Supplement of

Modeling of pollution in Fairbanks, Alaska, shows shallow trapping heights controlled by the surface-based temperature inversion strength.

Meeta Cesler-Maloney et al.

Correspondence to: Meeta Cesler-Maloney (m.ceslermaloney@gmail.com), William R. Simpson (wrsimpson@alaska.edu)

Measurements of trace gases from the CTC site and Birch Hill

In addition to the SO_2 and CO_2 gases discussed in the text, CO, O_3 and NO_x were also measured in the same larger stationary trailer parked next to the CTC building at the CTC site where SO_2 was measured. The same 3 m AGL inlet was used to deliver air to the Thermo Scientific CO (48C), O_3 (49C), NO_x (42C) and SO_2 (43C) gas analyzers. The CO analyzer was calibrated using the same EPA certified mixed standard of 5.190 micromole mole^{-1} SO_2 and 508.4 micromole mole^{-1} CO and the same calibration procedure as described in the text for SO_2; an overflow of either zero air, or standard gas diluted in zero air at multiple calibration mixing ratios, was sent to the inlet of the analyzers at calibration times.

To calibrate the O_3 analyzer, O_3 was generated using the Environics 9100 calibration dilution system, which contains an O_3 generator. A zero and multipoint calibration was performed by overflowing the inlet with zero air, or air containing O_3 generated by the calibration dilution system at multiple mixing ratios. The NO_x analyzer was calibrated in the same way as the other instruments, by overflowing the inlet with either zero air or standard gas diluted in zero air. An EPA certified NO standard of 50.12 micromole mole^{-1} NO and 50.16 micromole mole^{-1} NO_x was used to calibrate the NO measurement on the analyzer or was mixed with O_3 generated by the calibration dilution system to produce a known mixing ratio of NO_2 to calibrate the NO_2

measurement on the analyzer. All four analyzers (CO, O_3, NO_x and SO_2) were corrected in the same way as described in the text for SO_2, by first subtracting the instrument's average measurement during the zero and then applying a correction factor to the data, which is the slope from the zero-intercept linear correlation of the instrument observations to the known calibration standard mixing ratios from the multipoint calibrations. Calibration zeroes and slopes fits were linearly interpolated through the data between calibrations.

There were times in the CTC site O_3 time series where O_3 was present at non-zero mixing ratios when O_3 was expected to be fully titrated by the large amounts of NO present. This may be due to an interference from species that absorb light in the same region as O_3. To account for this discrepancy, a secondary correction was applied to the CTC site O_3 data in addition to the multipoint calibration correction. The median value of O_3 at the CTC site at times when there was enough NO available to fully titrate O_3 (NO > 20 nanomole mole^{-1}) was subtracted from the O_3 data to account for possible interferences.

A second O_3 analyzer (Teledyne 400E) was deployed at Birch Hill in a building with an inlet at 158 m AGL. There was only one O_3 generator available during the field campaign, so the O_3 analyzer at Birch Hill did not undergo routine zeroes and multipoint calibrations. Instead, the Teledyne 400E O_3 analyzer at was brought down from Birch Hill to the CTC site at 158 m AGL and placed on the same 3 m inlet as the Thermo Scientific 49C O_3 analyzer for inter-comparison for roughly ten days from March 3rd to March 17th, 2022 at the CTC site. The Teledyne 400E O_3 was subtracted from the Thermo 49C O_3 to obtain an offset during the period of co-location and the average offset during the colocation of 6.56 nanomole mole^{-1} O_3 was subtracted from the full Teledyne 400E O_3 dataset to obtain the corrected Birch Hill O_3 observation.

Determination of CO_2 background mixing ratio

Figure S1 shows a plot of hourly CO_2 versus SO_2 mixing ratios, both measured at 3 m at the CTC building. The intercept is interpreted to be the CO_2 background mixing ratio surrounding Fairbanks, so a background CO_2 mixing ratio of 420 micromole mole^{-1} was used in the model. The slope in Figure S1 represents the empirical emissions ratio of 4300 moles CO_2 to 1 mole SO_2 that was used in the model.

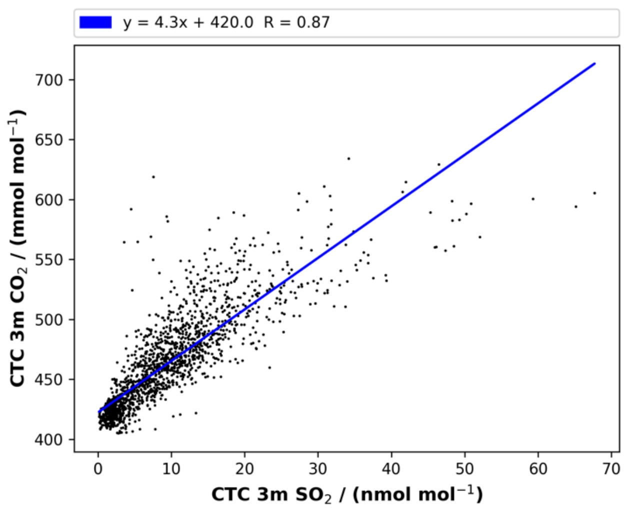

Figure S1. Free-intercept linear correlation plot of hourly CO_2 in micromole mole^{-1} (mmol mol^{-1} is an abbreviation for micromole mole^{-1}) versus SO_2 in nanomole mole^{-1}, both measured at the 3 m at the CTC building.

Additional model diagnostics

Table S1 shows the free-intercept linear correlation slopes, intercepts and R values for the "Base" model simulation and each model sensitivity test.

Table S1. Free intercept linear correlation coefficients. Intercepts are in nanomole mole^{-1}.

Variation	LP-DOAS Free intercept R	LP-DOAS Slope and intercept	3 m in-situ Free intercept R	3 m in-situ Slope and intercept	Free intercept Slope ratio P1/P0
Base	0.88	1.02 + 0.79	0.81	1.01 + 3.73	0.75
$h = \frac{2}{3} h_{base}$	0.87	1.56 – 0.66	0.82	1.66 + 2.93	0.42
$h = 1.5\ h_{base}$	0.86	0.68 + 1.58	0.80	0.63 + 3.94	1.21
$L = \frac{2}{3} L_{base}$	0.88	0.76 + 0.56	0.80	0.74 + 3.38	0.73
$L = 1.5\ L_{base}$	0.87	1.38 + 1.13	0.82	1.38 + 3.95	0.77
$h_{neutral} = \frac{2}{3}$ base	0.88	1.03 + 0.93	0.81	0.99 + 4.17	0.78
$h_{neutral}$ =1.5 base	0.87	1.02 + 0.69	0.81	1.02 + 3.40	0.73
$u* = 0.25$ m s^{-1}	0.88	1.11 + 0.77	0.82	1.10 + 4.88	0.71
$u* = 0.60$ m s^{-1}	0.87	0.96 + 0.84	0.80	0.95 + 2.95	0.78
$E = \frac{2}{3} E_{base}$	0.88	0.69 + 0.63	0.81	0.68 + 2.60	0.75
$E = 1.5\ E_{base}$	0.88	1.54 + 1.04	0.81	1.51 + 5.44	0.75

Figure S2 shows that the *Kz* profile in the region near ground level is similar when calculated using a SBL height, *h*, of 400 m or 600 m using Equation EQ1 for the SBL, and also when using the equation for a truly neutral boundary layer, which is equal to the von Hartmann constant multiplied by the friction velocity (0.4 m s^{-1} here) and the altitude, *z*.

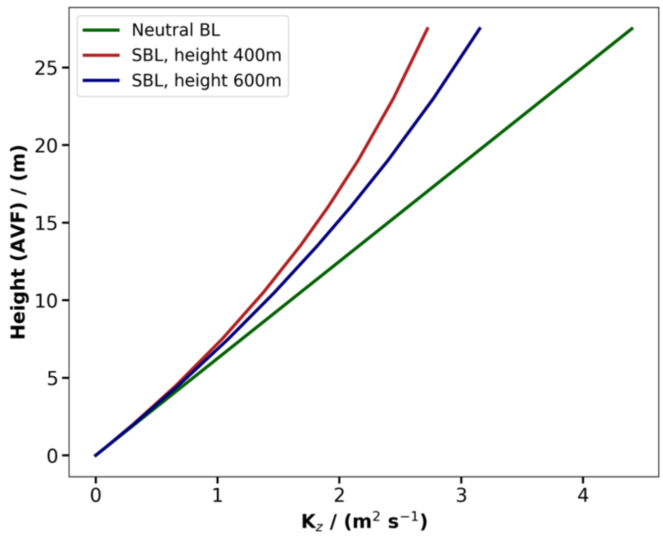

Figure S2. Comparison of *Kz* in the first 25 m AGL during stable boundary layer conditions, with an SBL height of 400 m and 600 m, as well as a *Kz* profile for the same altitude range calculated for a truly neutral boundary layer.

Figure S3 shows a zero-intercept linear correlation plot for the 3-hour modeled path 2 (P2) averaged SO_2 versus LP-DOAS observed path 2 averaged SO_2 in the left panel, with the same correlation plot for the 3-hour modeled path 3 (P3) averaged SO_2 versus LP-DOAS observed path 3 averaged SO_2 in the right panel.

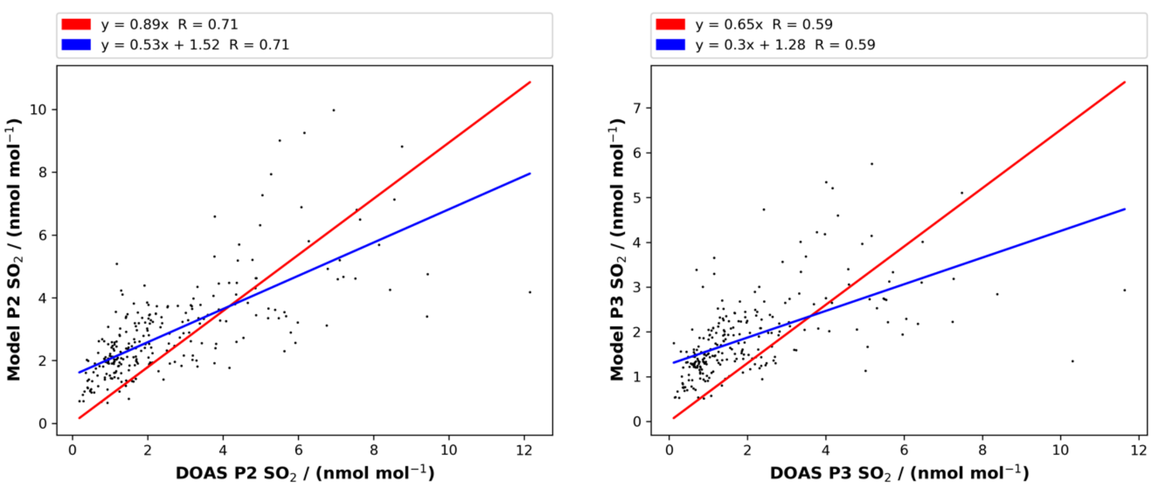

Figure S3. Linear correlation plots of 3-hour modeled path 2 (P2) averaged SO_2 versus the LP-DOAS observed path 2 averaged SO_2 (left panel) and 3-hour modeled path 3 (P3) averaged SO_2 versus the LP-DOAS observed path 3 averaged SO_2 (right panel).

The path 2 data in the left panel of Figure S3 has a zero-intercept *slope* = 0.89 and *R* = 0.71 and the path 3 data in the right panel has a zero-intercept *slope* = 0.65 and *R* = 0.59. While the statistics for path 2 and path 3 are not as close to the ideal *slope* = 1.0 and *R* = 1.0 as the statistics for path 0 and path 1 in Figure 7 in the text, there is overall much less pollution observed in path 2 and path 3, such that the overall model path average versus LP-DOAS observed path average statistics in Figure 7 are dominated by path 0 and path 1. Figure S4 shows the zero-intercept linear correlation plot for the LP-DOAS path 0 average SO_2 versus the CTC 3 m in-situ SO_2.

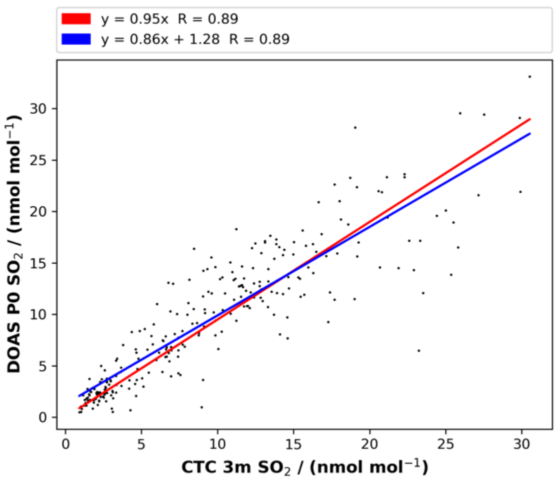

Figure S4. Linear correlation plot for the LP-DOAS path 0 (P0) average SO_2 versus the CTC 3 m in-situ SO_2. Data is averaged at 3-hour time resolution.

Figure S5 shows the 3-hour averaged zero-intercept correlation plots for the modeled versus in-situ CO_2 data at 3 m (left panel) and 23 m (right panel) at the CTC building. The slopes and R values in Figure S5 highlights that the model is also in good agreement with in-situ observations for another dispersion tracer, CO_2, across the CTC building height of 23 m. Figure S6 shows a time series of the steady state urban canopy and column export residence times calculated from the model flux outputs for the ALPACA "Base" simulation.

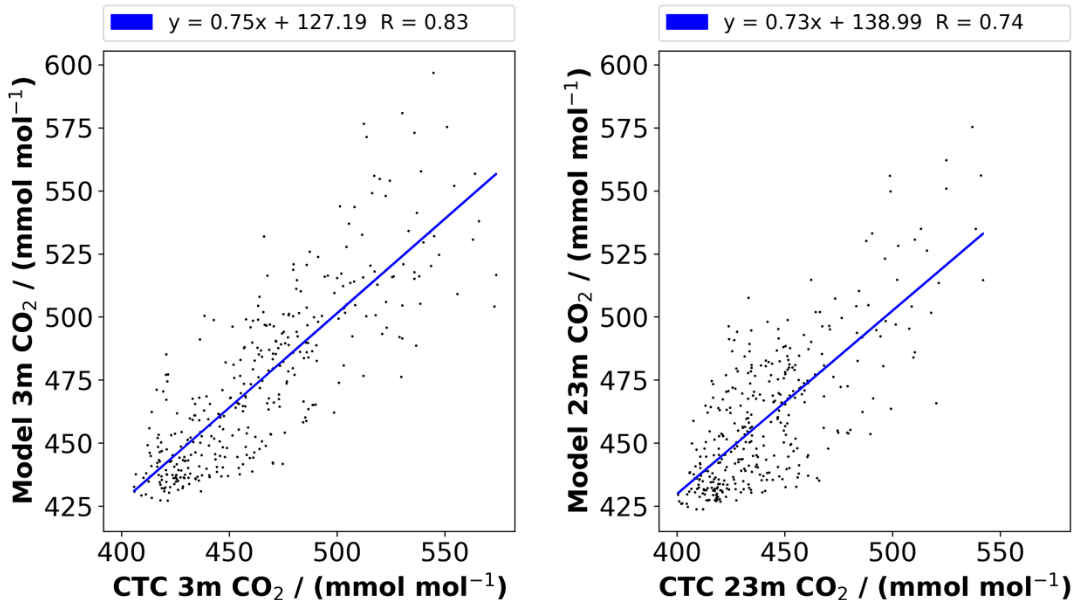

Figure S5. Free-intercept linear correlation plot for the modeled versus in-situ CO_2 in micromole mole^{-1} (mmol mol^{-1} is an abbreviation for micromole mole^{-1}) measured at the CTC building at both 3 m and 23 m AGL. Data is averaged at 3-hour time resolution.

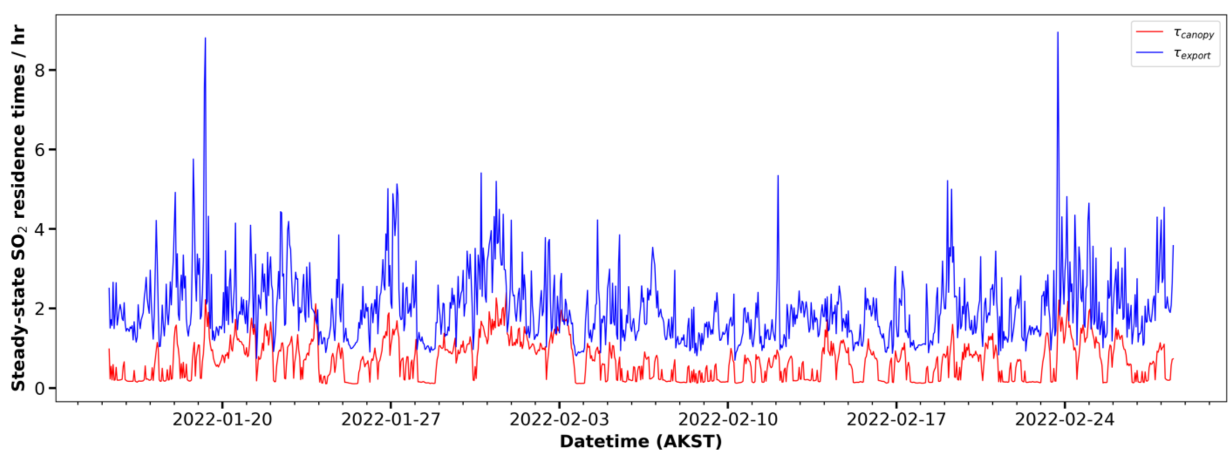

Figure S6: Time series of steady state calculated urban canopy (red) and column export (blue) pollution residence times for the ALPACA "Base" simulation.