Supplement of Atmos. Chem. Phys., 18, 14297–14325, 2018
https://doi.org/10.5194/acp-18-14297-2018-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Driving parameters of biogenic volatile organic compounds and consequences on new particle formation observed at an eastern Mediterranean background site

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Section S1 Planetary boundary layer (PBL) assimilated data

In order to investigate the PBL height effect on BVOC concentrations, this parameter was evaluated using PBL assimilated data generated by the European Centre for Medium-Range Weather Forecast (ECMWF) Interim Re-Analysis (ERA-Interim) global atmospheric reanalysis at the location corresponding to the Troodos station (32.88° E - 34.92° N, ~20 km westerly from the CAO station).

The ERA-Interim dataset starts from 1979 and continues to provide information until present in near real-time. Gridded data products include a large variety of 3-hourly surface parameters, describing weather as well as ocean-wave and land-surface conditions, and 6-hourly upper-air parameters covering the troposphere and stratosphere. Vertical integrals of atmospheric fluxes, monthly averages for many of the parameters, and other derived fields have also been produced. Berrishford et al. (2011) provide a detailed description of the ERA-Interim product archive. ERA-Interim products are normally updated once per month, with a delay of two months to allow for quality assurance and for correcting technical problems. The ERA-Interim atmospheric model has a spatial resolution of 0.75°x0.75° and expands vertically with 60 atmospheric layers. The reanalysis product is produced with a sequential data assimilation scheme, using 12-hourly analysis cycles , a time-window when available observations are assimilated into the information from the forecast model as described in Dee et al. (2011).

The ERA-Interim model includes a PBL height parameter calculated from the Bulk Richardson number (Troen and Mahrt, 1986), which is based on ratios of both dynamic and thermodynamic vertical gradients and hence characterizes the degree of turbulence. Given the fact that the boundary layer is often associated with stronger mixing (as compared to the free troposphere) due to increased levels of turbulence, it would be natural to investigate properties associated with turbulence. Essentially, the PBL height is defined as the level where the bulk Richardson number reaches a critical value of 0.25, based on the difference between quantities at this level and the lowest model level as an estimator for the vertical stability. Bulk Richardson number is available a 6-h and 12-h forecasts.

However, as reported in von Engeln and Teixeira (2013) this method of estimating the stability from dry thermodynamic variables (not moist), tends to provide estimates of PBL height that are often closer to the cloud-base height in marine cloudy boundary layers, rather than the PBL height itself (Janssen and Bidlot, 2003). Seidel et al. (2012) reports that for their scope of assessing the climatology of the PBL over the continental United States and Europe with the use of ERA-Interim datasets, they did not employ the estimates of the BLH from ERA-Interim itself, because they are computed using an algorithm not applicable to radiosonde data (due to the fact that turbulence parameters are required for this application). With a preliminary analysis, they report that the ERA-interim PBL height product (i.e., with the ECMWF algorithm) shows higher heights, especially over high elevation regions, than the algorithm used in their study on the radiosonde data. Differences were below 100 m at night and of several 100 m during daytime.

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Table S1: Statistics ($\mu g.m^{-3}$), detection limits (DL - $\mu g.m^{-3}$) and relative uncertainties u(X)/X (Unc. - %) of selected VOC concentrations measured at the site.

	Species	Min	25 %	50 %	Mean	75 %	Max	σ	DL	Unc.
DIENE	**Isoprene**	4	26	38	46	53	219	28	21	11
TERPENES	**α-Pinene**	8	8	18	58	58	1874	131	16	10
	β-Pinene	6	6	18	61	57	1962	142	12	12
	Camphene	<1	5	11	25	29	275	37	1	ND
	Myrcene	<1	2	4	6	8	43	7	2	ND
	Δ^3-Carene	<1	4	8	11	15	91	11	1	ND
	α-Terpinene	<1	1	2	3	5	32	4	1	ND
	γ-Terpinene	<1	<1	<1	<1	1	12	2	1	ND
	Limonene	<1	8	17	27	32	347	37	1	ND
ALCOHOL	**Methanol**	654	1658	2426	2765	3452	9074	1452	180	21
CARBONYL COMPOUNDS	**Formaldehyde**	399	678	909	986	1170	2416	409	25	ND
	Acetaldehyde	102	277	390	431	531	1533	209	44	10
	Acetone	423	861	1048	1083	1214	2662	335	17	9
	MVK+MACR	3	19	26	30	35	139	18	3	12
	MEK	59	154	196	210	242	653	84	13	9

ND: not determined

Figure S1: Agreement between on-line and off-line measurements of α-pinene, β-pinene and the sum of monoterpenes

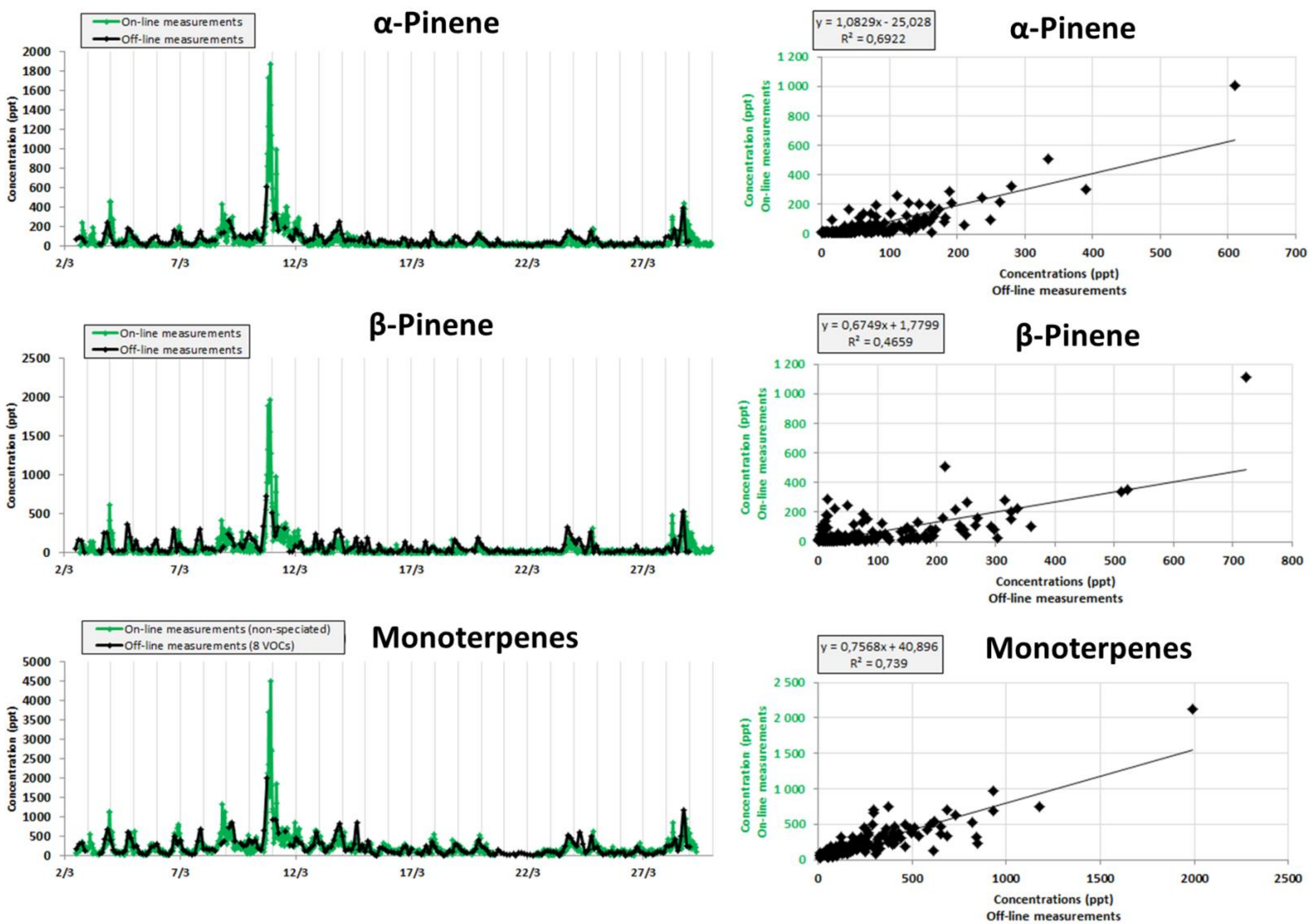


Figure S2: Agreement between on-line and off-line measurements of acetaldehyde, acetone and MEK

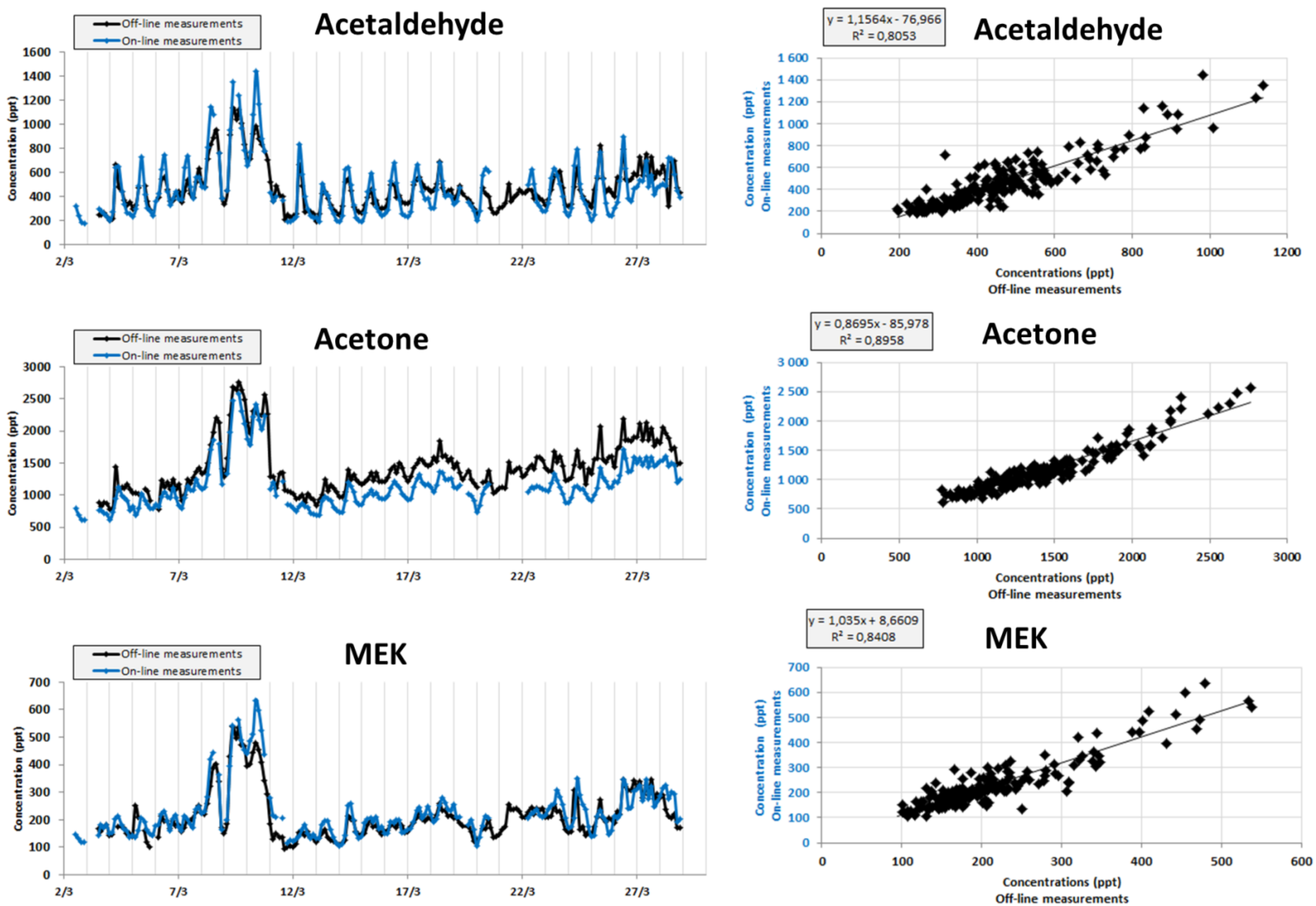


Figure S3: Mean diel variation of isoprene and its oxidation products (in green colors) in comparison with mean diel variation of meteorological parameters (solar radiation, temperature displayed as red lines and orange boxes, respectively). This figure includes all measurement days with a PTR-MS (i.e. from 1 to 29 March 2015).

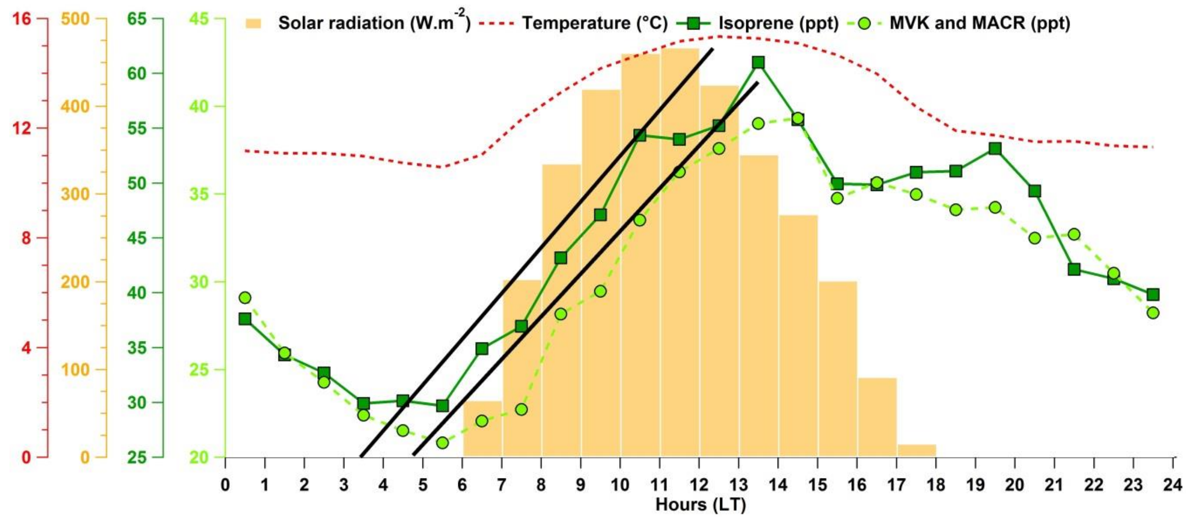
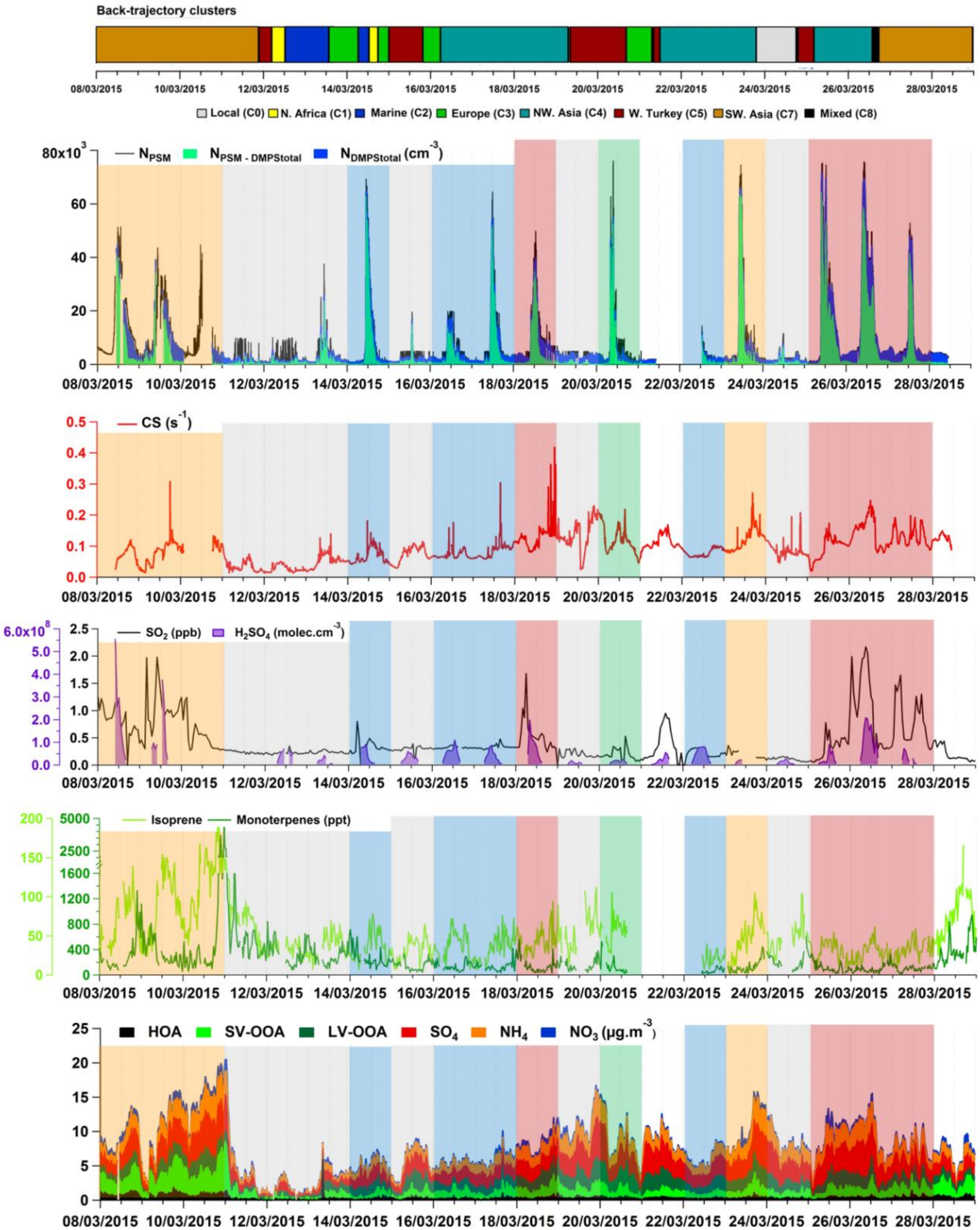


Figure S4: Time series of particle number N_{PSM}, N_{DMPS} and CS in comparison with suspected parameters controlling NPF events (SO_2, H_2SO_4, isoprene and monoterpenes) and accumulated time series of PM_1 contribution.

The color code highlights NPF event days and non-event days (grey periods). Red periods represent NPF1 event days with anthropogenic origin. Orange periods represent NPF2 event days both with mixed origins (anthropogenic and biogenic). Blue and green periods are respectively for NPF events of marine (NPF3) and biogenic origin (NPF4). Organic aerosol (OA) factors: HOA - hydrogen-like OA; SV-OOA – semi-volatile oxygen-like OA; LV-OOA – low-volatile oxygen-like OA. Time is given in local time (UTC + 2 h).


Back-trajectory clusters
08/03/2015
10/03/2015
12/03/2015
14/03/2015
16/03/2015
18/03/2015
20/03/2015
22/03/2015
24/03/2015
26/03/2015
28/03/2015
Local (C0)
N. Africa (C1)
Marine (C2)
Europe (C3)
NW. Asia (C4)
W. Turkey (C5)
SW. Asia (C7)
Mixed (C8)
$80x10^3$
60
40
20
0
N_{PSM}
$N_{PSM - DMPStotal}$
$N_{DMPStotal}$ (cm^{-3})
CS (s^{-1})
0.5
0.4
0.3
0.2
0.1
0.0
SO_2 (ppb)
H_2SO_4 (molec.cm^{-3})
$6.0x10^8$
5.0
4.0
3.0
2.0
1.0
0.0
2.5
2.0
1.5
1.0
0.5
0.0
Isoprene
Monoterpenes (ppt)
200
150
100
50
0
5000
2500
1600
1200
800
400
0
HOA
SV-OOA
LV-OOA
SO_4
NH_4
NO_3 ($\mu g.m^{-3}$)
25
20
15
10
5
0