Supplemental materials for "Comparison and evaluation of updates to WRF-Chem (v3.9) biogenic emissions using MEGAN"

Table S1: Soil-related wilting point (θ_w) (m^3 m^{-3}) used by MEGAN soil moisture emission activity factor. Adapted from Chen and Dudhia, 2001.

Soil type	Wilting point
Sand	0.01
Loamy sand	0.028
Sandy loam	0.047
Silt loam	0.084
Silt	0.084
Loam	0.066
Sandy clay loam	0.067
Silty clay loam	0.12
Clay loam	0.103
Sandy clay	0.1
Silty clay	0.126
Clay	0.138
Organic material	0.06
Water	n.a.
Bedrock	0.094
Other (land–ice)	0.028

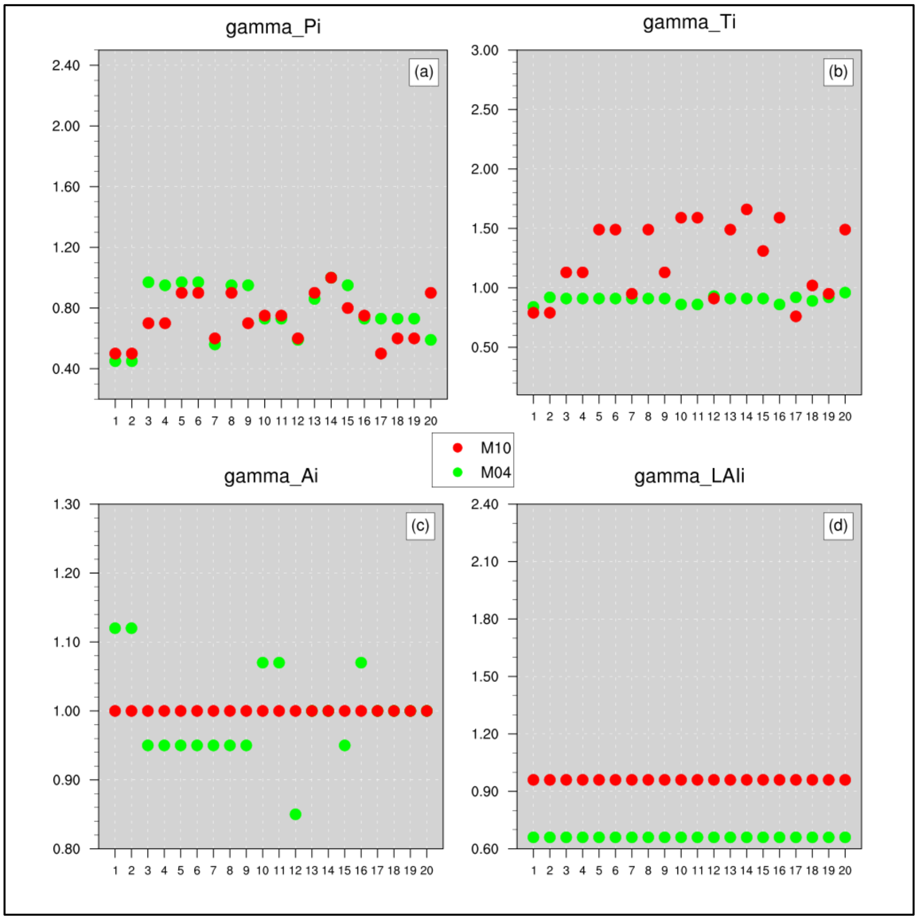

Figure S1: Comparison between M04 and M10 run of the emission activity factors (dimensionless) (a) photosynthetic photon flux density (γP, GAMMA_P), (b) temperature (γT, GAMMA_T), (c) leaf age (γage, GAMMA_A), and (d) leaf area index (γLAI, GAMMA_LAI) classified by classes compound (x-axis). The factors refer to the city of Kiev (Ukraine) in August 13th (12:00 UTC), 2015.

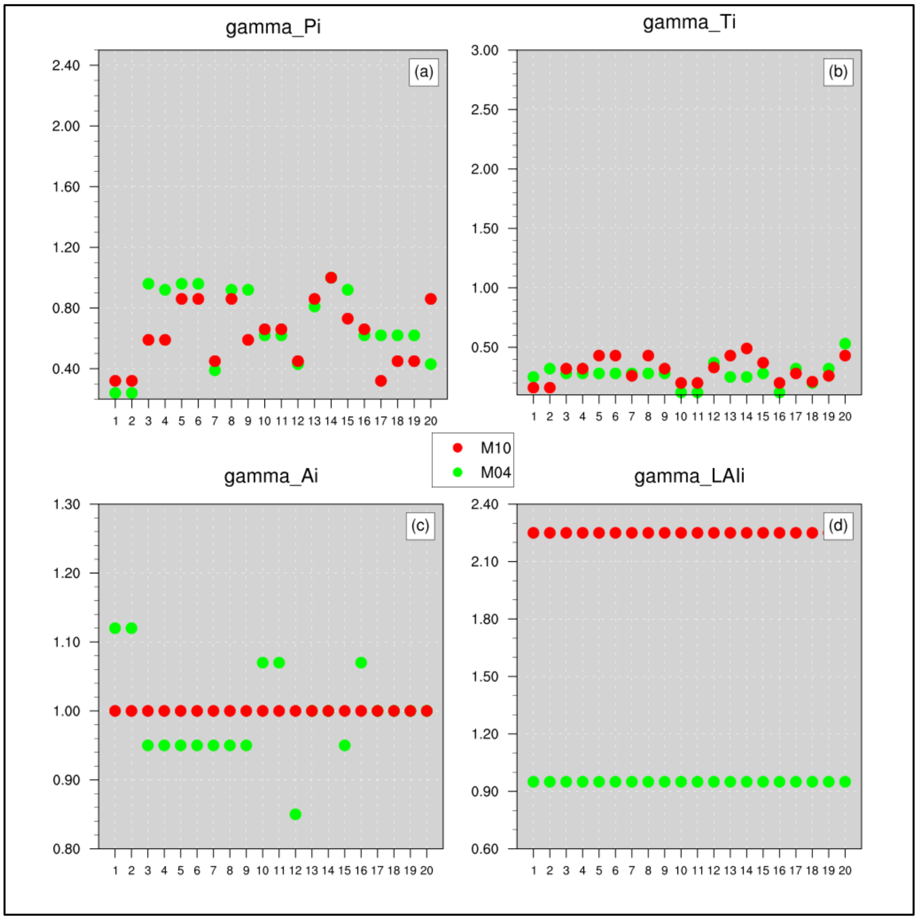

Figure S2: Comparison between M04 and M10 run of the emission activity factors (dimensionless) (a) photosynthetic photon flux density (γ_P, GAMMA_P), (b) temperature (γ_T, GAMMA_T), (c) leaf age (γ_{age}, GAMMA_A), and (d) leaf area index (γ_{LAI}, GAMMA_LAI) classified by classes compound (x-axis). The factors refer to the city of Porto (Portugal) in August 13th (12:00 UTC), 2015.

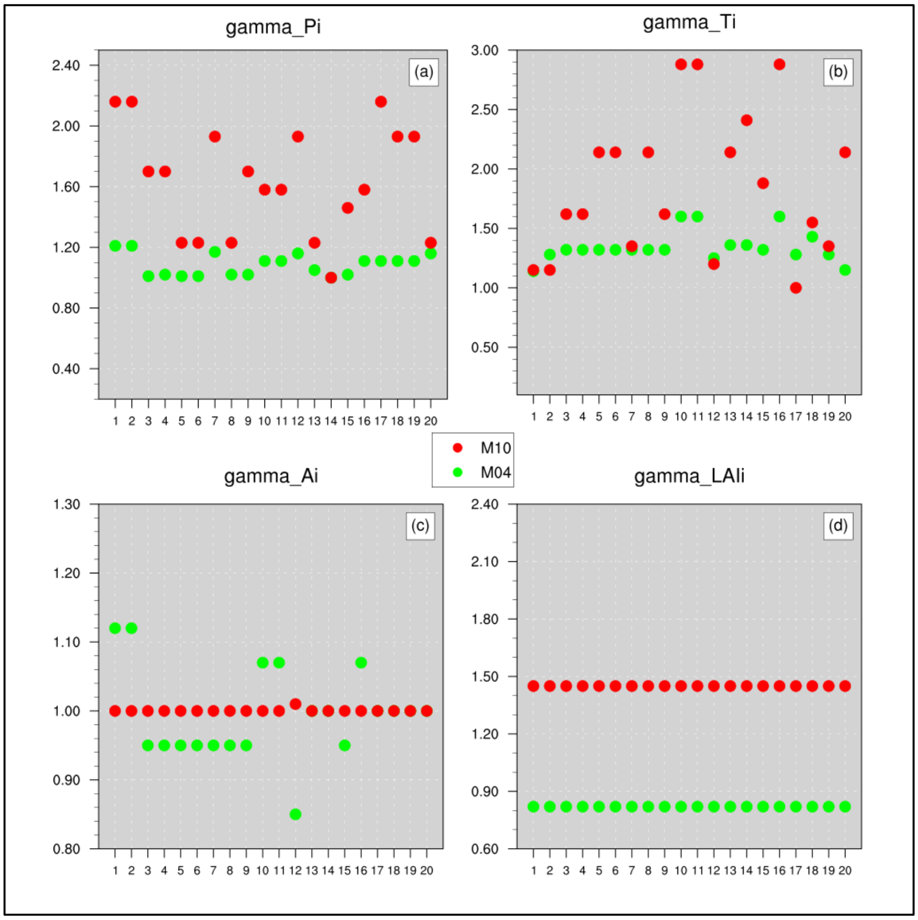

Figure S3: Comparison between M04 and M10 run of the emission activity factors (dimensionless) (a) photosynthetic photon flux density (γ_P, GAMMA_P), (b) temperature (γ_T, GAMMA_T), (c) leaf age (γ_{age}, GAMMA_A), and (d) leaf area index (γ_{LAI}, GAMMA_LAI) classified by classes compound (x-axis). The factors refer to the city of Zagreb (Croatia) in August 13th (12:00 UTC), 2015.

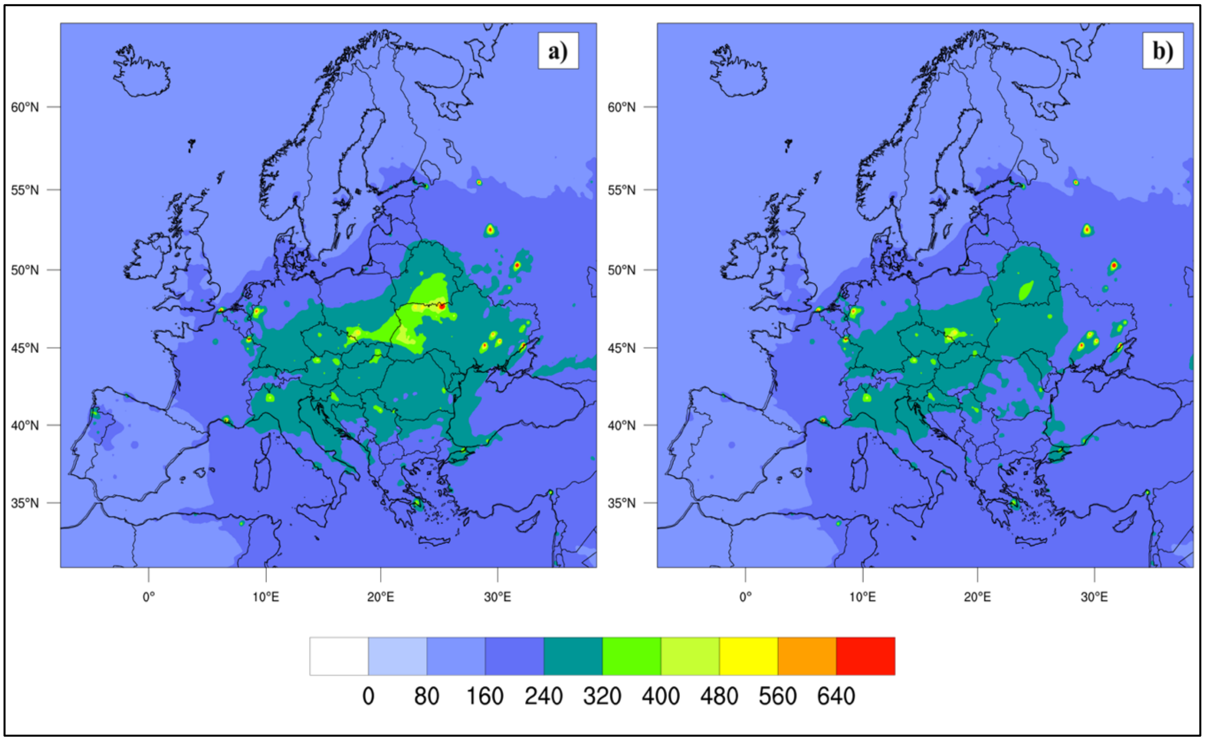

Figure S4: Comparison of the predicted spatial distribution of CO concentration (µg m^{-3}) of the last two simulations done: (a) with all the MEGAN updates (M10 run), and (b) the same simulation without including the biomass burning emissions in the calculation (b - "M10_noFINN"). The maps represent the weekly averages (from August 10th, 2015 at 0000 UTC to August 16th, 2015 at 0000 UTC), extrapolated from WRF-Chem model.

Table S2: Gas-phase reactions involving isoprene (ISOP) for the formation of methacrolein (MACR), and methyl vinyl ketone (MVK) in the MOZART-4 chemical mechanism. The table is adapted from Emmons et al., 2010.

Reactants	Products
ISOP + OH	$\rightarrow$ $ISOPO_2$
ISOP + O_3	$\rightarrow$ 0.4·MACR + 0.2·MVK + 0.07·C_3H_6 + 0.27·OH + 0.06·HO_2 + 0.6·CH_2O + 0.3·CO + 0.1·O_3 + 0.2·MCO_3 + 0.2·CH_3COOH
$ISOPO_2$ + NO	$\rightarrow$ 0.08·ONITR + 0.92·NO_2 + HO_2 + 0.55·CH_2O + 0.23·MACR + 0.32·MVK + 0.37·HYDRALD
$ISOPO_2$ + NO_3	$\rightarrow$ HO_2 + NO_2 + 0.6·CH_2O + 0.25·MACR + 0.35·MVK + 0.4·HYDRALD
$ISOPO_2$ + HO_2	$\rightarrow$ ISOPOOH
ISOPOOH + OH	$\rightarrow$ 0.5·XO_2 + 0.5·$ISOPO_2$
$ISOPO_2$ + CH_3O_2	$\rightarrow$ 1.2·CH_2O + 0.19·MACR + 0.26·MVK + 0.3·HYDRALD + 0.25·CH_3OH + HO_2
$ISOPO_2$ + CH_3CO_3	$\rightarrow$ 0.6·CH_2O + 0.25·MACR + 0.35·MVK + 0.4·HYDRALD + CH_3O_2 + HO_2 + CO_2
ISOP + NO_3	$\rightarrow$ $ISOPNO_3$
$ISOPNO_3$ + NO	$\rightarrow$ 10.206·NO_2 + 0.072·CH_2O + 0.167·MACR + 0.039·MVK + 0.794·ONITR + 0.794·HO_2
$ISOPNO_3$ + NO_3	$\rightarrow$ 10.206·NO_2 + 0.072·CH_2O + 0.167·MACR + 0.039·MVK + 0.794·ONITR + 0.794·HO_2
$ISOPNO_3$ + HO_2	$\rightarrow$ 0.206·NO_2 + 0.008·CH_2O + 0.167·MACR
ISOPOOH + hν	$\rightarrow$ 0.402·MVK + 0.288·MACR + 0.69·CH_2O + HO_2
TERPOOH + hν	$\rightarrow$ OH + 0.1·CH_3COCH_3 + HO_2 + MVK + MACR

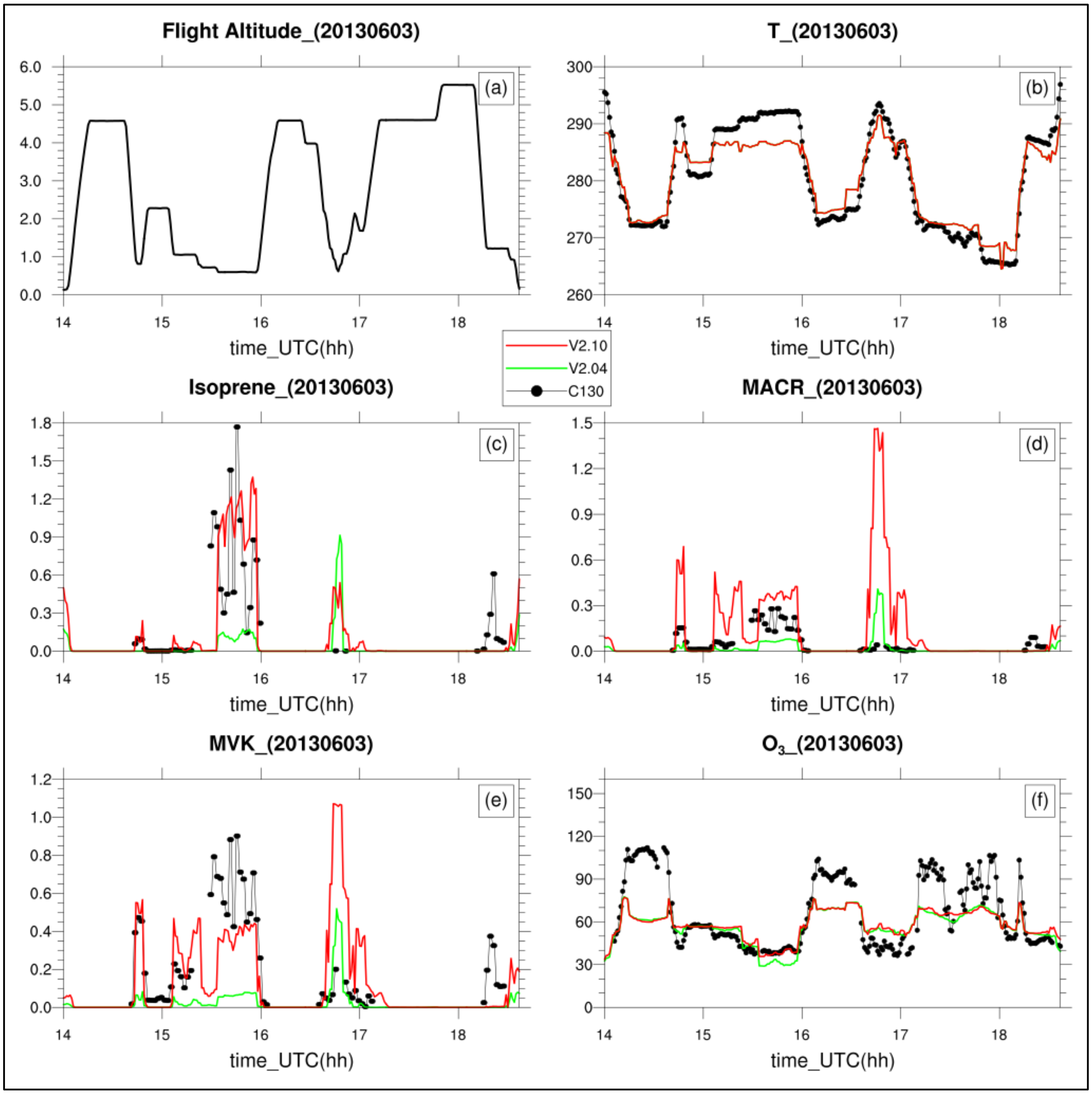

Figure S5: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the first NOMADSS flight (rf01). The black line shows the C-130 aircraft measurements, the green and red lines indicate the WRF-Chem model results using MEGAN version 2.04 (M2.04 run) and MEGAN updated to the version 2.10 (M2.10 run), respectively. In the panel b) the green line is not showed since it is overlapped by the red line, they have identical values.

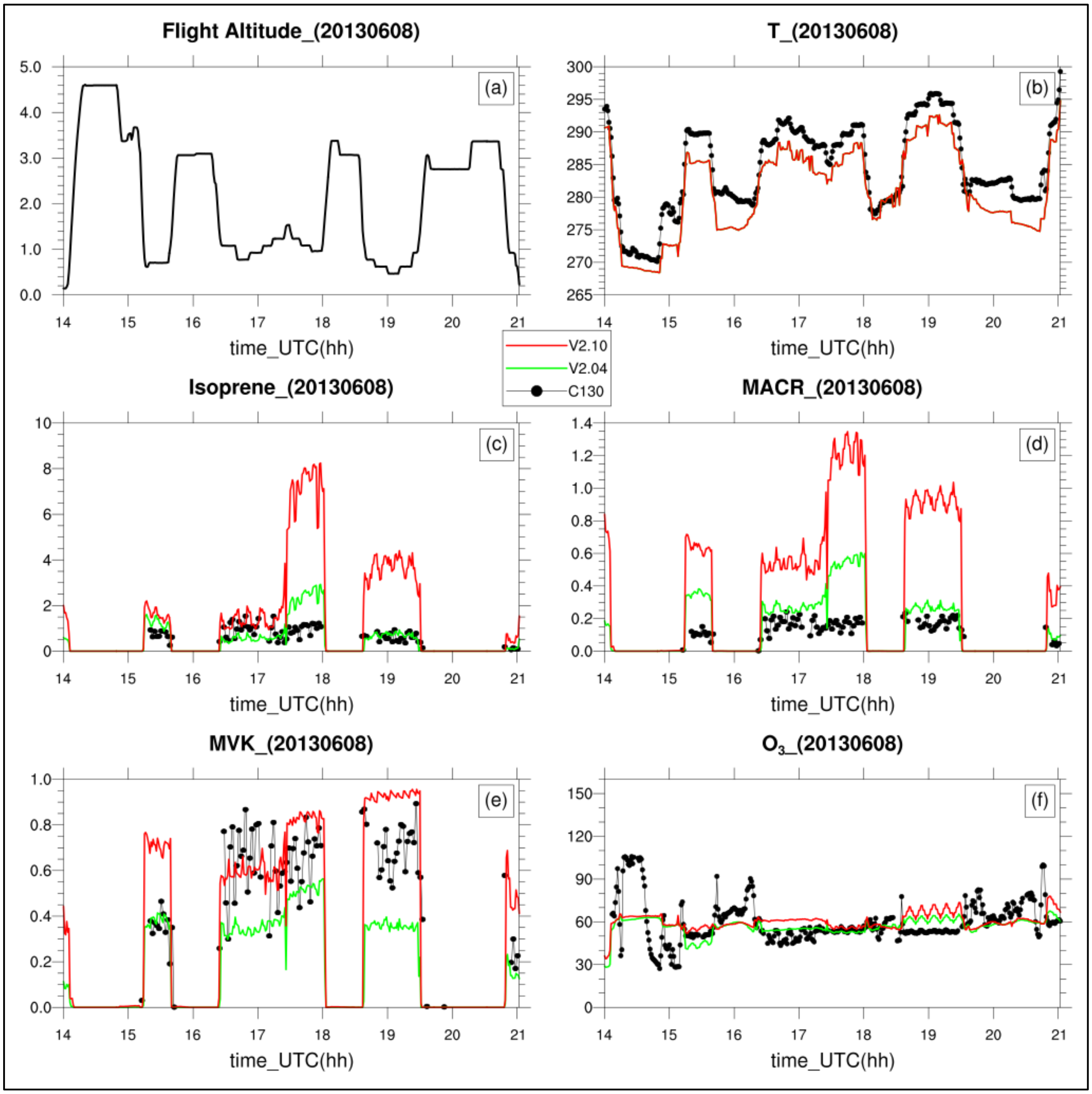

Figure S6: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the third NOMADSS flight (rf03). The black line shows the C-130 aircraft measurements, the green and red lines indicate the WRF-Chem model results using MEGAN version 2.04 (M04 run) and MEGAN updated to the version 2.10 (M10 run), respectively. In the panel b) the green line is not showed since it is overlapped by the red line, they have identical values.

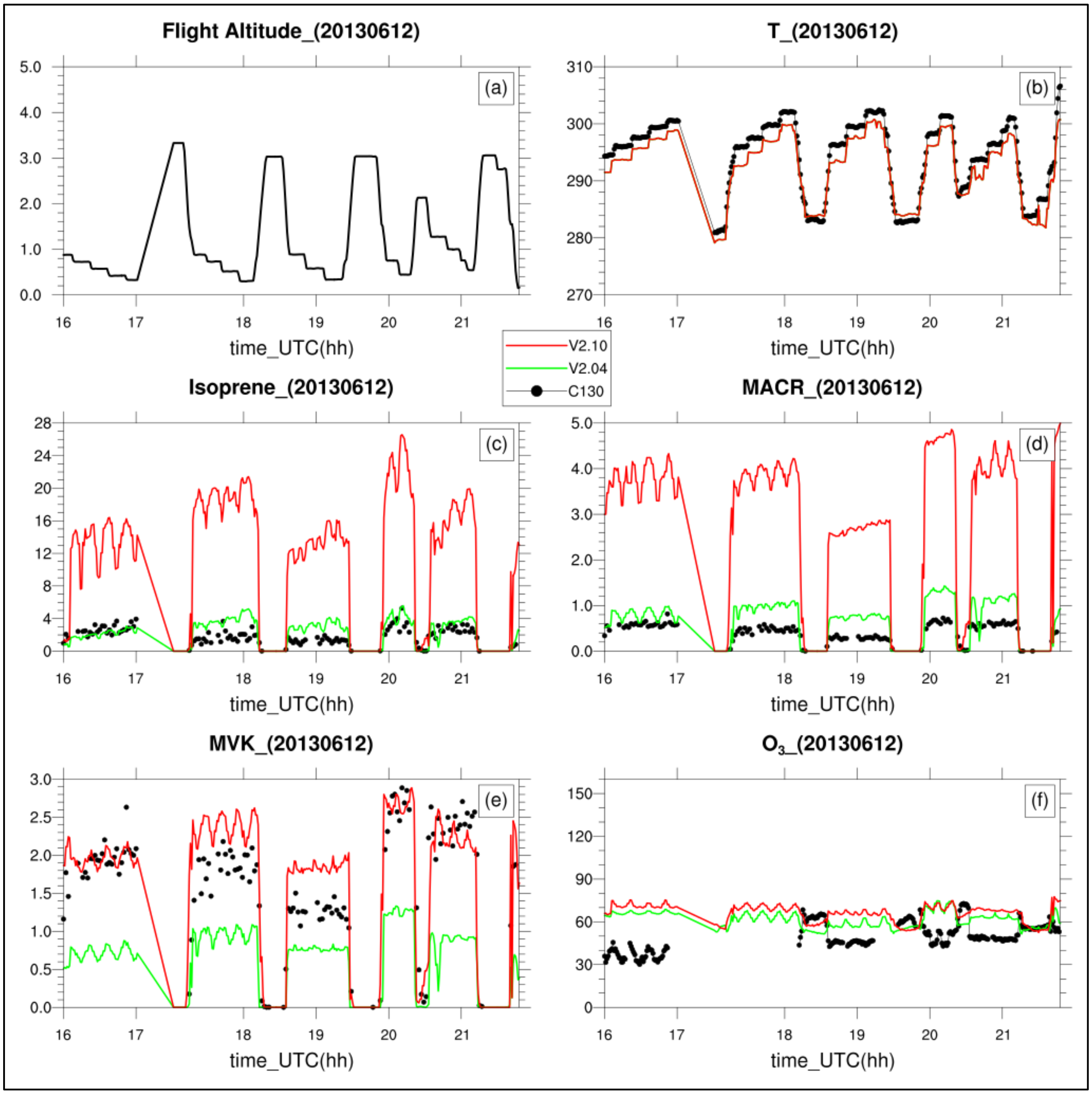

Figure S7: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the fourth NOMADSS flight (rf04). The black line shows the C-130 aircraft measurements, the green and red lines indicate the WRF-Chem model results using MEGAN version 2.04 (M04 run) and MEGAN updated to the version 2.10 (M10 run), respectively. In the panel b) the green line is not showed since it is overlapped by the red line, they have identical values.

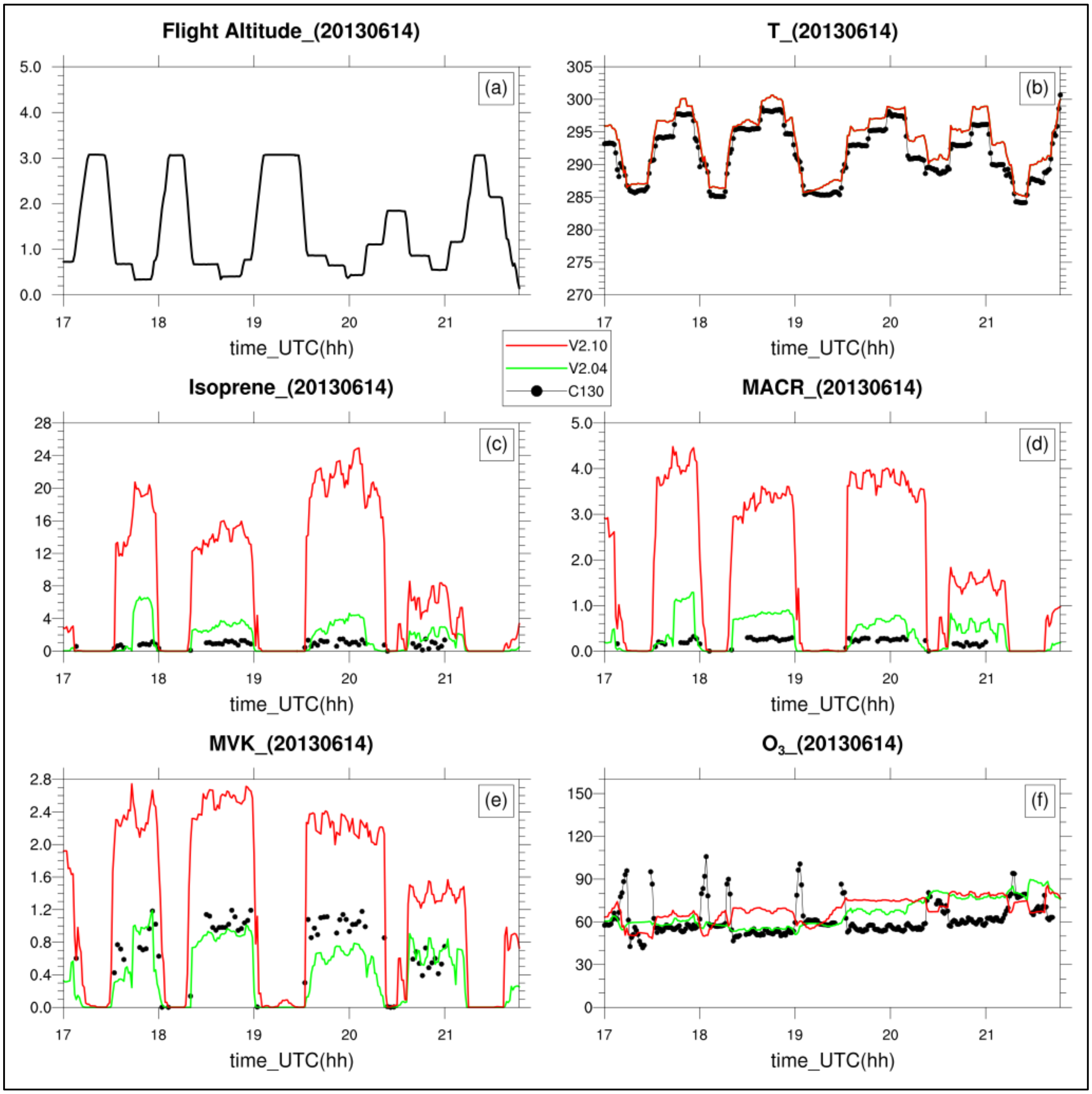

Figure S8: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the fifth NOMADSS flight (rf05). The black line shows the C-130 aircraft measurements, the green and red lines indicate the WRF-Chem model results using MEGAN version 2.04 (M04 run) and MEGAN updated to the version 2.10 (M10 run), respectively. In the panel b) the green line is not showed since it is overlapped by the red line, they have identical values.