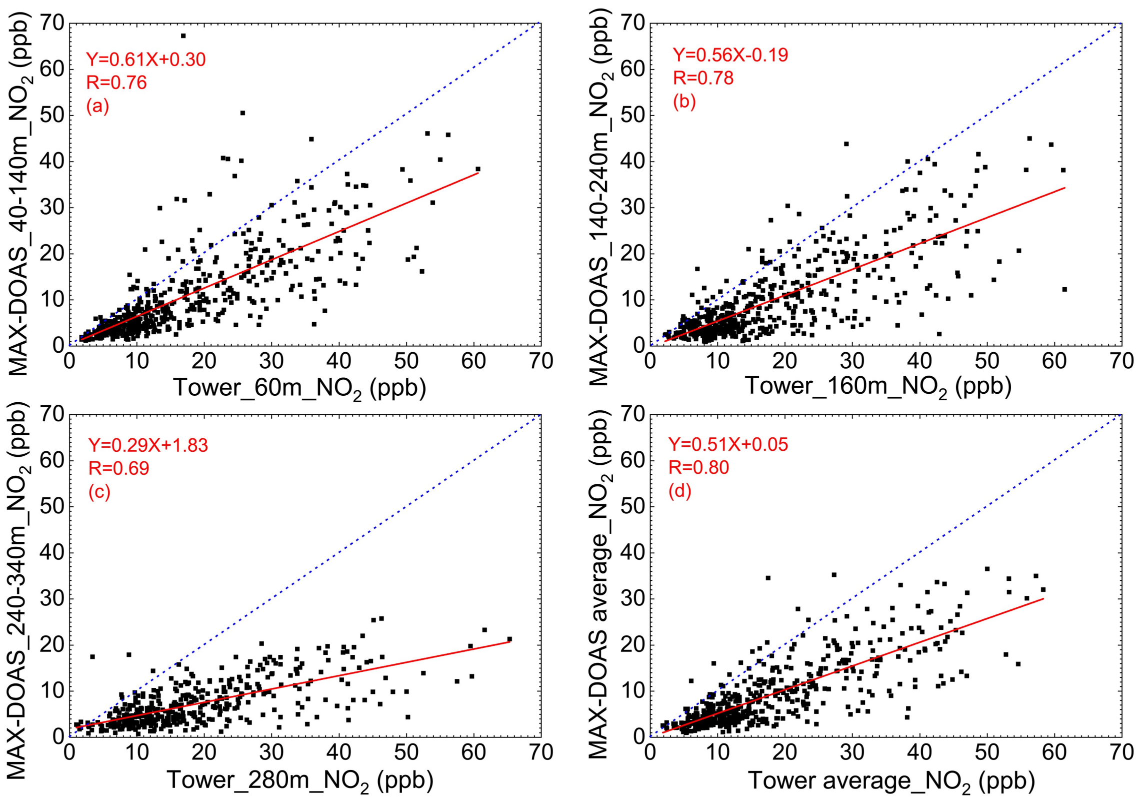

Fig. S1. Correlation analysis of the MAX-DOAS and tower-based in situ VMR results in the case where the cloud is not removed.

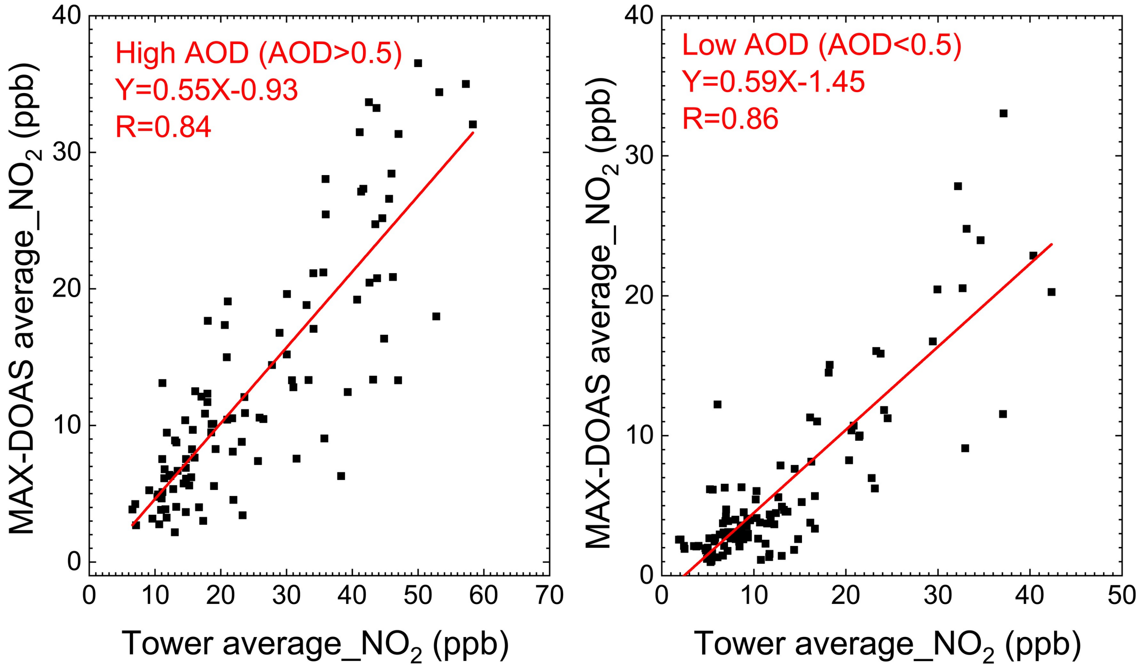

Fig. S2. Correlation analysis of the MAX-DOAS and tower-based in situ VMR results in the cases of high AOD and low AOD.

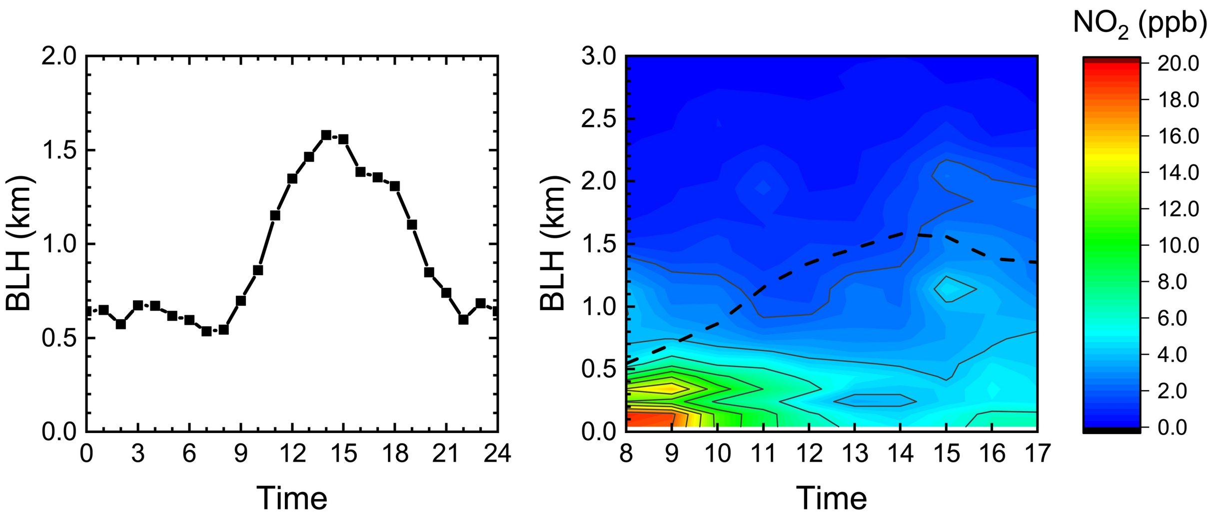

Fig. S3. Diurnal variation of boundary layer height (BLH) from 1 April to 31 May 2019.

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