



Supplement of

Constraining light dependency in modeled emissions through comparison to observed biogenic volatile organic compound (BVOC) concentrations in a southeastern US forest

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Emission Factors for VFRL

Table S1. Emission factors for grid cell at standard conditions.

Categories	Emission Factor ($nmol.m^{-2}.s^{-1}$)
isoprene	15.16
MBO	0.46
pinenes	0.27
ocimenes	0.22
carene	0.20
limonene	0.21
cymene	0.03
camphor	0.05
b-caryophyllene	0.07
longifolene	0.04
methanol	1.60
acetone	0.40
acetaldehyde and ethanol	0.70
formic acid; acetic acid; pyruvic acid	0.40
ethene; ethane	1.27
methacrolein	0.10
linalool	0.20
other VOC	0.04
CO	1

Tree Species composition at VFRL

Table S2. Tree species composition at VFRL with the fraction of the grid occupied by the corresponding species.

Species	Grid Fraction	Type
<i>Quercus alba</i>	0.2364	Broadleaf tree
<i>Pinus virginiana</i>	0.2006	Needleleaf tree
<i>Quercus falcata</i>	0.1186	Broadleaf tree
<i>Acer rubrum</i>	0.1146	Broadleaf tree
<i>Liriodendron tulipifera</i>	0.1026	Broadleaf tree
<i>Carya</i>	0.0453	Broadleaf tree
<i>Fagus grandifolia</i>	0.0443	Broadleaf tree
<i>Quercus rubra</i>	0.0389	Broadleaf tree
<i>Pinus taeda</i>	0.0277	Needleleaf tree
<i>Liquidambar styraciflua</i>	0.02	Broadleaf tree
<i>Nyssa sylvatica</i>	0.0178	Broadleaf tree
<i>Quercus marilandica</i>	0.0104	Broadleaf tree
<i>Cornus florida</i>	0.008	Broadleaf tree
<i>Juniperus virginiana</i>	0.0047	Needleleaf tree
<i>Quercus prinus</i>	0.0025	Broadleaf tree
<i>Sassafras albidum</i>	0.0018	Broadleaf tree
<i>Platanus occidentalis</i>	0.0018	Broadleaf tree
<i>Populus deltoides</i>	0.0015	Broadleaf tree
<i>Carpinus caroliniana</i>	0.0012	Broadleaf tree
<i>Quercus stellata</i>	0.0008	Broadleaf tree
<i>Ilex opaca</i>	0.0002	Broadleaf tree
<i>Castanea pumila</i>	0.0001	Broadleaf tree

Correlation of meteorological data at VFRL with those from Weather Underground

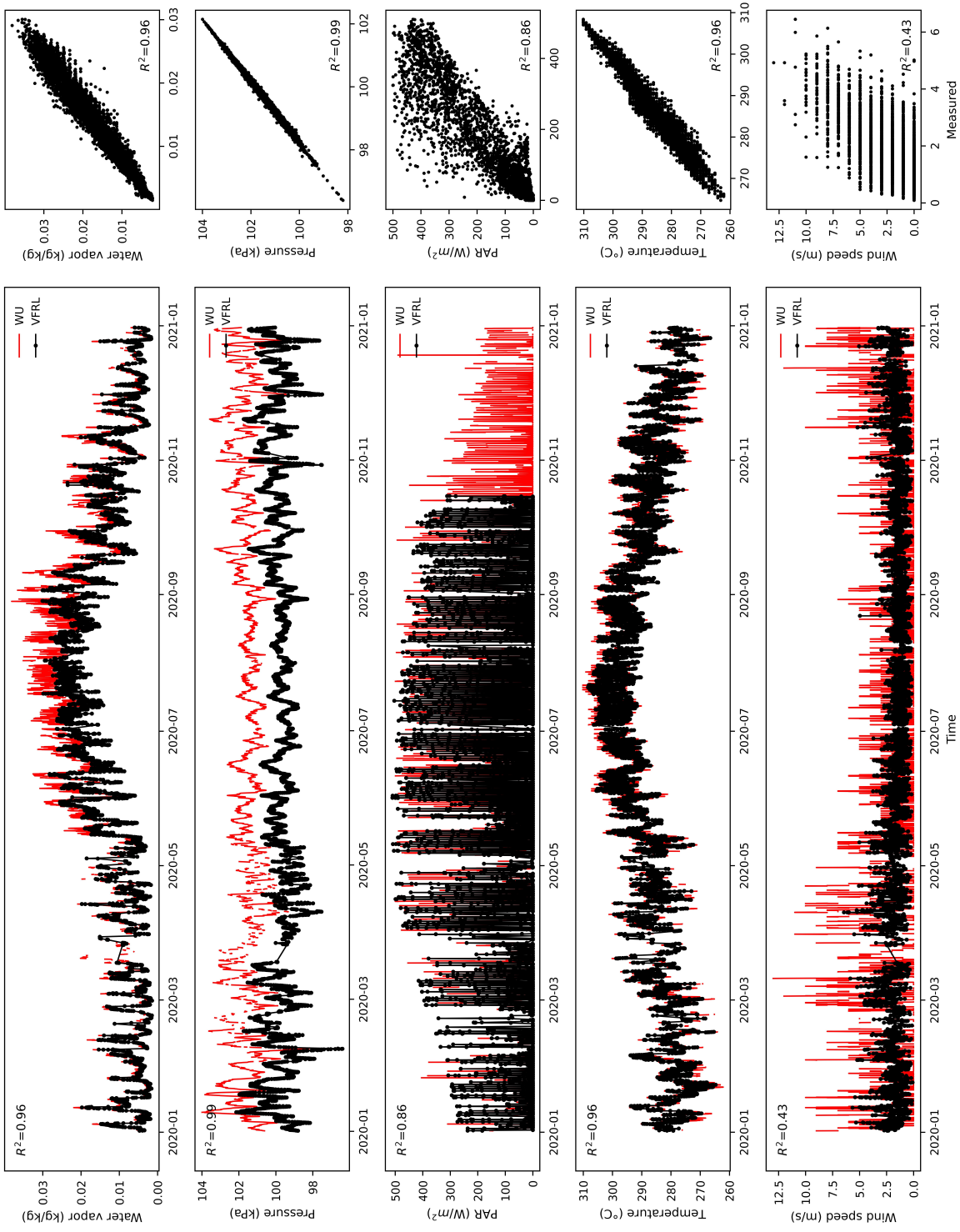


Figure S1. Timeseries of meteorological parameters measured at the Virginia Forest Research Laboratory (VFRL, black lines) and those obtained from Weather Underground identifiers as mentioned in Section 2.2 (in red). The Pearson Correlation coefficient is denoted by R^2 .

Timeseries of α -pinene with adjusted LDF values.

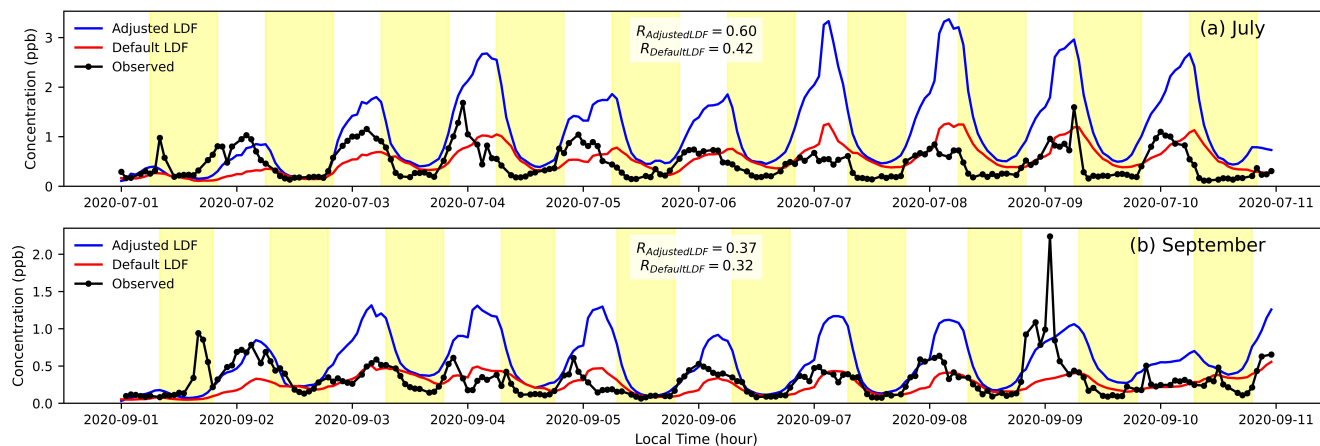


Figure S2. A snapshot of α -pinene concentrations (in ppb) for January, July, and September of 2020 using the monthly LDF as shown in Figure 6. The Pearson correlation coefficient values of the adjusted and default modeled (refer to Table 1) concentrations against the observed concentrations are reported as $R_{\text{AdjustedLDF}}$ and $R_{\text{DefaultLDF}}$.

Rates of reaction for additional BVOCs added to MCMv3.3.1.

Table S3. Rates of reaction of BVOCs added to MCMv3.3.1 where $k_{\text{OH}-i}$ and k_{O_3-i} are the second order reaction rates of compound *emphi* with OH and O₃ in $\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$

Compound (<i>i</i>)	k_{O_3-i} ($\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$)	$k_{\text{OH}-i}$ ($\text{cm}^3 \cdot \text{molecule}^{-1} \cdot \text{s}^{-1}$)	References
β -phellandrene	4.77×10^{-17}	1.68×10^{-10}	Shorees et al. (1991)
Camphene	5.10×10^{-19}	5.30×10^{-11}	Gaona-Colmán et al. (2017)
Tricyclene	None	3.54×10^{-12}	US EPA (2024)
β -Thujene	1.13×10^{-17}	6.09×10^{-11}	US EPA (2024)
α -Fenchene	1.13×10^{-17}	5.96×10^{-11}	US EPA (2024)
Sabinene	8.60×10^{-17}	1.17×10^{-10}	Atkinson et al. (1990b, a)
α -Cymene	None	8.54×10^{-12}	US EPA (2024)
γ -terpinene	1.40×10^{-16}	1.77×10^{-10}	Atkinson et al. (1990b)
α -Cedrene	2.78×10^{-17}	6.70×10^{-11}	Shu and Atkinson (1994, 1995)
β -cedrene	1.70×10^{-16}	6.53×10^{-11}	Richters et al. (2015)

Monthly variation of LDF throughout the year for other BVOCs.

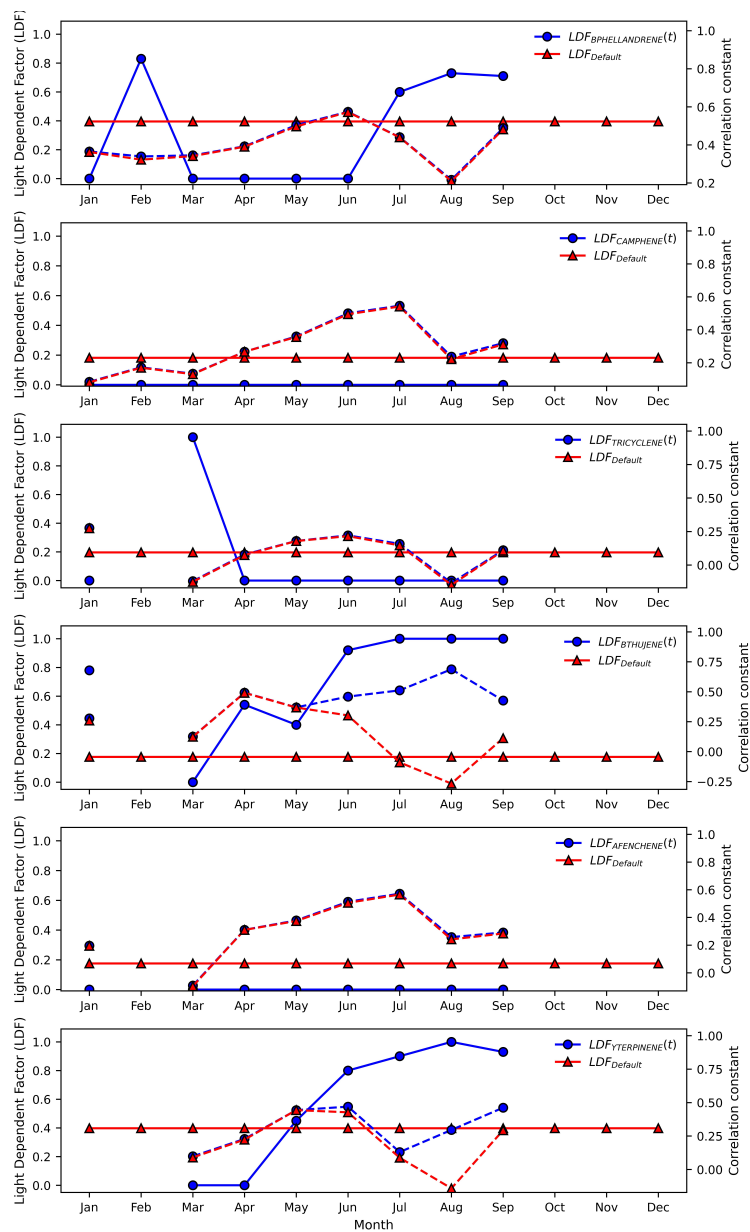


Figure S3. Monthly variation of LDF for α -fenchene, β -phellandrene, β -thujene, camphene, tricyclene and γ -terpinene estimated by maximizing the correlation between observed concentrations and those estimated by MEGANv3.2 and FOAM at VFRL. The blue markers represent the adjusted LDF values, the red line represents the LDF used by default in MEGANv3.2. The blue and red solid lines present the LDF values and the dashed lines represent the corresponding Pearson correlation coefficients.

Variation of correlation constant with LDF throughout the seasons for all BVOCs simulated.

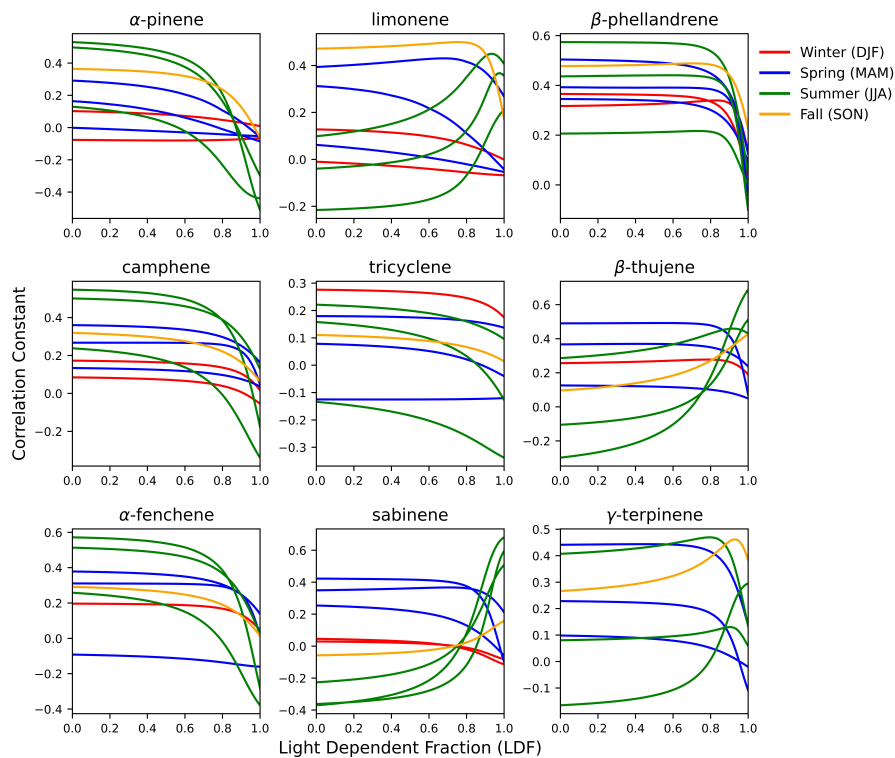


Figure S4. Variation of the Pearson correlation coefficient between modeled and measured concentration with LDF for α -pinene, limonene, β -phellandrene, camphene, tricyclene, β -thujene, α -fenchene, sabinene, and γ -terpinene at VFRL. The red lines represent winter (Dec, Jan, Feb), blue lines spring (Mar, Apr, May), green lines summer (Jun, Jul, Aug), and orange lines fall (Sep, Oct, Nov) months.

Seasonal LDFs for all BVOCs simulated.

Table S4. Seasonal variation of Light-dependent Factors for α -pinene, limonene, β -phellandrene, camphene, tricyclene, β -thujene, α -fenchene, sabinene, and γ -terpinene at VFRL.

Compound	Winter (DJF)	Spring (MAM)	Summer (JJA)	Fall (SON)
α -pinene	0	0	0	0
limonene	0	0.23	0.97	0.76
β -phellandrene	0.42	0	0.44	0.71
camphene	0	0	0	0
tricyclene	0	0.33	0	0
β -thujene	0.78	0.31	0.97	1
α -fenchene	0	0	0	0
sabinene	0	0.24	1	1
γ -terpinene		0.15	0.90	0.93

Comparison of Ozone Concentrations at VFRL and EPA Albemarle High School Station.

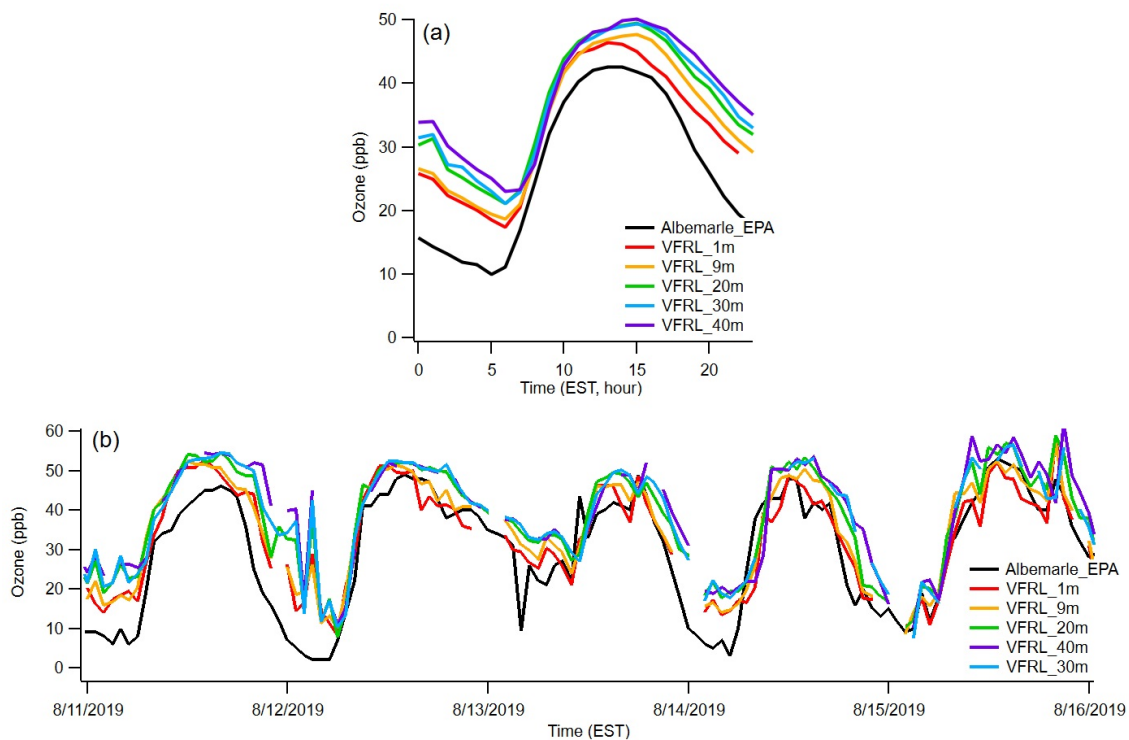


Figure S5. Ozone measured at the Virginia Forest Research Laboratory (VFRL) at different heights from the ground (1, 9, 20, 30, 40 m) and at the EPA monitoring station in Albemarle, VA: (a) average diurnal for all data June through November of 2019, and (b) Sample five-day period showing similar day-to-day variability.

Model sensitivity to ozone concentrations.

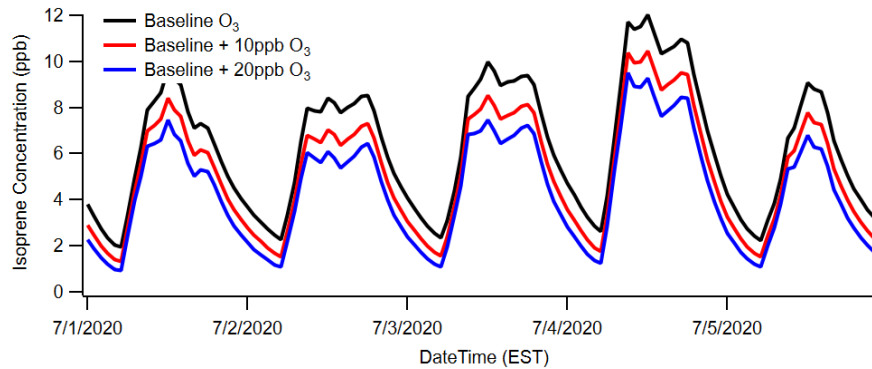


Figure S6. Simulated concentrations of isoprene (in ppb) over 5 days in July, 2020 with the ozone used in our model (Baseline O₃ denoted by a black line) and at elevated ozone levels (Baseline + 10ppb O₃ and Baseline + 20ppb O₃ denoted by red and blue lines respectively).