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Quantifying forest canopy shading and turbulence effects on boundary layer ozone over the United States

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Supplementary document

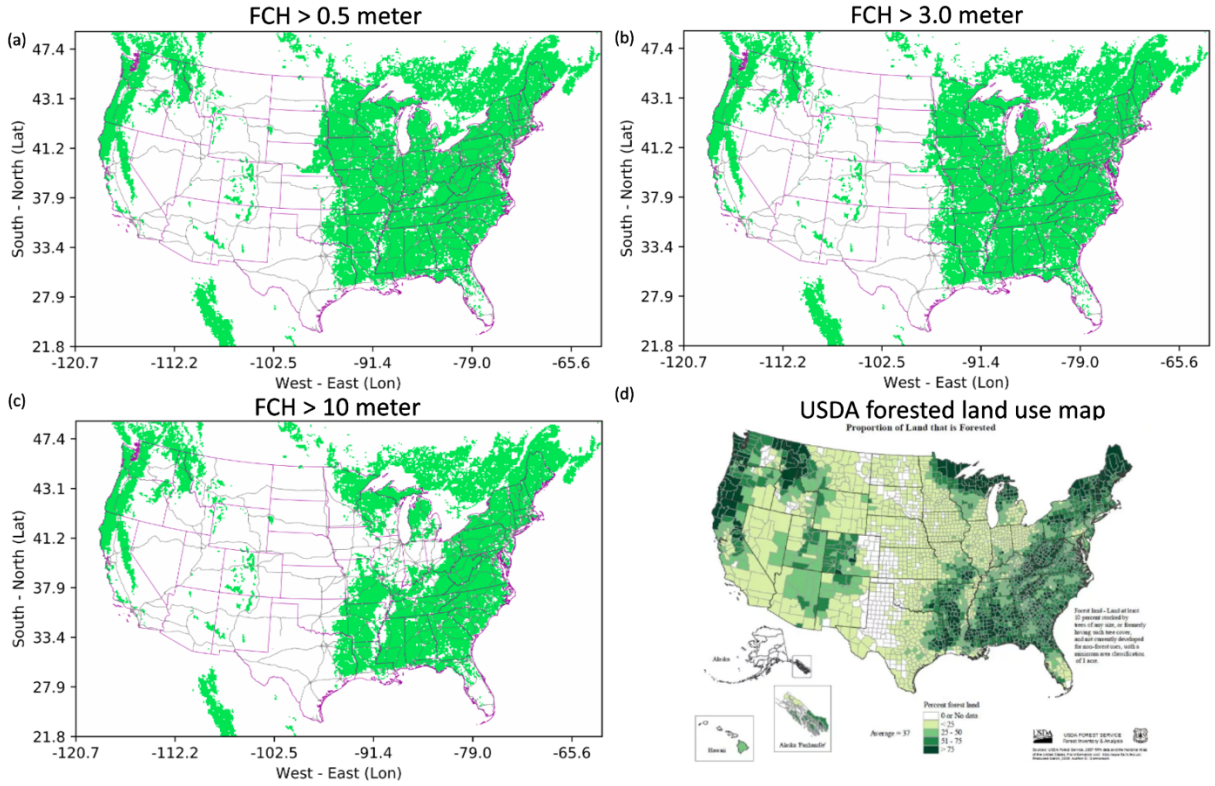

Fig S1. Contiguous canopy threshold regions (green shading) based on Section 2.1 and Figure 1 using different test conditions for FCH > a) 0.5 m, b) 3.0 m, and c) 10.0 m, and d) compared to a USDA forested land use map (https://research.fs.usda.gov/). We note that the contiguous canopy threshold regions in green shading best agree with the USDA map when using c) FCH > 10.0.

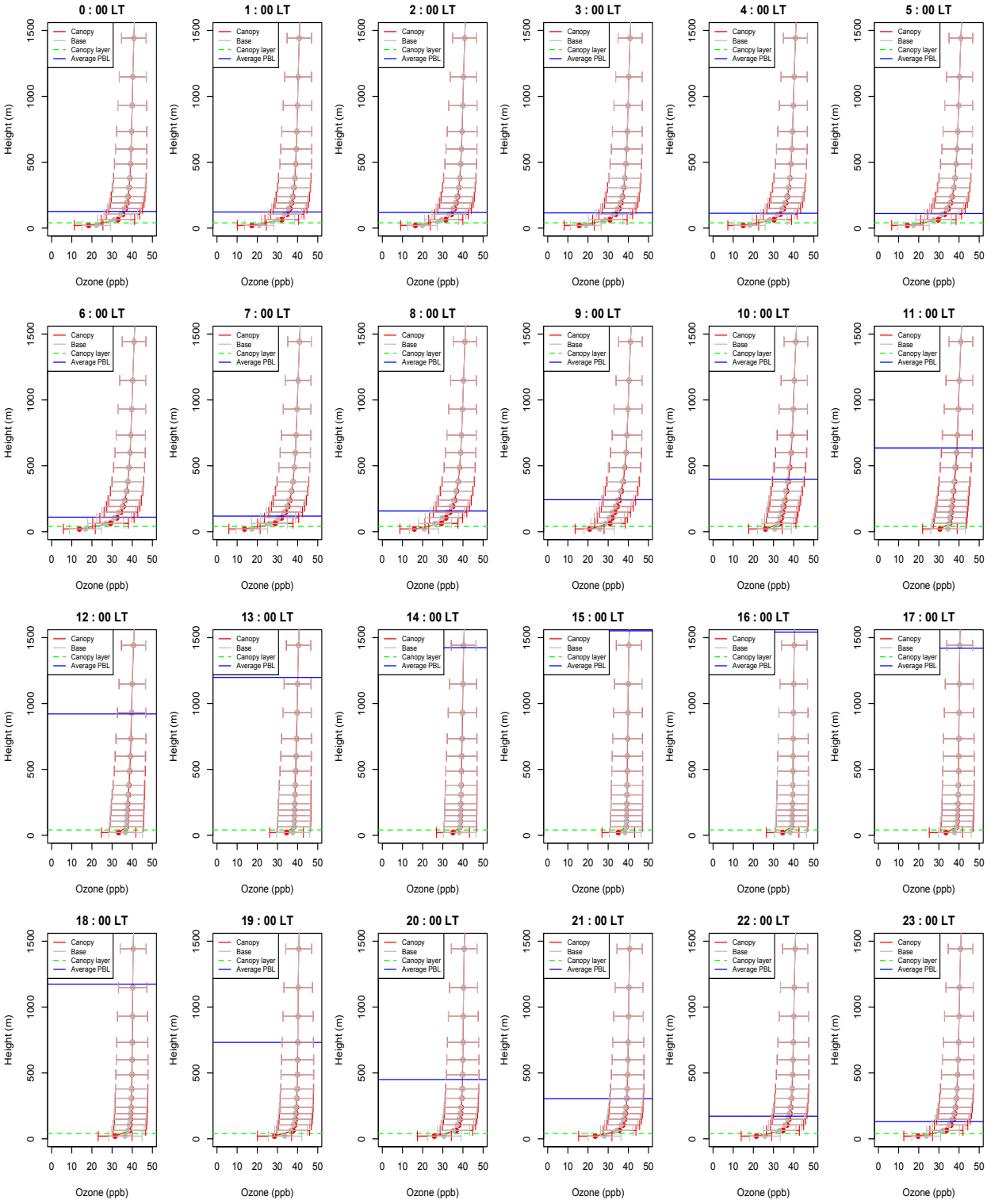

Fig. S2 The diurnal hourly vertical O_3 profiles of Base (gray) and Canopy (red). The dots in each layer are average O_3 concentration in regions of canopy effects in Fig. 2 and the range bars are the standard deviation range. The blue Line is the hourly average PBL height, and below the green dash line is the canopy effect layer.

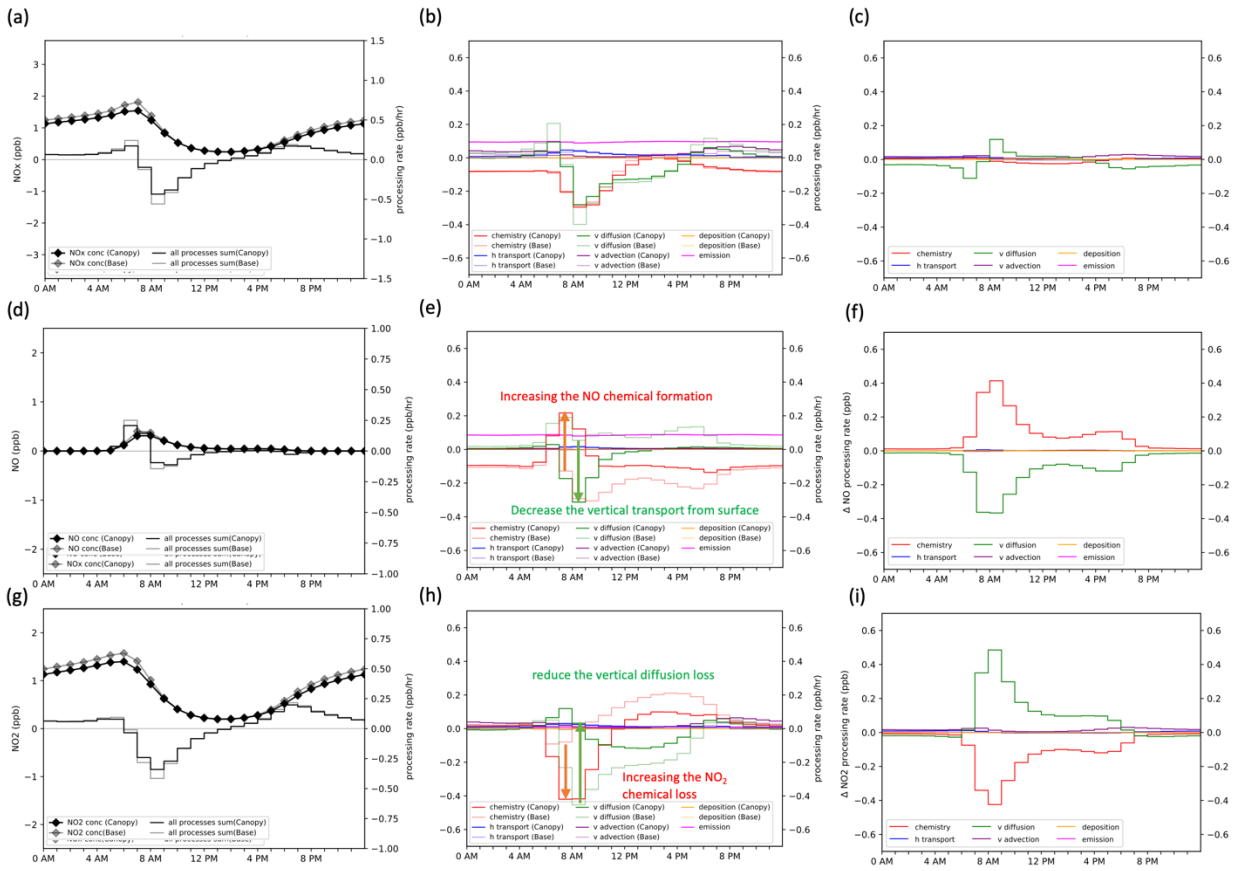

Fig. S3 Hourly average second layer (40 - 80 m AGL) process analysis result for (a) NO_x concentration and net process; (b) NO_x explicit processing rates; (c) delta (Canopy- Base) NO_x processing rate (d) is NO concentration and net process; (e) is NO explicit processing rates; (f) delta (Canopy- Base) NO processing rate (g) is NO_2 concentration and net process; (h) is NO_2 explicit processing rate and (i) delta (Canopy- Base) NO_2 processing rates at Canopy effect locations in August 2019 for two scenarios.

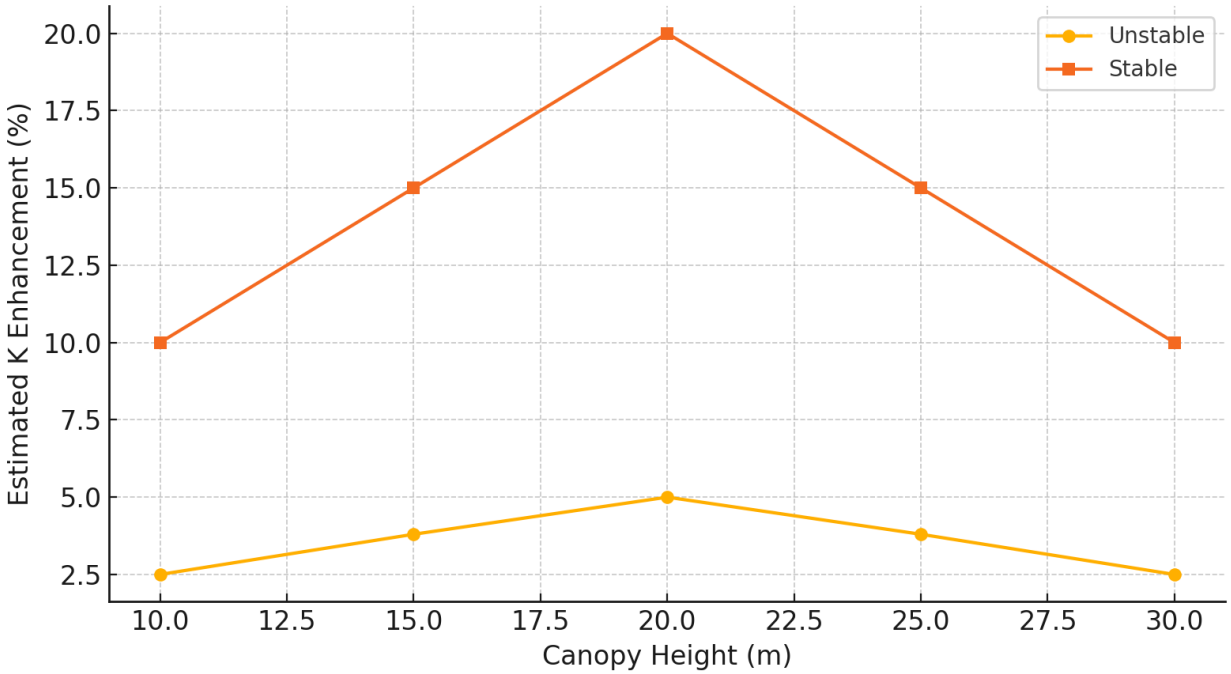

Fig S4. Estimated enhancement (%) of vertical diffusivity (K) in the first model layer (Y-Axis) as a function of canopy height (X-Axis), under unstable (Yellow line) and stable atmospheric conditions (Orange line). The enhancement is based on the fractional overlap between the Roughness SubLayer (RSL, defined as $z \in [h, 2h]$) and at the first model layer (0–40 m), multiplied by characteristic increases in K reported by Harman and Finnigan (2007): about 10% in unstable and 40% in stable conditions. Results show that moderate canopy heights (15–25 m) produce the greatest relative impact on K due to substantial overlap with the RSL. For taller canopies (e.g., 30 m), the first layer is dominated by in-canopy processes, which are already parameterized, leaving less room for additional RSL-driven enhancement.

Table S1 Ozone average daily daytime and nighttime process analysis summary tables.

Daytime	O_3 process (ppb)	Base	Canopy	Difference	
First Model layer	O_3 vertical transport	168	170	2	1.2%
	O_3 horizontal transport	0.14	0.03	-0.11	-78.6%
	O_3 deposition (-)	-164	-150	14	-8.5%
	Net chemical Ozone process	**14**	**-6**	**-20**	**-142.9%**
	O_3 chemical production	629	157	-472	-75.0%
	O_3 chemical reduction	615	163	-452	-73.5%
Second layer	O_3 vertical transport	-3.89	-7.82	-3.93	101.0%
	O_3 horizontal transport	0.46	0.4	-0.06	-13.0%
	O_3 deposition	0	0	0	0%
	Net chemical Ozone process	**14.1**	**16.8**	**2.7**	**19.1%**
	O_3 chemical production	632.8	634.1	1.3	0.2%
	O_3 chemical reduction	618.7	617.3	-1.4	-0.2%

Nighttime	O_3 process (ppb)	Base	Canopy	Difference	
First Model layer	O_3 vertical transport	45	38	-7	-15.6%
	O_3 horizontal transport	3.53	9.58	6.05	171.4%
	O3 deposition	-60	-53	7	-11.7%
	Net chemical Ozone process	-7.1	-8	**-0.9**	**12.7%**
	O_3 chemical production	44	10	-34	-77.3%
	O_3 chemical reduction	51	18	-33	-64.7%
Second layer	O_3 vertical transport	-13.11	-11.38	1.73	-13.2%
	O_3 horizontal transport	3.95	3.03	-0.92	-23.3%
	O_3 deposition	0	0	0	0%
	Net chemical Ozone process	-2.35	-2.23	**0.12**	**-5.1%**
	O_3 chemical production	44.9	45.1	0.2	0.4%
	O_3 chemical reduction	47.25	47.33	0.08	0.2%

Table S2 The average daily total VOC + O_3 reactivity and major individual VOC contribution on surface and second layer at canopy effect regions (see Figure 2).

	Reactions	Base (ppb d^{-1})	Canopy (ppb d^{-1})	Diff (ppb d^{-1})	Diff (%)
First Model layer	R143 & R147: O3 + Alkenes	2	2.51	0.51	25.50%
	R156: O3+ISOP	0.56	1.23	0.67	119.64%
	R173: O3+TERP	1.18	1.48	0.3	25.42%
	Total VOC + O3	4.05	5.53	1.48	36.54%
Second Model layer	R143 & R147: O3 + Alkenes	1.02	0.96	-0.06	-5.88%
	R156: O3+ISOP	0.45	0.56	0.11	24.44%
	R173: O3+TERP	0.55	0.52	-0.03	-5.45%
	Total VOC + O3	2.35	2.4	0.05	2.13%

Table S3 Hourly mean bias (MB) and fraction bias (FB) for all sites, the **bold** font indicates the significant improvement hours in canopy case.

	Hourly MB and FB averaged across all 235 AQS sites				Hourly MB and FB median values across all 235 AQS sites			
	MB (ppb)		FB (%)		MB (ppb)		FB (%)	
Hour	BASE	CANOPY	BASE	CANOPY	BASE	CANOPY	BASE	CANOPY
0	0.58	-2.45	21.91	**6.02**	2.33	**-1.20**	23.60	**4.59**
1	1.32	-1.68	29.20	**12.92**	3.27	**-0.56**	30.98	**9.54**
2	1.53	-1.44	33.32	**16.40**	3.41	**-0.32**	36.36	**13.91**
3	0.89	-1.86	31.99	**15.09**	2.64	**-0.39**	32.87	**13.36**
4	1.61	-1.08	37.88	**20.51**	3.45	**0.15**	45.58	**23.24**
5	1.26	-1.41	37.21	**18.51**	3.25	**-0.11**	44.16	**17.80**
6	2.59	**-1.65**	38.34	**10.88**	3.98	**-1.11**	41.13	**2.83**
7	5.44	**-0.92**	34.58	**4.09**	5.80	**-1.09**	32.44	**-0.92**
8	6.65	**1.09**	27.51	**7.38**	6.39	**0.88**	23.60	**4.83**
9	6.28	**1.98**	21.02	**7.94**	6.25	**2.03**	20.08	**7.42**
10	5.11	**1.57**	15.64	**5.81**	5.19	**1.88**	15.46	**5.84**
11	3.94	**0.83**	11.89	**3.63**	3.95	**0.69**	11.22	**2.64**
12	3.06	**0.08**	9.51	**1.81**	3.03	**-0.19**	9.12	**0.66**
13	2.55	**-0.50**	8.29	**0.47**	2.83	**-0.40**	8.27	**0.23**
14	2.16	**-1.27**	7.39	**-1.41**	2.46	**-1.25**	6.77	**-2.17**
15	1.94	-2.12	6.92	**-3.58**	2.02	-2.27	6.16	-4.52
16	1.64	-3.24	6.35	-6.68	1.34	-3.46	4.97	-7.97
17	0.71	-4.84	4.49	-11.56	0.29	-5.36	3.18	-13.29
18	-0.48	-5.73	2.52	-14.98	-0.56	-5.86	0.76	-17.29
19	-0.31	-4.84	5.24	-11.91	0.32	-4.58	4.25	-14.97
20	0.18	-3.84	9.83	-6.75	1.31	-3.02	10.27	-8.42
21	0.54	-3.16	14.18	**-2.16**	2.37	-1.71	16.08	**-1.50**
22	0.82	-2.65	18.15	**1.87**	2.20	-1.26	17.73	**1.88**
23	1.05	-2.24	22.11	**5.90**	2.68	-1.07	22.86	**6.67**

Model performance metric formula definitions:

Common Variables:

M = predicted concentration

O = observed concentration

X = predicted or observed concentration

σ = standard deviation

I. Mean Bias, Mean Error, and Root Mean Square Error (ppb)

$$\text{Mean Bias} = \frac{1}{n}\sum_{1}^{n}(M - O)$$

$$\text{Mean Error} = \frac{1}{n}\sum_{1}^{n}|M - O|$$

$$\text{Root Mean Square Error} = \sqrt{\frac{\sum_{1}^{n}(M - O)^2}{n}}$$

II. Normalized Mean Bias and Error (unitless)

$$\text{Normalized Mean Bias} = \frac{\sum_{1}^{n}(M - O)}{\sum_{1}^{n}(O)}$$

$$\text{Normalized Mean Error} = \frac{\sum_{1}^{n}|M - O|}{\sum_{1}^{n}(O)}$$

III. Fractional Bias and Error (unitless)

Fractional Bias = $$\frac{1}{n}\left(\frac{\sum_{1}^{n}(M-O)}{\sum_{1}^{n}\left(\frac{(M+O)}{2}\right)}\right)$$

Fractional Error = $$\frac{1}{n}\left(\frac{\sum_{1}^{n}|M-O|}{\sum_{1}^{n}\left(\frac{(M+O)}{2}\right)}\right)$$

IV. Correlation Coefficient (unitless)

Correlation = $$\frac{1}{(n-1)}\sum_{1}^{n}\left(\left(\frac{O-\overline{O}}{\sigma_o}\right)*\left(\frac{M-\overline{M}}{\sigma_m}\right)\right)$$

V. Standard Deviation (ppb)

Standard Deviation (σ) = $$\sqrt{\frac{1}{n}\sum_{1}^{n}(X-\bar{X})^2}$$

Underlying turbulence and photolysis parameterizations used in the CMAQ canopy implementation (from Makar et.al., 2017)

$$T_{\mathrm{L}}\left(\frac{z}{h_{\mathrm{c}}}\right)=\frac{h_{\mathrm{c}}}{u^{*}}\left[0.256\left(\frac{z-0.75h_{\mathrm{c}}}{h_{\mathrm{c}}}\right)+0.492\exp\left(\frac{-0.256z/h_{\mathrm{c}}}{0.492}\right)\right], \quad (4)$$

$$\sigma_{\mathrm{w}}\left(\frac{z}{h_{\mathrm{c}}}\right)=\begin{cases}1.25u^{*} & , \frac{z}{h_{\mathrm{c}}}>1.0\\ u^{*}\left[0.75+0.5*\cos\left(\pi\left(1-\frac{z}{h_{\mathrm{c}}}\right)\right)\right] & , \frac{z}{h_{\mathrm{c}}}\le 1.0\end{cases}, \quad (5)$$

$$(-0.1\le h_{\mathrm{c}}/L<+0.1):$$
$$\sigma_{\mathrm{w}}\left(\frac{z}{h_{\mathrm{c}}}\right)=\left\{\begin{array}{cc}1.0u^{*} & , \frac{z}{h_{\mathrm{c}}}>1.25\\ u^{*}\left[0.625+0.375*\cos\left(\frac{\pi}{1.06818}\left(1.25-\frac{z}{h_{\mathrm{c}}}\right)\right)\right] & , 0.175\le\frac{z}{h_{\mathrm{c}}}\le 1.25)\\ 0.25u^{*} & , \frac{z}{h_{\mathrm{c}}}\le 0.175\end{array}\right\}, \quad (6)$$

$$h_{\mathrm{c}}/L\ge 0.9:$$
$$\sigma_{\mathrm{w}}=0.25u^{*}, \quad (7)$$

$$0.1\le h_{\mathrm{c}}/L<0.9:$$
$$\sigma_{w}\left(\frac{z}{h_{\mathrm{c}}}\right)=\left\{\begin{array}{cc}0.25\left(4.375-3.75\frac{h_{\mathrm{c}}}{L}\right)u^{*} & , \frac{z}{h_{\mathrm{c}}}>1.25\\ u^{*}\left[A+B^{*}\cos\left(\frac{\pi}{1.06818}\left(1.25-\frac{z}{h_{\mathrm{c}}}\right)\right)\right] & , 0.175\le\frac{z}{h_{\mathrm{c}}}\le 1.25\\ 0.25u^{*} & , \frac{z}{h_{\mathrm{c}}}\le 0.175\\ \text{where} & \\ A=0.125R+0.125 & \\ B=0.125R-0.125 & \\ R=4.375-3.75\frac{h_{\mathrm{c}}}{L} & \end{array}\right\}, \quad (8)$$

$$h_{\mathrm{c}}/L<-0.1:$$
$$\sigma_{\mathrm{w}}\left(\frac{z}{h_{\mathrm{c}}}\right)=\left\{\begin{array}{cc}1.25u^{*} & , \frac{z}{h_{\mathrm{c}}}>1.25\\ u^{*}\left[0.75+0.5*\cos\left(\frac{\pi}{1.06818}\left(1.25-\frac{z}{h_{\mathrm{c}}}\right)\right)\right] & , 0.175\le\frac{z}{h_{\mathrm{c}}}\le 1.25\\ 0.25u^{*} & , \frac{z}{h_{\mathrm{c}}}\le 0.175\end{array}\right\}, \quad (9)$$

Reference:

Makar, P. A., Staebler, R. M., Akingunola, A., Zhang, J., McLinden, C., Kharol, S. K., Pabla, B., Cheung, P., and Zheng, Q.: The effects of forest canopy shading and turbulence on boundary layer ozone, Nature Communications, 8, 15243, 10.1038/ncomms15243, 2017.