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

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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

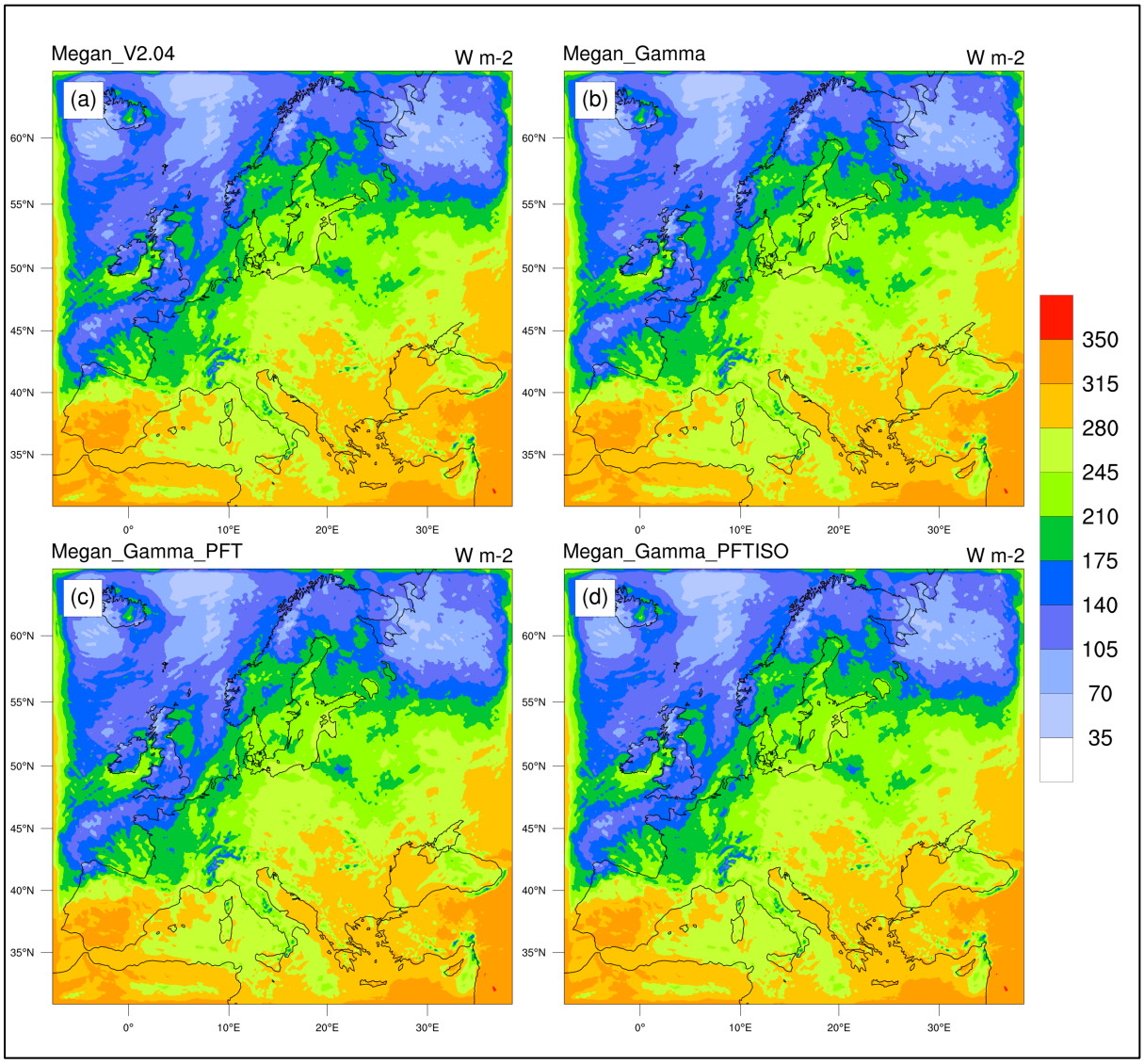

Figure S1: Downward shortwave radiation flux (W m^{-2}) averaged for the time period from August 10, 2015 at 0000 UTC to August 16, 2015 at 0000 UTC for the different WRF-Chem simulations, namely (a) control simulation (M2.04), (b) activity factors (γ_i) updated (MG), (c) PFTs emission factors updated (MGPFT), and (d) the isoprene emission factor updated (M2.10).

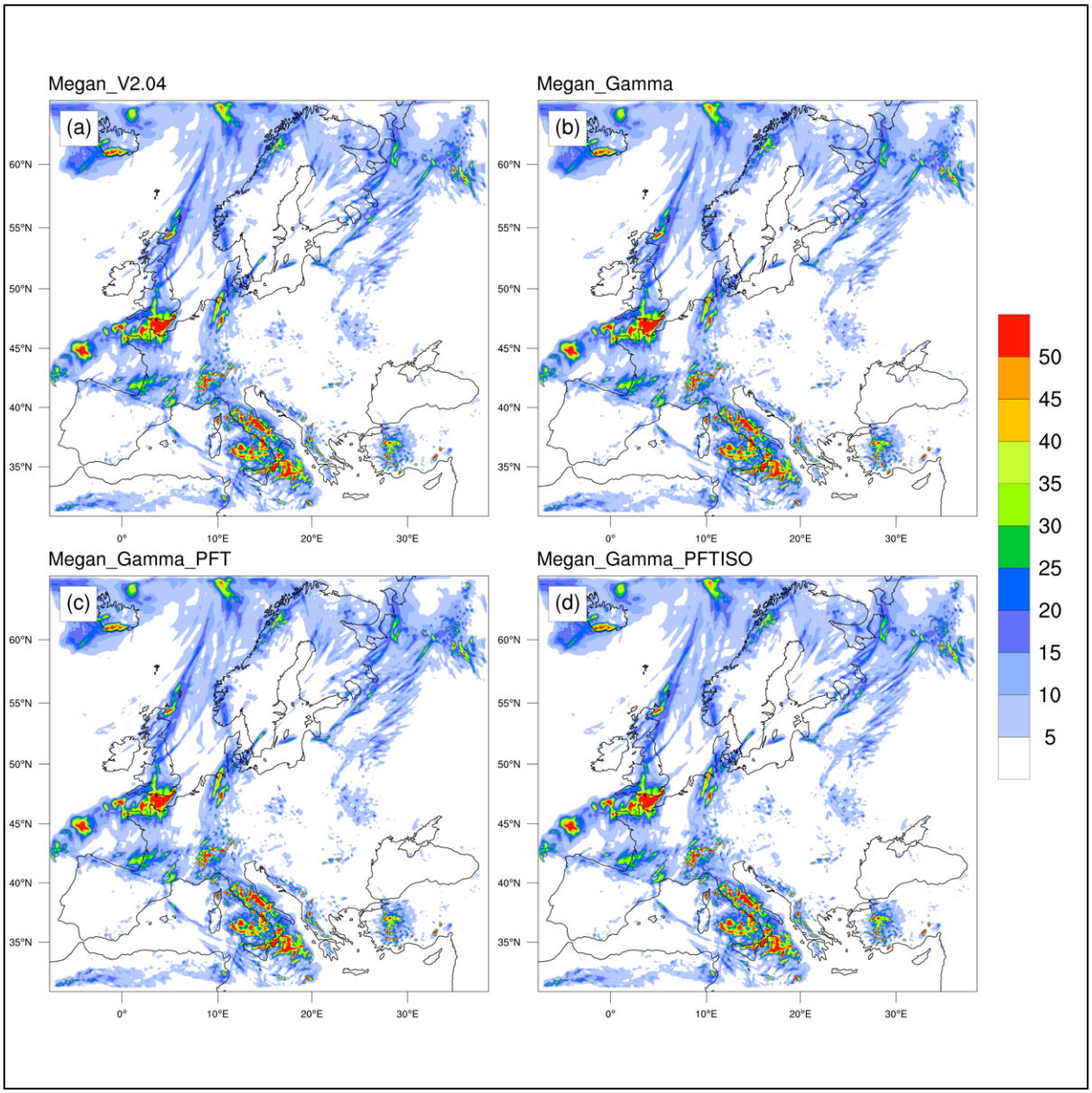

Figure S2: Total precipitation (mm) averaged for the time period from August 10, 2015 at 0000 UTC to August 16, 2015 at 0000 UTC for the different WRF-Chem simulations, namely (a) control simulation (M2.04), (b) activity factors (γ_i) updated (MG), (c) PFTs emission factors updated (MGPFT), and (d) the isoprene emission factor updated (M2.10).

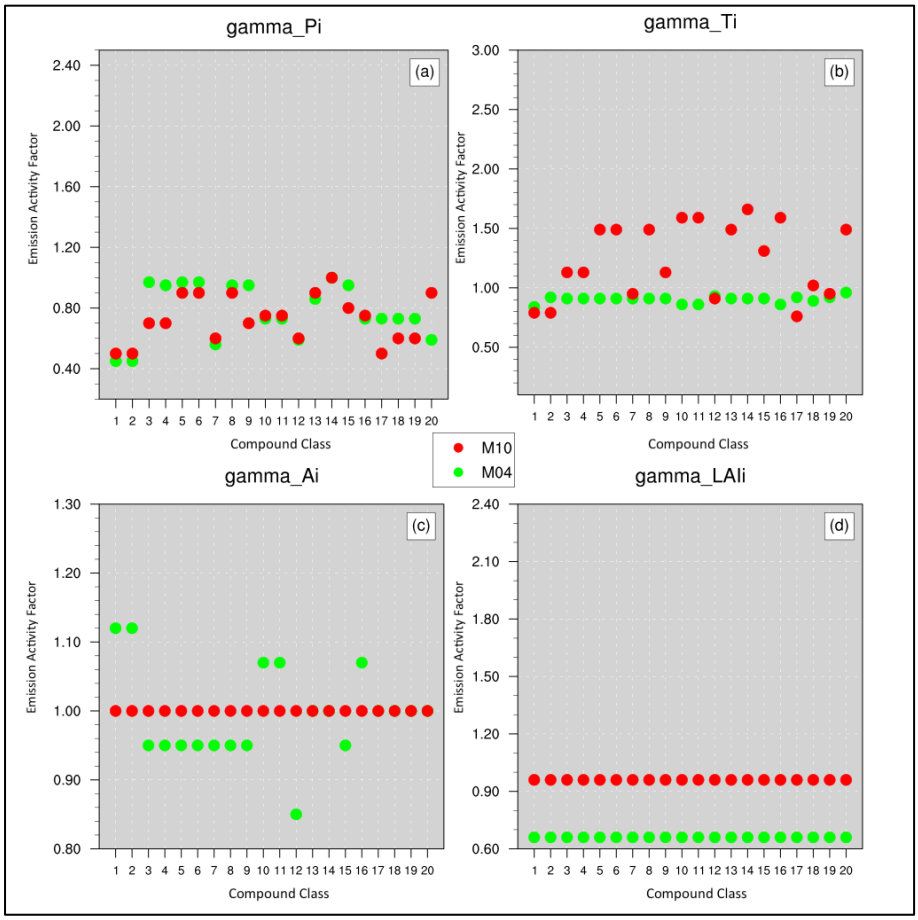

Figure S3: Emission activity factors (y-axis, dimensionless) from M2.04 (M04) and M2.10 (M10) for different compound classes (1. Isoprene, 2. Myrcene, 3. Sabinene, 4. Limonene, 5. 3-Carene, 6. t-β-Ocimene, 7. β-Pinene, 8. α-Pinene, 9. Other Monoterpenes, 10. α-Farnesene, 11. β-Caryophyllene, 12. Other Sesquiterpenes, 13. 232-MBO, 14. Methanol, 15. Acetone, 16. Carbon Monoxide, 17. Nitric Oxide, 18. Bidirectional VOC, 19. Stress VOC and 20. other VOC). Each panel is for a different meteorological factor: (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). The factors refer to the city of Kiev (Ukraine) on August 13th 885 (12:00 UTC), 2015.

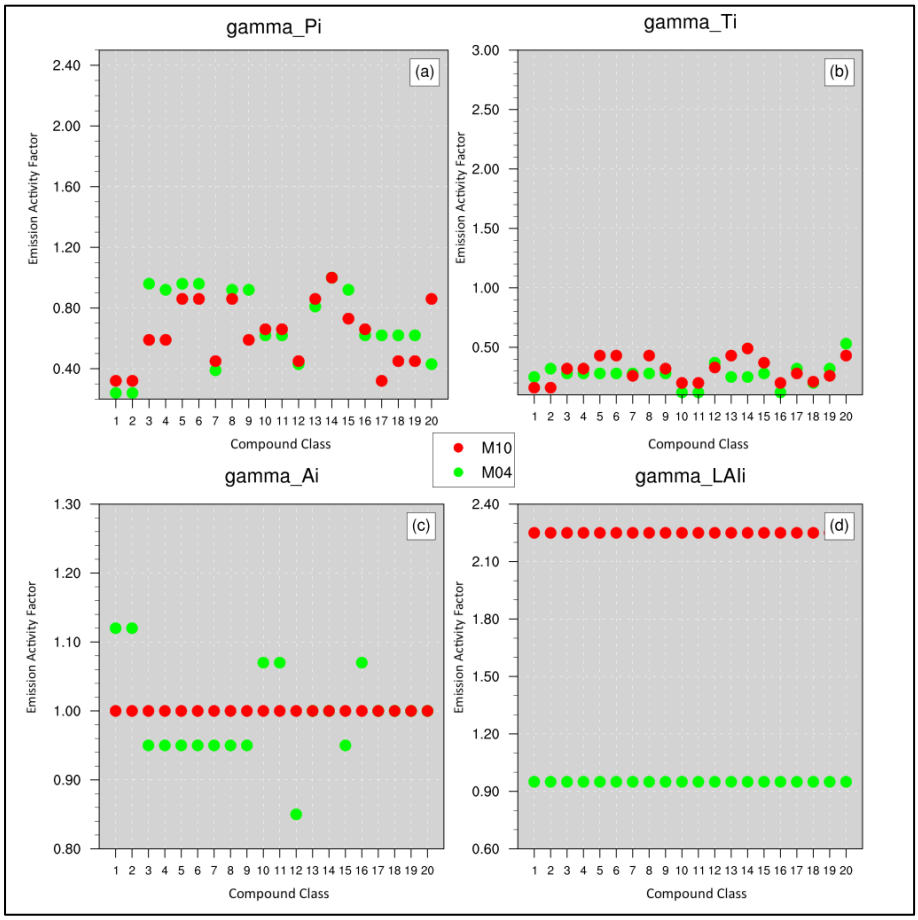

Figure S4: Emission activity factors (y-axis, dimensionless) from M2.04 (M04) and M2.10 (M10) for different compound classes (1. Isoprene, 2. Myrcene, 3. Sabinene, 4. Limonene, 5. 3-Carene, 6. t-β-Ocimene, 7. β-Pinene, 8. α-Pinene, 9. Other Monoterpenes, 10. α-Farnesene, 11. β-Caryophyllene, 12. Other Sesquiterpenes, 13. 232-MBO, 14. Methanol, 15. Acetone, 16. Carbon Monoxide, 17. Nitric Oxide, 18. Bidirectional VOC, 19. Stress VOC and 20. other VOC). Each panel is for a different meteorological factor: (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). The factors refer to the city of Porto (Portugal) on August 13th 885 (12:00 UTC), 2015.

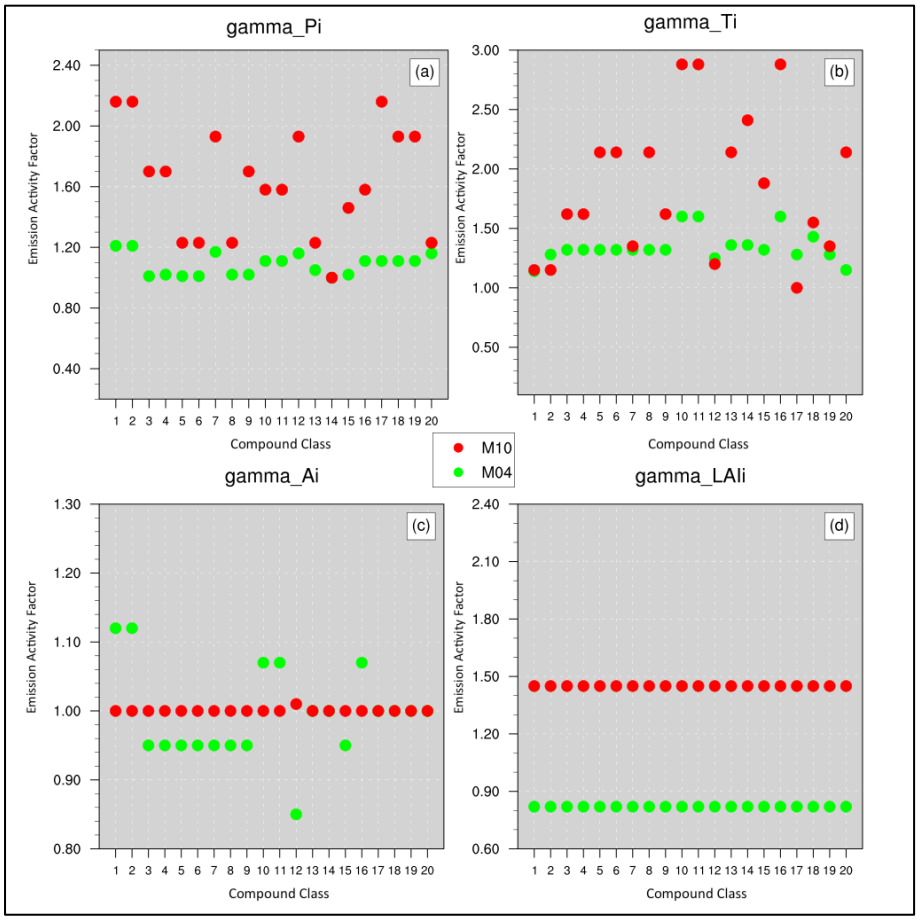

Figure S5: Emission activity factors (y-axis, dimensionless) from M2.04 (M04) and M2.10 (M10) for different compound classes (1. Isoprene, 2. Myrcene, 3. Sabinene, 4. Limonene, 5. 3-Carene, 6. t-β-Ocimene, 7. β-Pinene, 8. α-Pinene, 9. Other Monoterpenes, 10. α-Farnesene, 11. β-Caryophyllene, 12. Other Sesquiterpenes, 13. 232-MBO, 14. Methanol, 15. Acetone, 16. Carbon Monoxide, 17. Nitric Oxide, 18. Bidirectional VOC, 19. Stress VOC and 20. other VOC). Each panel is for a different meteorological factor: (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). The factors refer to the city of Zagreb (Crotia) on August 13th 885 (12:00 UTC), 2015.

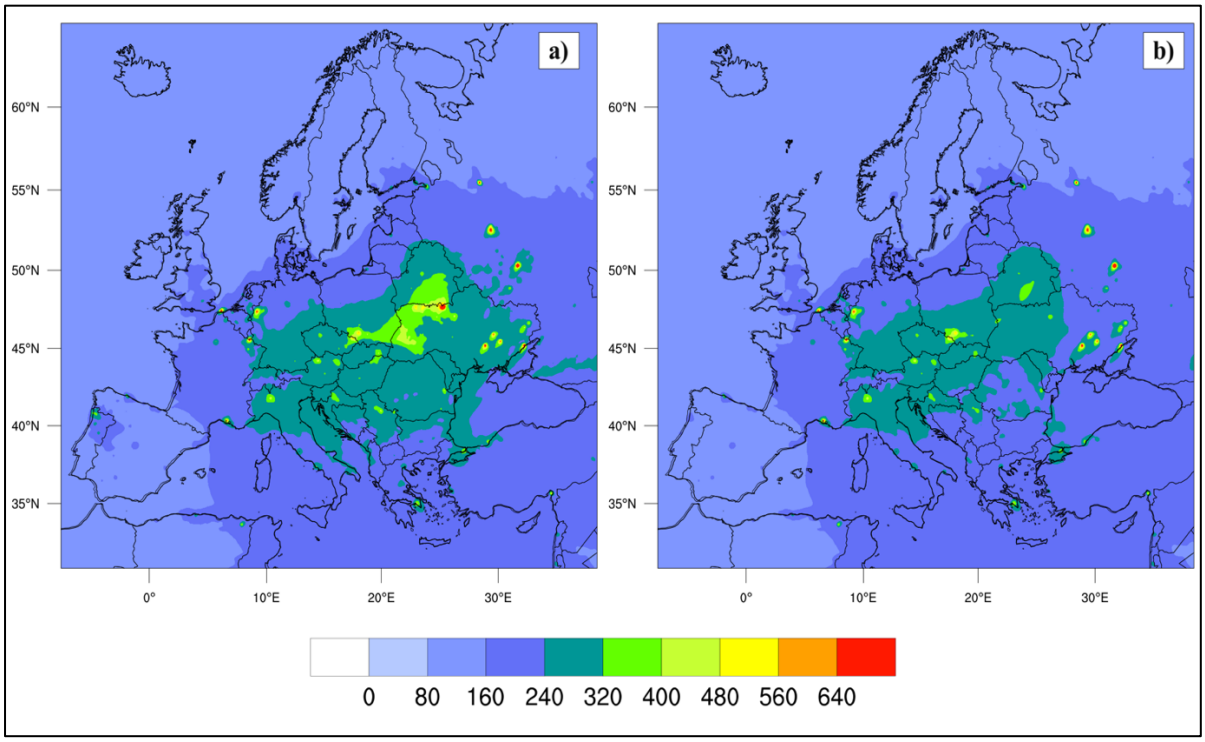

Figure S6: CO concentration (μg m^{-3}) for the simulations (a) with all the MEGAN updates (M2.10 run), and (b) with all the MEGAN updates but without including the biomass burning emissions in the calculation (b - "M10_noFINN"). The maps represent the weekly averages (from August 10th, 2015 at 0000 UTC to August 16th, 2015 at 0000 UTC), extrapolated from WRF-Chem model.

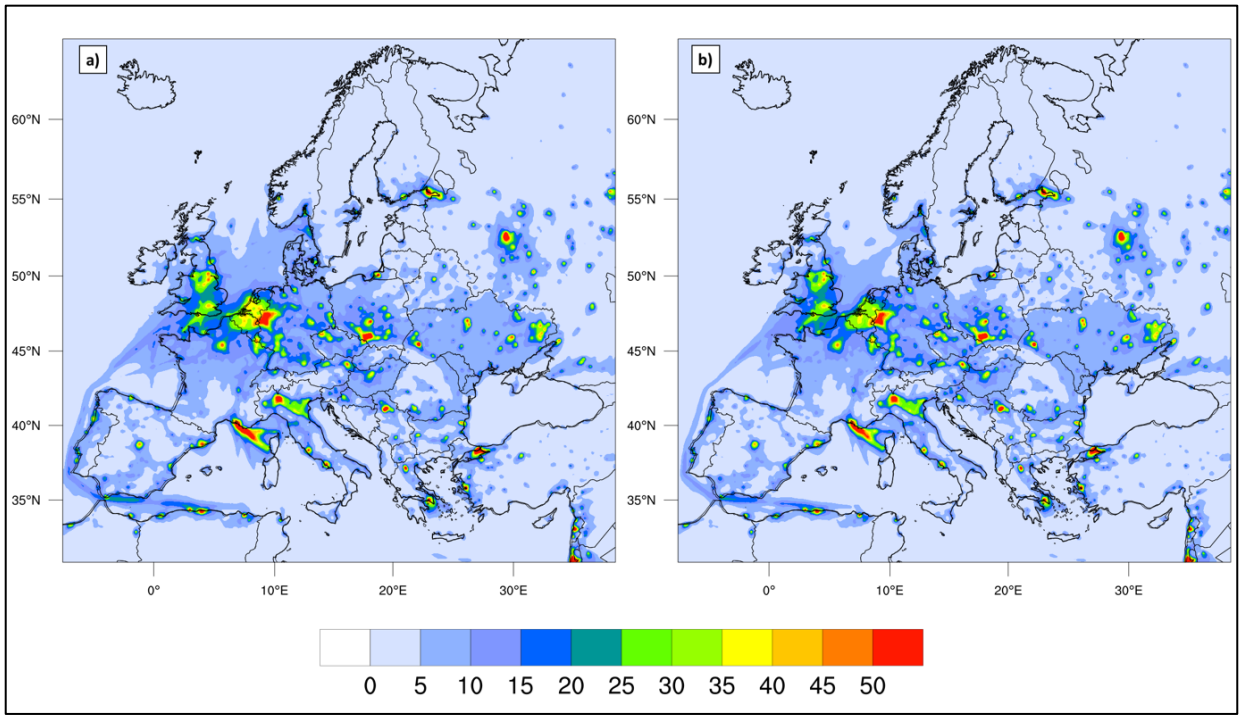

Figure S7: NO2 concentration (µg m^{-3}) for the simulations (a) with all the MEGAN updates (M2.10 run), and (b) with all the MEGAN updates but without including the biomass burning emissions in the calculation (b - "M10_noFINN"). The maps represent the weekly averages (from August 10th, 2015 at 0000 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	→ $ISOPO_2$
ISOP + O_3	→ 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	→ 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	→ HO_2 + NO_2 + 0.6·CH_2O + 0.25·MACR + 0.35·MVK + 0.4·HYDRALD
$ISOPO_2$ + HO_2	→ ISOPOOH
ISOPOOH + OH	→ 0.5·XO_2 + 0.5·$ISOPO_2$
$ISOPO_2$ + CH_3O_2	→ 1.2·CH_2O + 0.19·MACR + 0.26·MVK + 0.3·HYDRALD + 0.25·CH_3OH + HO_2
$ISOPO_2$ + CH_3CO_3	→ 0.6·CH_2O + 0.25·MACR + 0.35·MVK + 0.4·HYDRALD + CH_3O_2 + HO_2 + CO_2
ISOP + NO_3	→ $ISOPNO_3$
$ISOPNO_3$ + NO	→ 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	→ 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	→ 0.206·NO_2 + 0.008·CH_2O + 0.167·MACR
ISOPOOH + hν	→ 0.402·MVK + 0.288·MACR + 0.69·CH_2O + HO_2
TERPOOH + hν	→ OH + 0.1·CH_3COCH_3 + HO_2 + MVK + MACR

Table S3: Summary of the statistics between predicted and measured ozone, isoprene, methyl vinyl ketone (MVK), and methacrolein (MACR), namely the (a) normalized mean bias (bias - %), (b) normalized root mean square errors (nrmse – dimensionless), (c) the correlation coefficient (r - dimensionless), and the relative number of points analyzed (n_{XY}). Values are shown according to the different NOMADSS flights (i.e., rf01, rf02, rf03, rf04, and rf05), and WRF-Chem model runs (M2.04, and M2.10).

		rf01		rf02		rf03		rf04		rf05	
		M2.04	**M2.10**	**M2.04**	**M2.10**	**M2.04**	**M2.10**	**M2.04**	**M2.10**	**M2.04**	**M2.10**
O_3	**nxy**	254	254	385	385	395	395	237	237	268	268
	nrmse	29.8	30.0	36.3	42.4	24.7	26.4	36.0	42.7	22.5	27.0
	r	0.8	0.8	-0.5	-0.7	0.2	0.0	-0.6	-0.6	0.2	-0.2
	bias	-13.4	-11.5	24.3	30.4	-3.6	2.0	22.6	31.4	7.8	11.9
Isoprene	**nxy**	88	88	162	162	168	168	121	121	59	59
	nrmse	161.3	128.4	59.8	500.3	97.3	427.9	78.4	697.9	274.8	1677.6
	r	0.2	0.6	0.6	0.6	0.4	0.3	0.5	0.6	0.4	0.5
	bias	-85.1	4.3	27.1	437.7	26.2	298.5	41.6	621.8	203.6	1485.2
MVK	**nxy**	118	118	164	164	178	178	126	126	64	64
	nrmse	131.4	115.4	61.0	73.8	53.6	45.5	64.4	31.1	40.0	159.9
	r	0.2	0.3	0.6	0.4	0.5	0.5	0.8	0.8	0.7	0.9
	bias	-86.7	-10.3	-39.6	35.6	-41.1	17.7	-56.8	12.3	-22.3	147.1
MACR	**nxy**	118	118	164	164	174	174	124	124	60	60
	nrmse	129.2	428.4	113.3	565.9	136.4	440.1	99.8	697.1	223.1	1397.4
	r	0.3	0.2	0.6	0.3	0.3	0.4	0.8	0.8	0.6	0.8
	bias	-64.7	204.6	87.2	493.8	95.5	382.8	79.8	645.8	178.0	1295.9

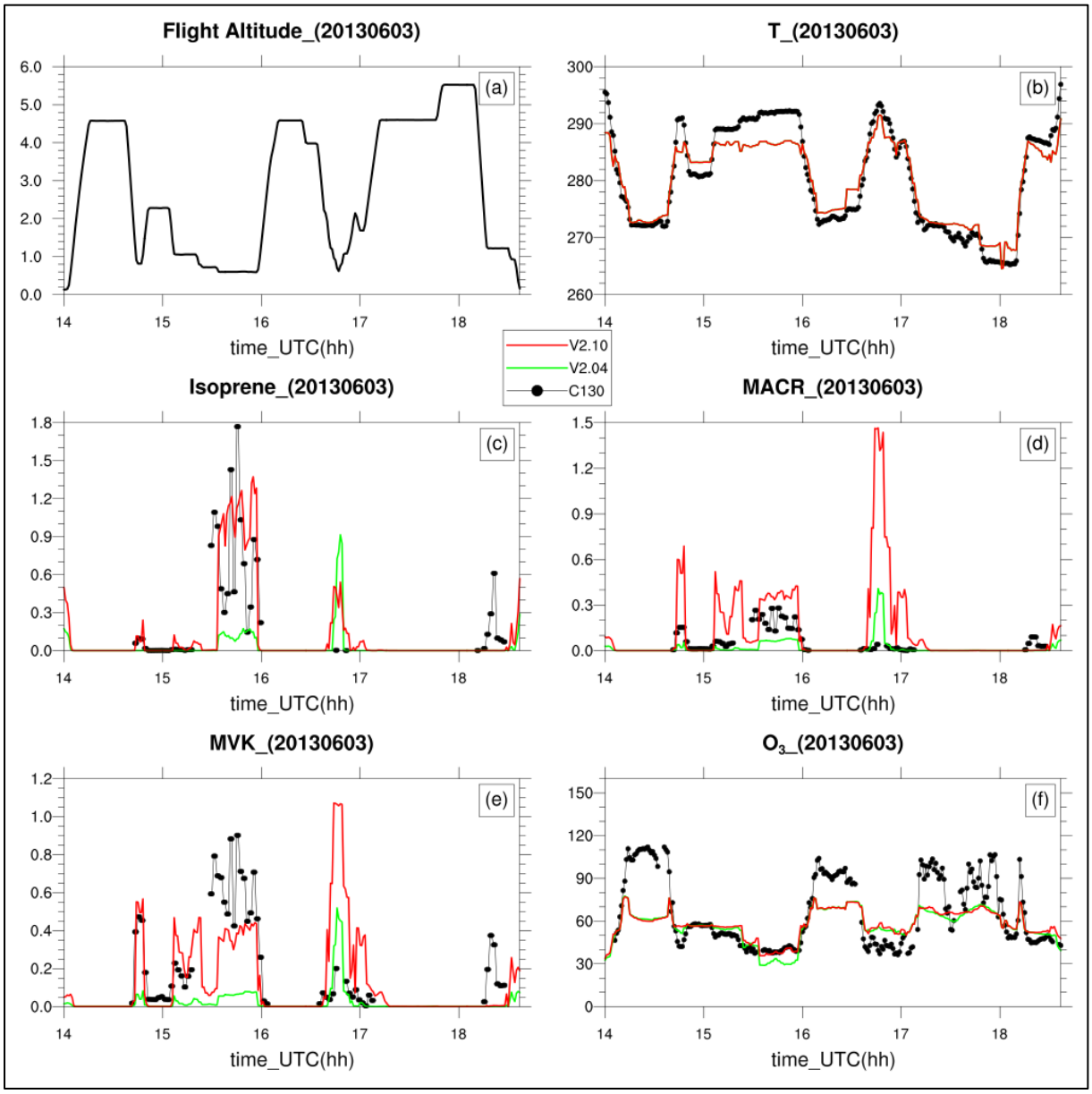

Figure S8: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the first NOMADSS flight (rf01). The black line shows the C-130 aircraft measurements, the green and 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.

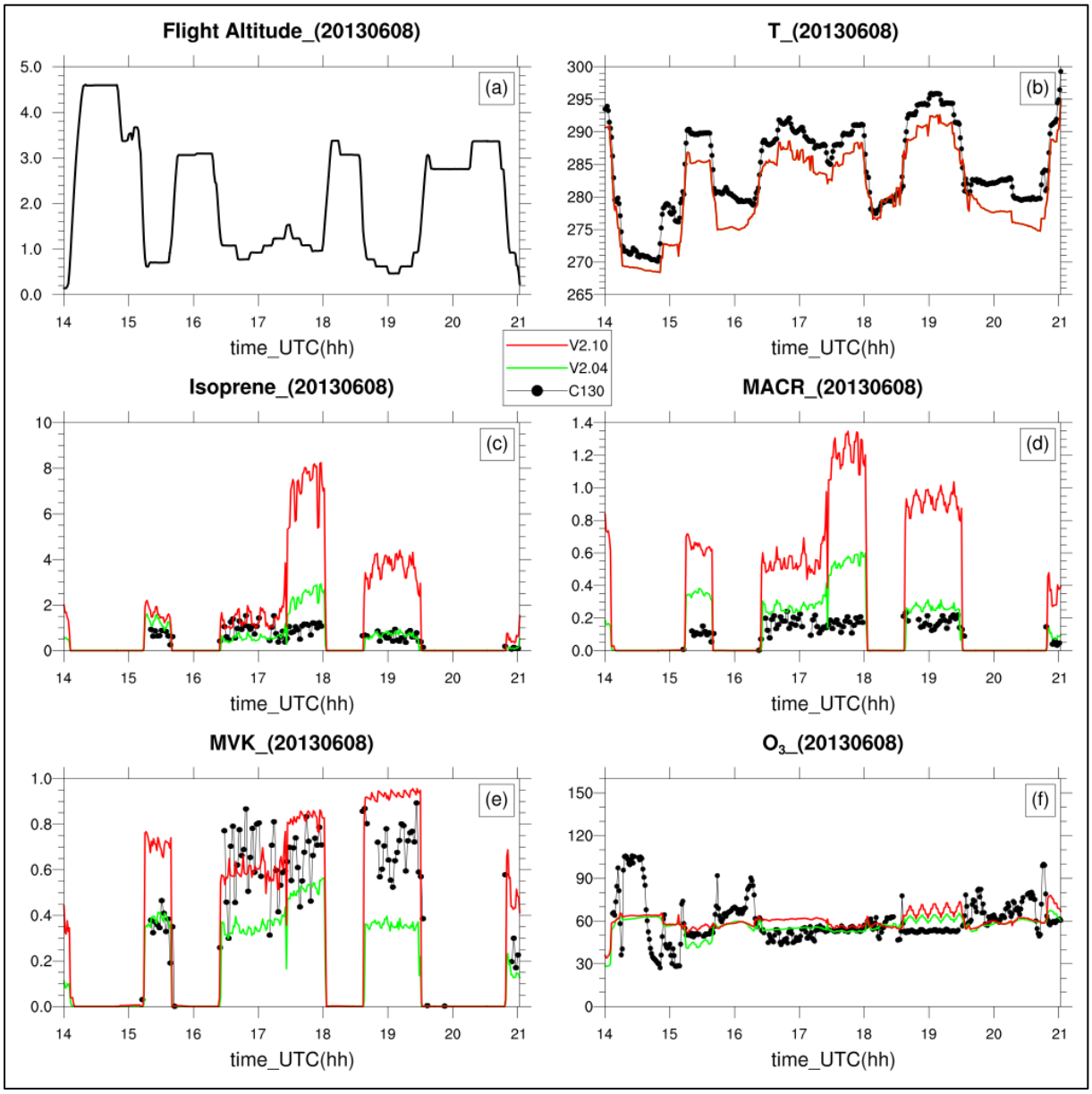

Figure S9: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the third NOMADSS flight (rf03). The black line shows the C-130 aircraft measurements, the green and 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.

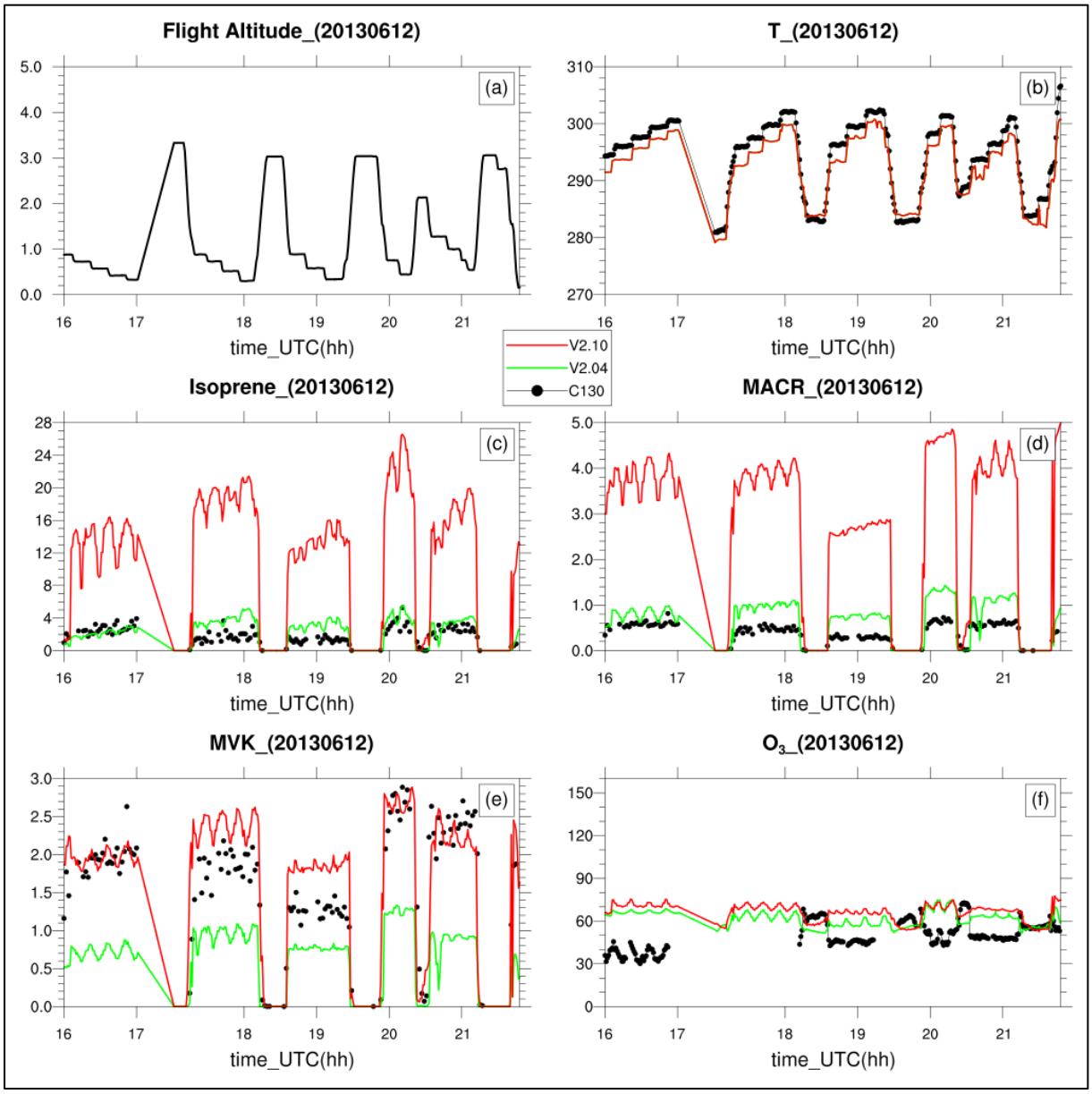

Figure S10: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the fourth NOMADSS flight (rf04). The black line shows the C-130 aircraft measurements, the green and 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.

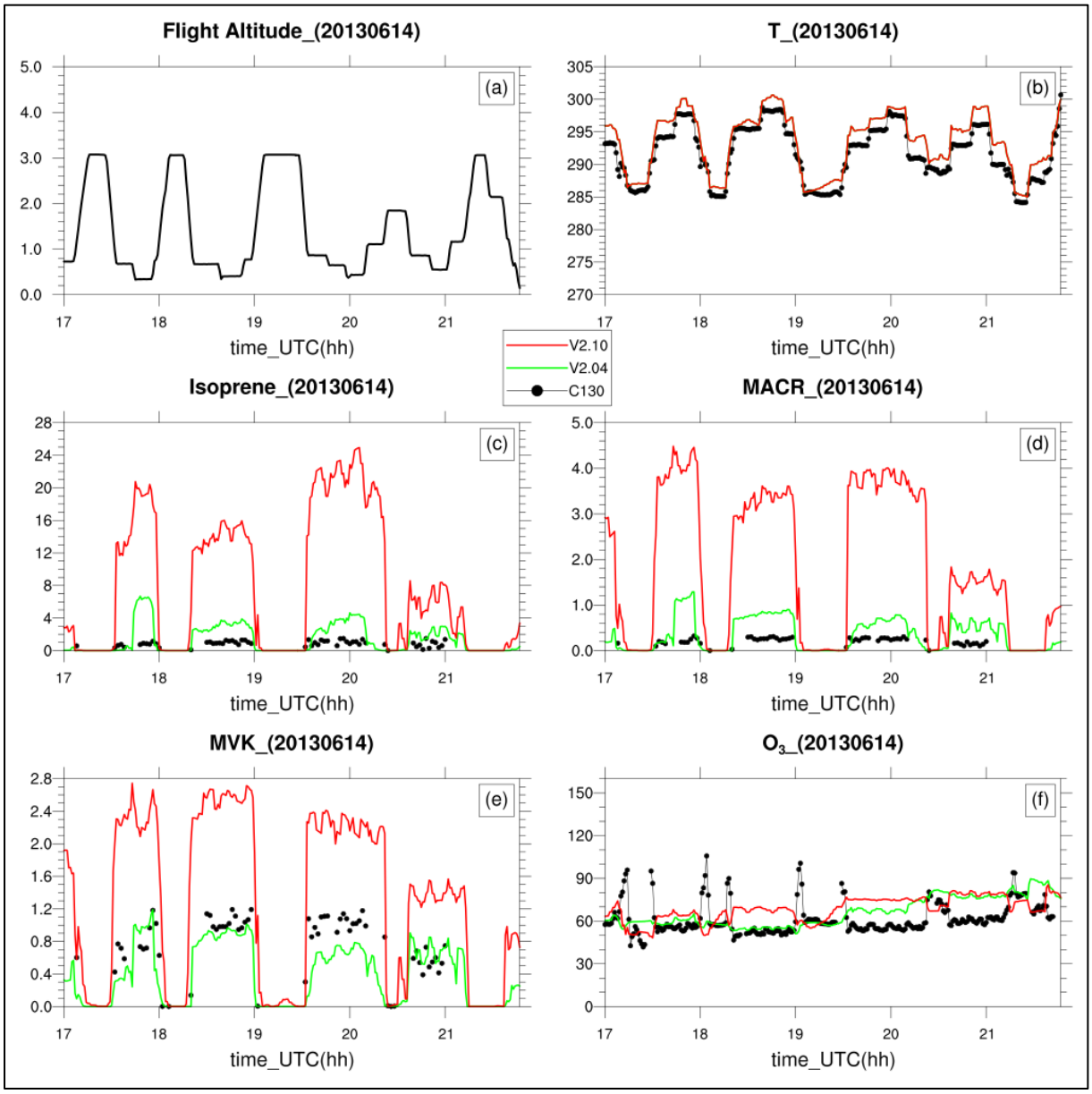

Figure S11: The flight altitude (a - km), the temperature (b - K), the concentration of isoprene (c - ppb), methacrolein (MACR) (d - ppb), methyl vinyl ketone (MVK) (e – ppb), and ozone (f - ppb), for the fifth NOMADSS flight (rf05). The black line shows the C-130 aircraft measurements, the green and 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.