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Supplement of

Secondary inorganic aerosols in Europe: sources and the significant influence of biogenic VOC emissions, especially on ammonium nitrate

Sebnem Aksoyoglu et al.

Correspondence to: Sebnem Aksoyoglu (sebnem.aksoyoglu@psi.ch)

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Supplementary Material

Table S1: Reactions and rate constants for biogenic VOCs in the CB05 mechanism (ENVIRON, 2011)

Isoprene reactions	Reaction products	k ₂₉₈ (ppm ⁻ⁿ min ⁻¹)
ISOP + O	0.75 ISPD + 0.5 FORM + 0.25 XO2 + 0.25 HO2 + 0.25 CXO3 + 0.25 PAR	5.318E+04
ISOP+OH	0.912 ISPD + 0.629 FORM + 0.991 XO2 + 0.912 HO2 + 0.088 XO2N	1.473E+05
ISOP + O3	0.65 ISPD + 0.6 FORM + 0.2 XO2 + 0.066 HO2 + 0.266 OH + 0.2 CXO3 + 0.15 ALDX + 0.35 PAR + 0.066 CO	1.898E-02
ISOP+NO3	0.2 ISPD + 0.8 NTR + XO2 + 0.8 HO2 + 0.2 NO2 + 0.8 ALDX + 2.4 PAR	9.954E+02
ISOP + NO2	0.2 ISPD + 0.8 NTR + XO2 + 0.8 HO2 + 0.2 NO + 0.8 ALDX + 2.4 PAR	2.216E-04
ISPD+OH	1.565 PAR + 0.167 FORM + 0.713 XO2 + 0.503 HO2 + 0.334 CO + 0.168 MGLY + 0.252 ALD2 + 0.21 C2O3 + 0.25 CXO3 + 0.12 ALDX	4.963E+04
ISPD + O3	0.114 C2O3 + 0.15 FORM + 0.85 MGLY + 0.154 HO2 + 0.268 OH + 0.064 XO2 + 0.02 ALD2 + 0.36 PAR + 0.225 CO	1.049E-02
ISPD+NO3	0.357 ALDX + 0.282 FORM + 1.282 PAR + 0.925 HO2 + 0.643 CO + 0.85 NTR + 0.075 CXO3 + 0.075 XO2 + 0.15 HNO3	1.477E+00
ISPD	0.333 CO + 0.067 ALD2 + 0.9 FORM + 0.832 PAR + 1.033 HO2 + 0.7 XO2 + 0.967 C2O3	photolysis
Terpene reactions		
TERP + O	0.15 ALDX + 5.12 PAR	5.318E+04
TERP+OH	0.75 HO2 + 1.25 XO2 + 0.25 XO2N + 0.28 FORM + 1.66 PAR + 0.47 ALDX	9.997E+04
TERP + O3	0.57 OH + 0.07 HO2 + 0.76 XO2 + 0.18 XO2N + 0.24 FORM + 0.001 CO + 7 PAR + 0.21 ALDX + 0.39 CXO3	1.128E-01
TERP+NO3	0.47 NO2 + 0.28 HO2 + 1.03 XO2 + 0.25 XO2N + 0.47 ALDX + 0.53 NTR	9.833E+03
OH	Hydroxyl radical	
HO2	Hydroperoxy radical	
NO2	Nitrogen dioxide	
NO3	Nitrate radical	
HNO3	Nitric acid	
NTR	Organic nitrate (RNO ₃)	
CO	Carbon monoxide	
FORM	Formaldehyde	
ALD2	Acetaldehyde	
ALDX	Propionaldehyde and higher aldehydes	
PAR	Paraffin carbon bond (C-C)	
XO2	NO to NO2 conversion from alkylperoxy (RO ₂) radical	
XO2N	NO to organic nitrate conversion from alkylperoxy (RO ₂) radical	
MGLY	Methylglyoxal and other aromatic products	
C2O3	Acetylperoxy radical	
CXO3	C3 and higher acylperoxy radicals	
ISOP	Isoprene	
ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)	
TERP	Terpene	

Table S2: Biogenic SOA precursor reactions included in CAMx (ENVIRON, 2011)

Precursor	Reaction	CG (condensable gas) products	k ₂₉₈ (ppm ⁻ⁿ min ⁻¹)
Isoprene	ISP + O	none	5.32E+04
	ISP + OH	0.015 CG3 + 0.12 CG4	1.47E+05
	ISP + O ₃	none	1.90E-02
	ISP + NO ₃	none	9.96E+02
Terpenes	TRP + O	0.065 CG5 + 0.29 CG6	4.12E+04
	TRP + OH	0.065 CG5 + 0.29 CG6	7.76E+04
	TRP + O ₃	0.065 CG5 + 0.29 CG6	1.33E-01
	TRP + NO ₃	0.065 CG5 + 0.29 CG6	9.18E+03
Sesquiterpenes	SQT + OH	0.85 CG7	2.91E+05
	SQT + O ₃	0.85 CG7	1.71E+01
	SQT + NO ₃	0.85 CG7	2.81E+04

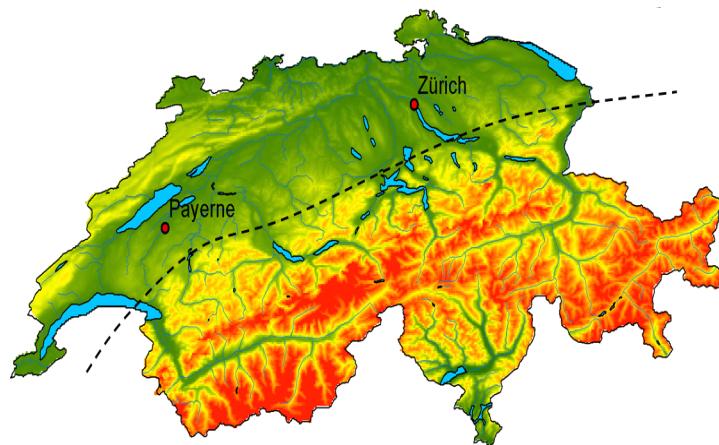


Figure S1: The Swiss Plateau (the region above the dashed line) used as receptor in PSAT calculations.

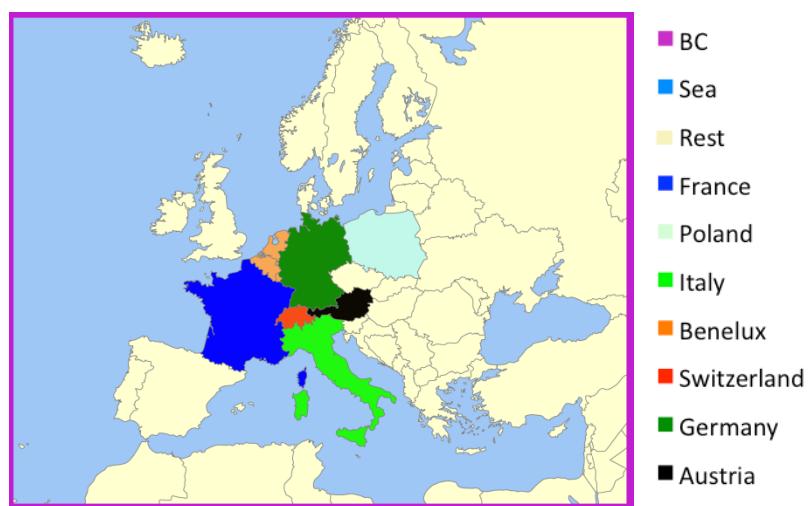


Figure S2: Source regions used in PSAT calculations. Note that this map was only used for illustration of the regions and their colors and it doesn't have the same projection used in the model simulations.

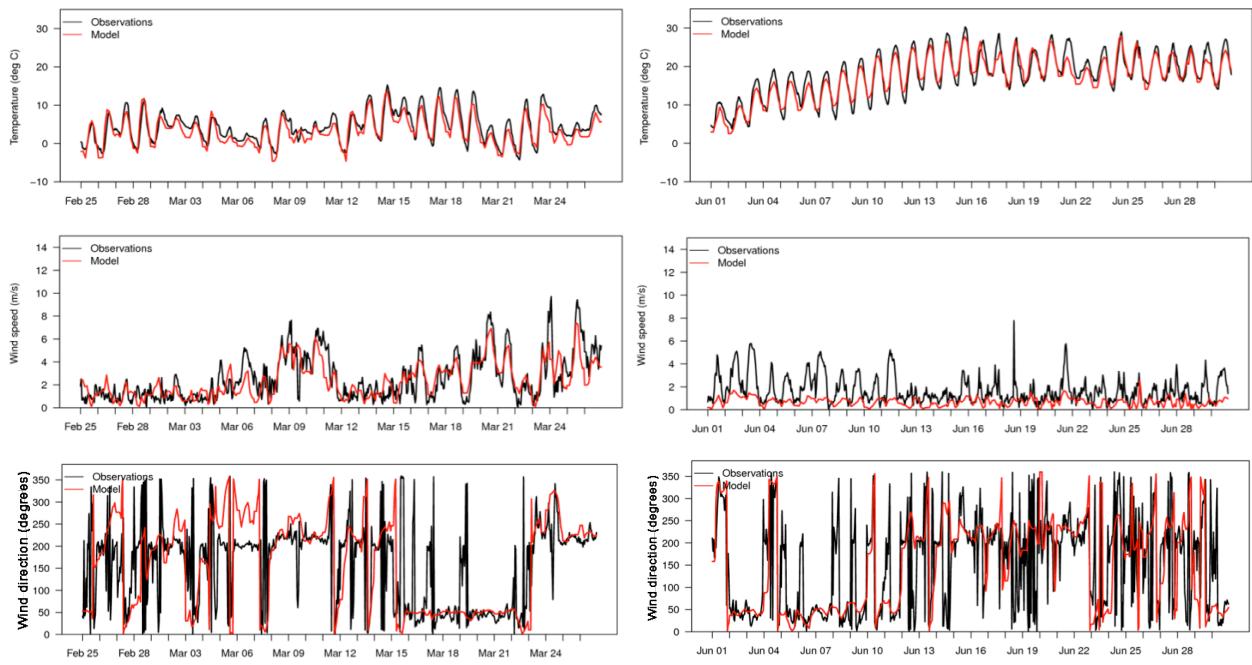


Figure S3: Modelled (red) and measured (black) temperature, wind speed and wind direction for the cold season in Feb-Mar 2009 (left) and the warm season in June 2006 (right) in Payerne, Switzerland.

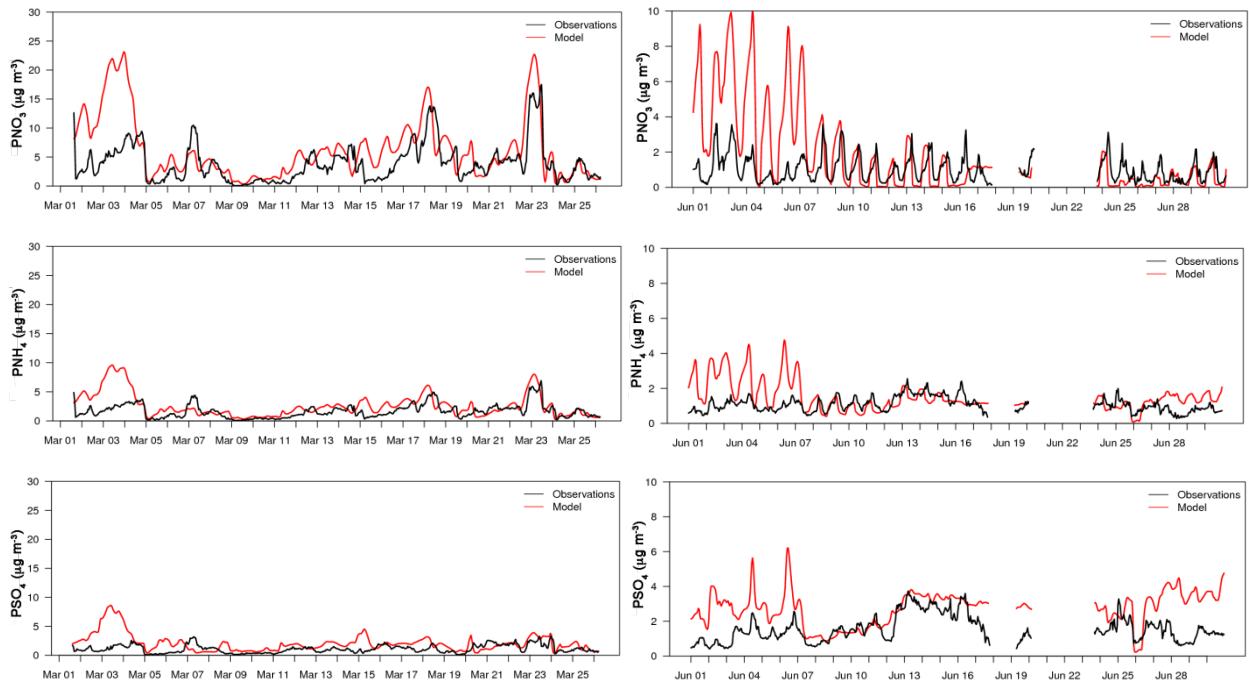


Figure S4: Modelled (red) and measured (black) nitrate (PNO_3), ammonium (PNH_4) and sulfate (PSO_4) for the cold season in Mar 2009 (left) and the warm season in June 2006 (right) in Payerne, Switzerland.

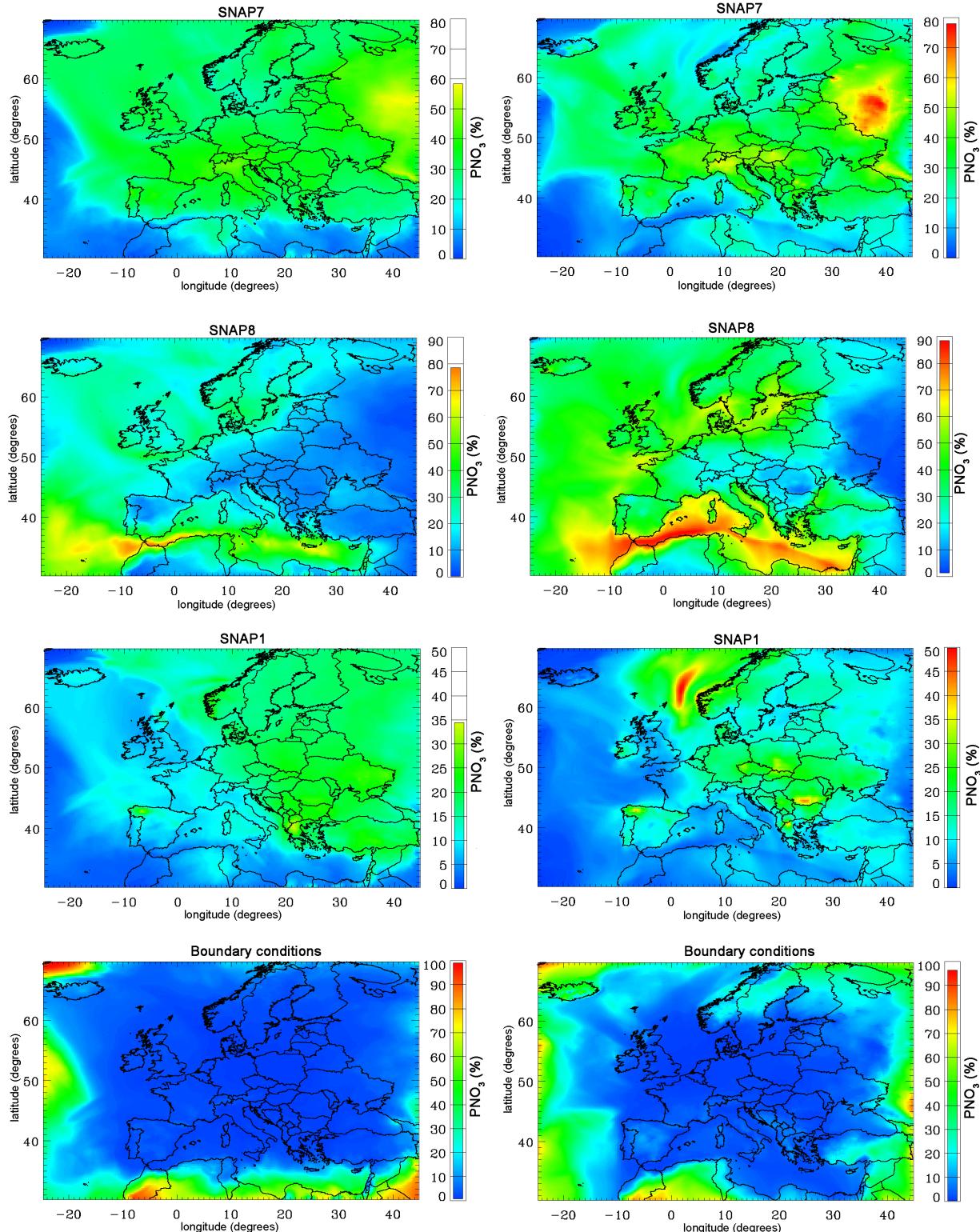


Figure S5: Relative contributions to PNO_3 from road transport (SNAP7), ships (SNAP8), combustion in energy and transformation industries (SNAP1) and boundary conditions in February-March 2009 (left) and in June 2006 (right).

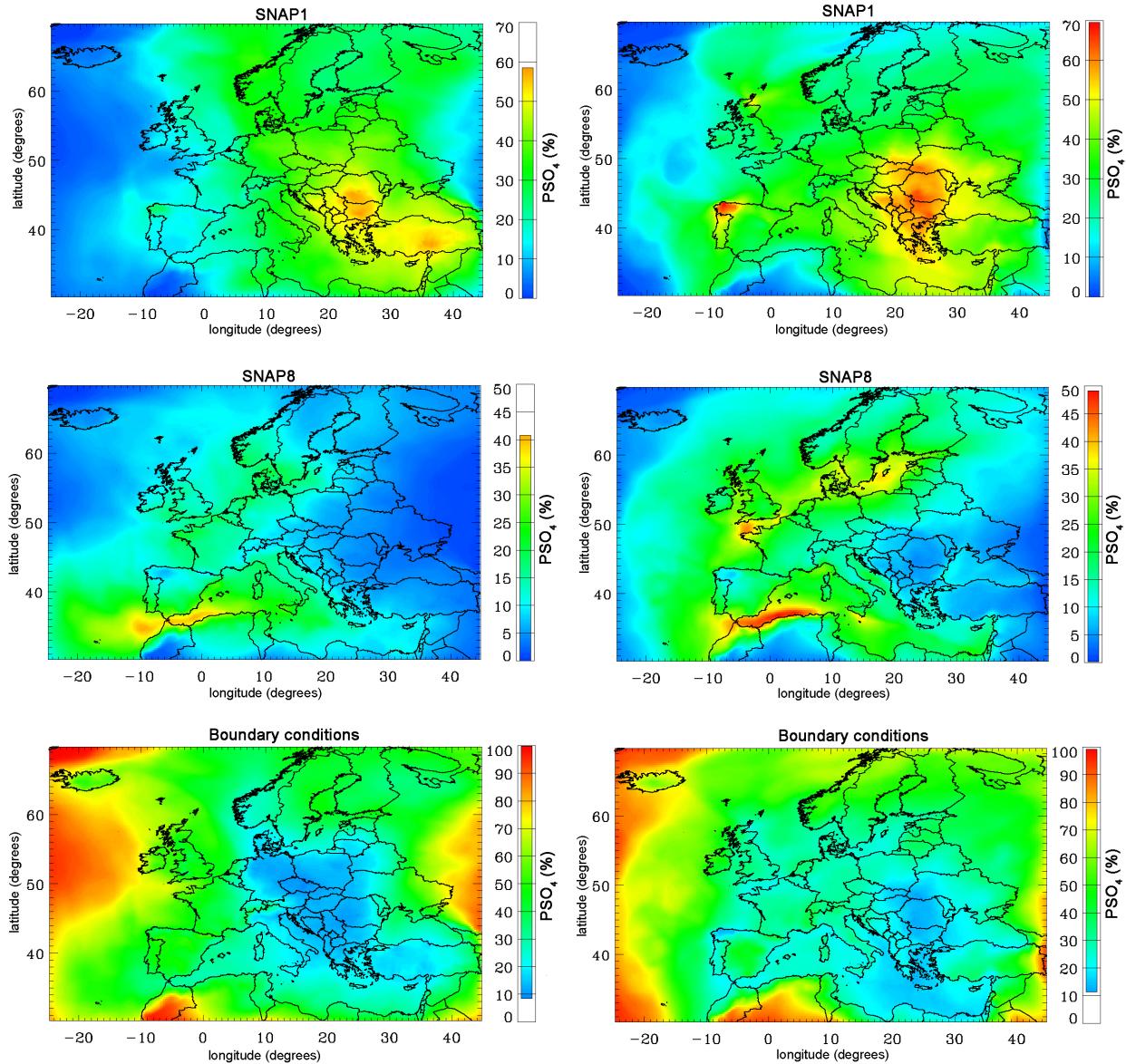


Figure S6: Relative contributions to PSO_4 from combustion in energy and transformation industries (SNAP1), ships (SNAP8) and boundary conditions in February–March 2009 (left) and in June 2006 (right).

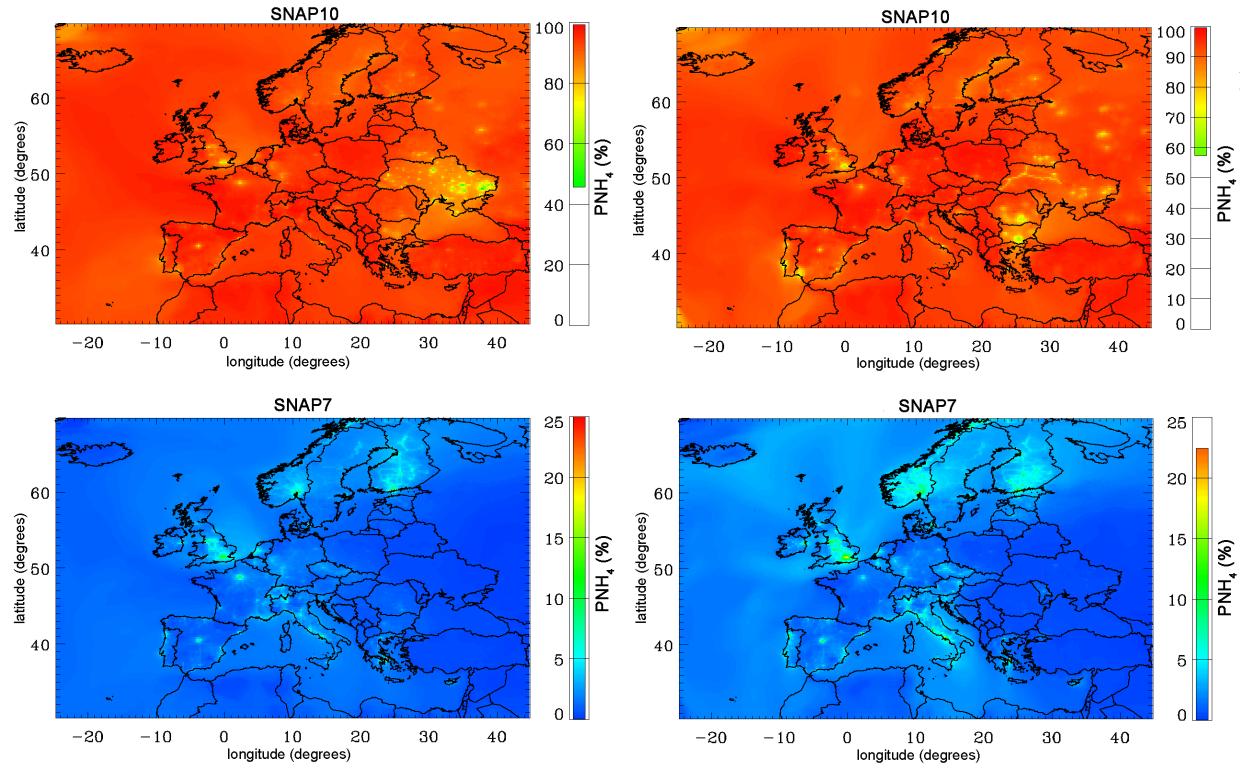


Figure S7: Relative contributions to PNH_4 from agriculture (SNAP10) and road transport (SNAP7) in February-March 2009 (left) and in June 2006 (right).

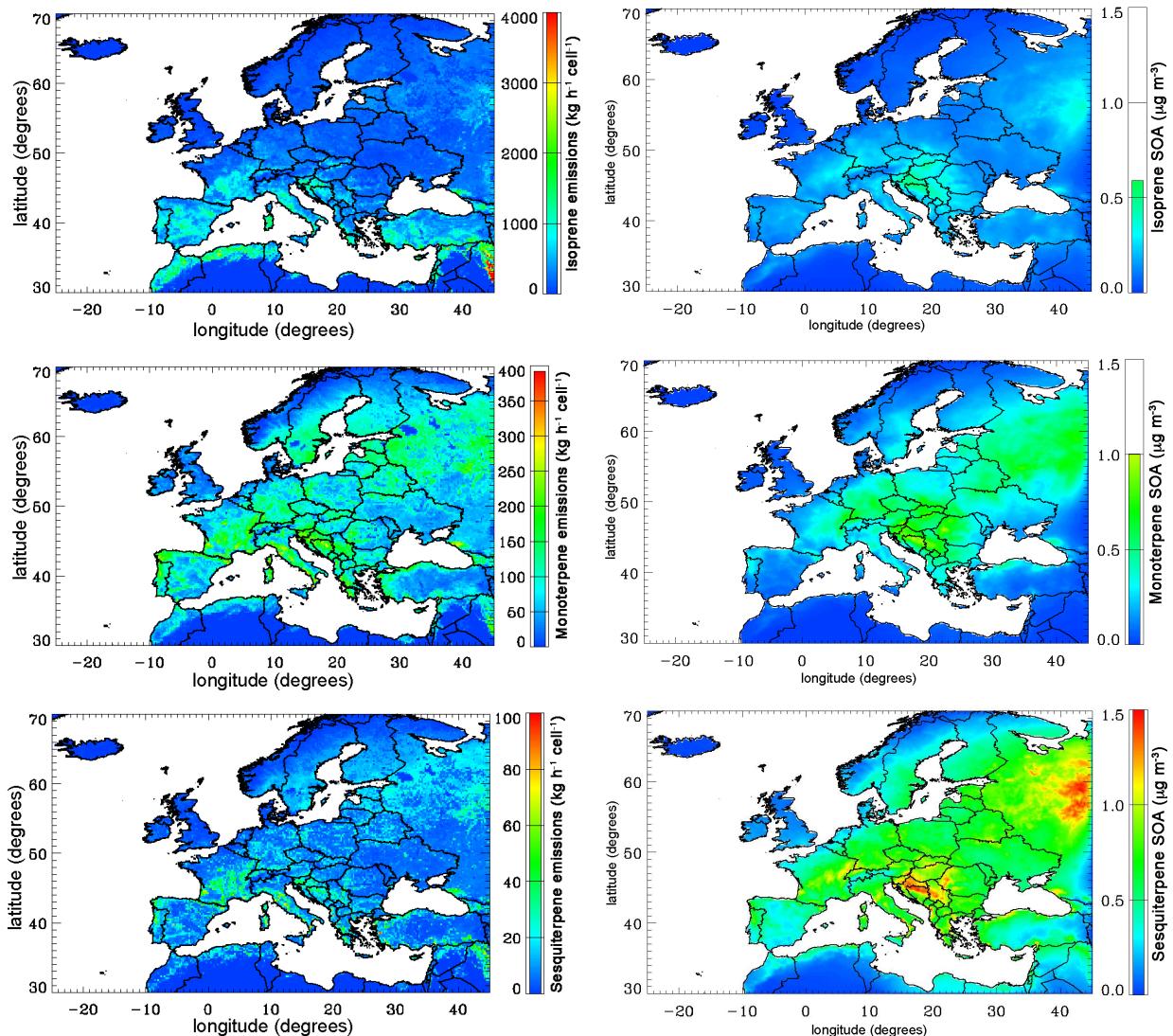


Figure S8: Monthly average emissions of biogenic species (left) and their SOA products (right); isoprene (top), monoterpenes (middle) and sesquiterpenes (bottom) in June 2006.

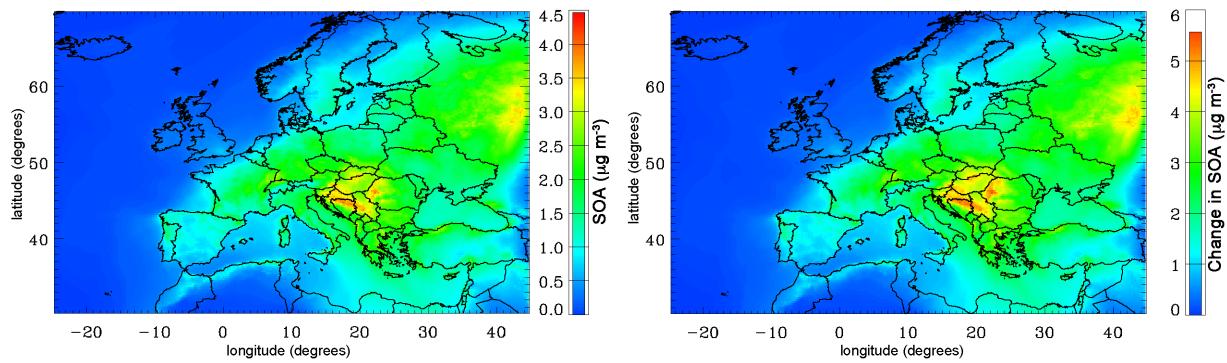


Figure S9: Total SOA concentrations in the base case (left) and changes in SOA when BVOC emissions were doubled (right) in June 2006.

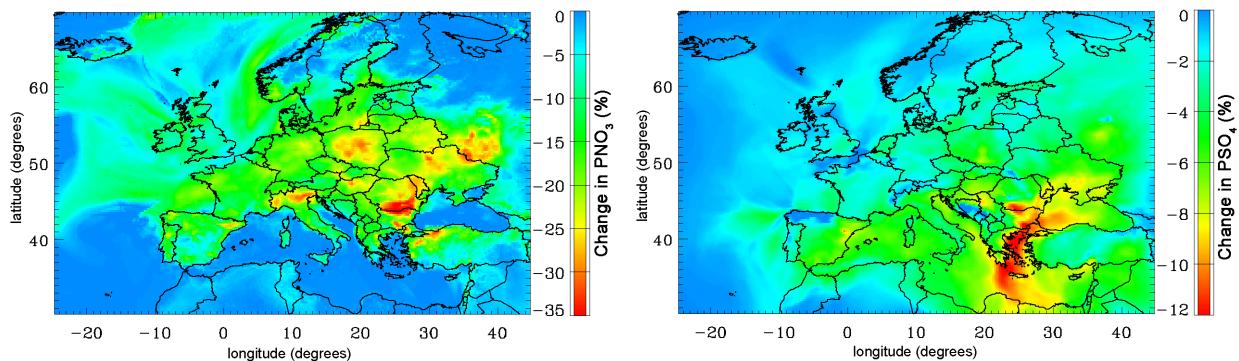


Figure S10: Relative changes in PNO_3 (left) and PSO_4 (right) concentrations in June 2006 when BVOC emissions were doubled.

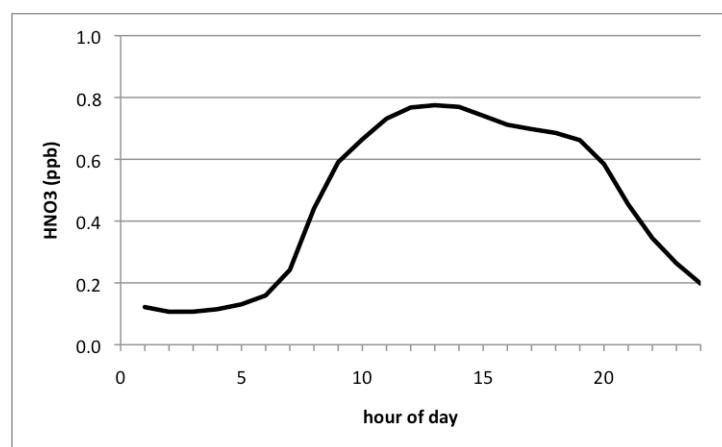


Figure S11: Diurnal cycle of modeled HNO_3 concentrations (ppb) at Payerne (June 2006).

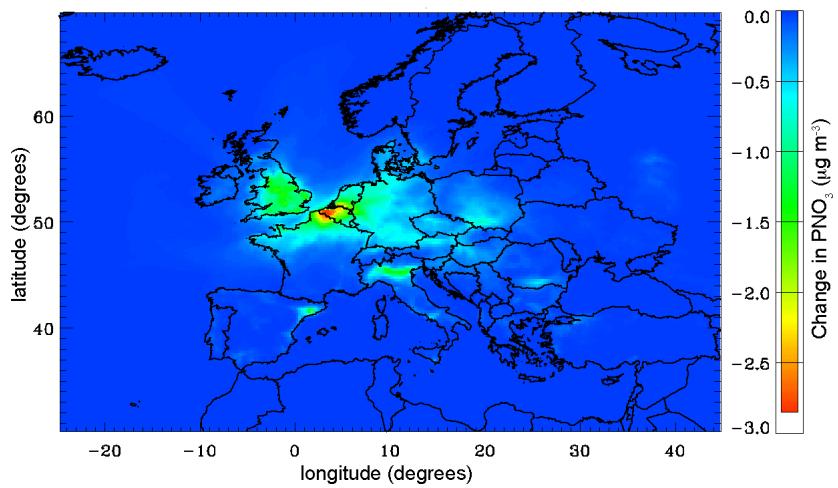


Figure S12: Change in PNO₃ concentrations (in $\mu\text{g m}^{-3}$) in June 2006 when hydrolysis reaction of N₂O₅ was switched off.

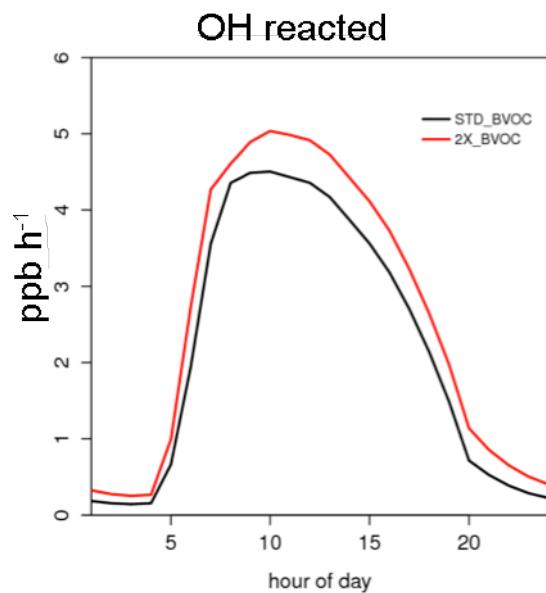


Figure S13: Changes in diurnal variation of reacted OH radical (June 2006, Payerne). Black: with standard BVOC emissions, red: with doubled BVOC emissions.