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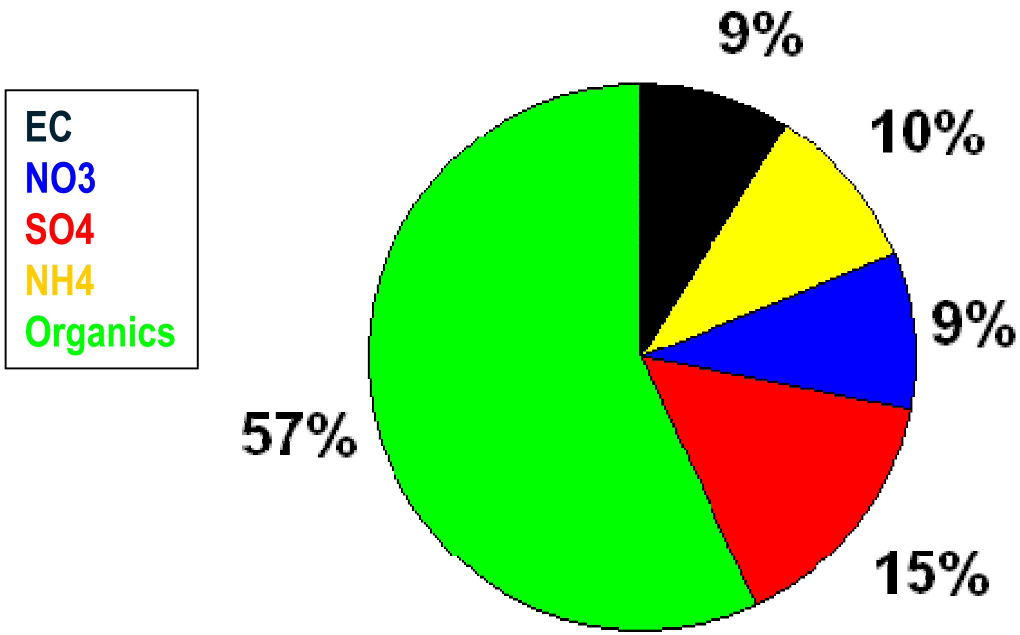
Sensitivity of modelled secondary organic aerosols (SOA) to biogenic VOC (BVOC) emissions in Switzerland

Motivation

Motivation – OA is important in Switzerland

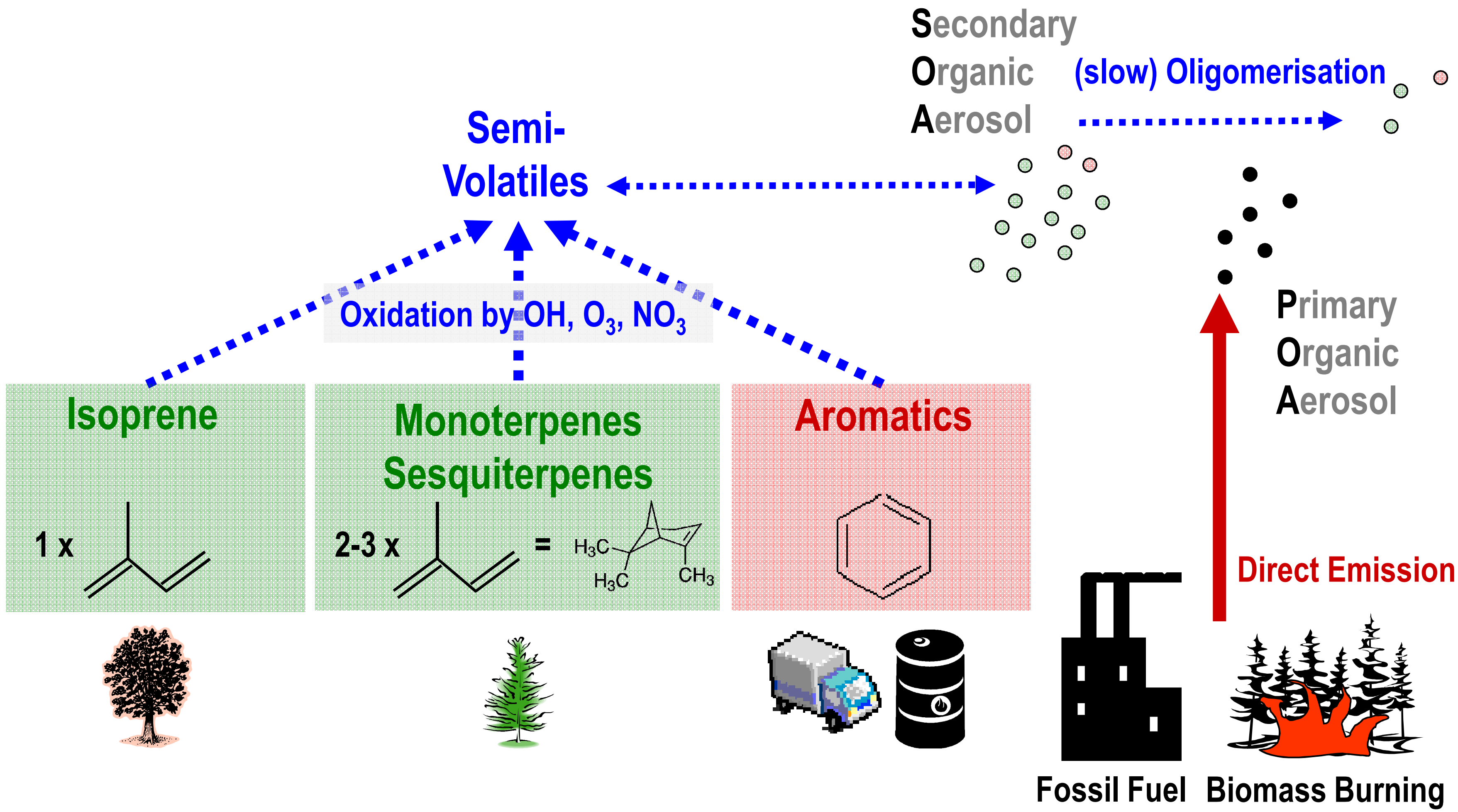
- Organic aerosol accounts for 30-80% of PM1 in Switzerland
- In summer, values are around 60%
- Further analyses suggest **BVOC** as important precursors



PM1 Measured (Aethalometer and AMS)
June 2006, Payerne (Rural Background site)

Lanz et al., ACPD 2010

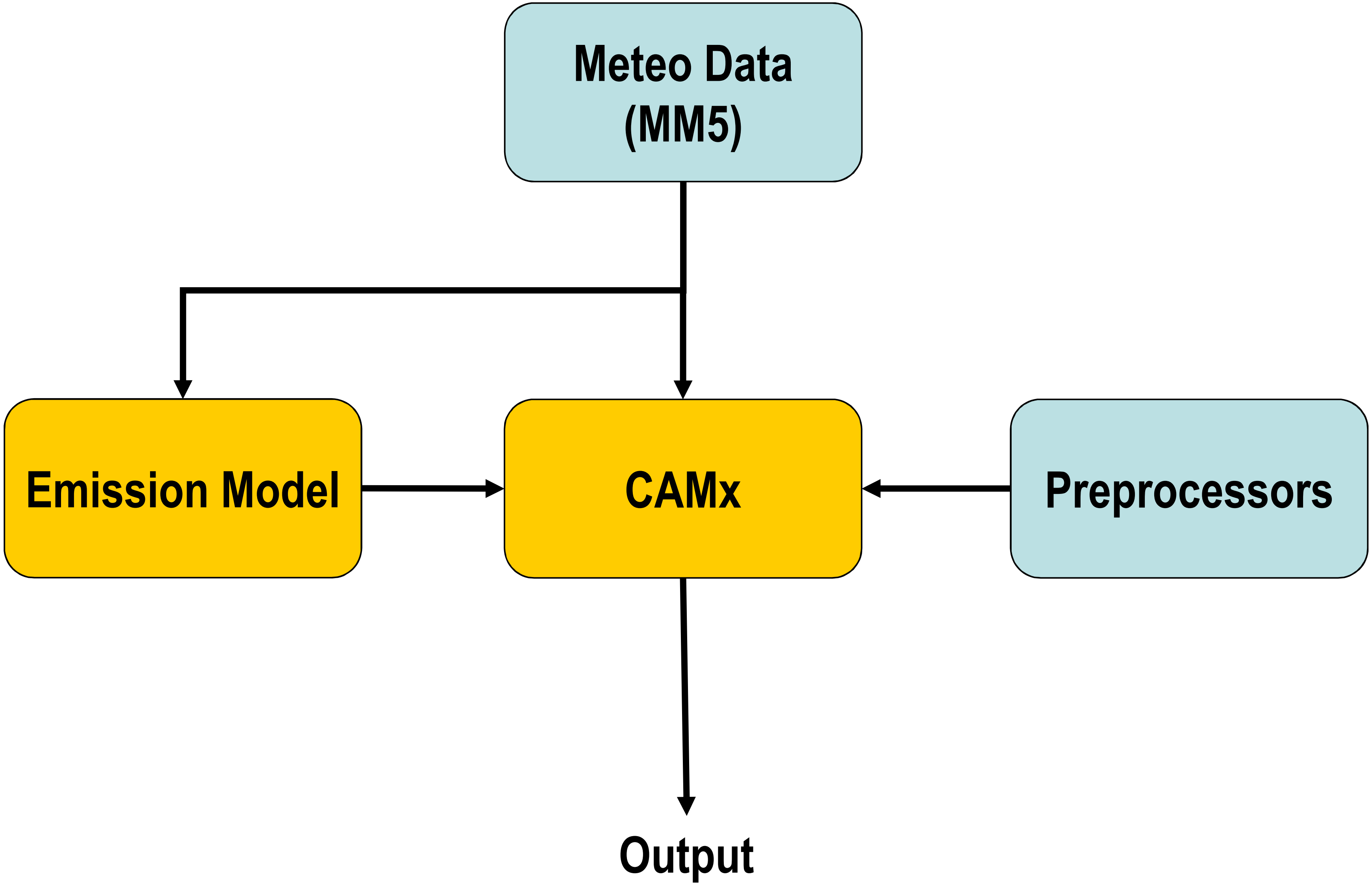
Organic aerosol in CAMx



Adapted from Heald (Telluride 2008)

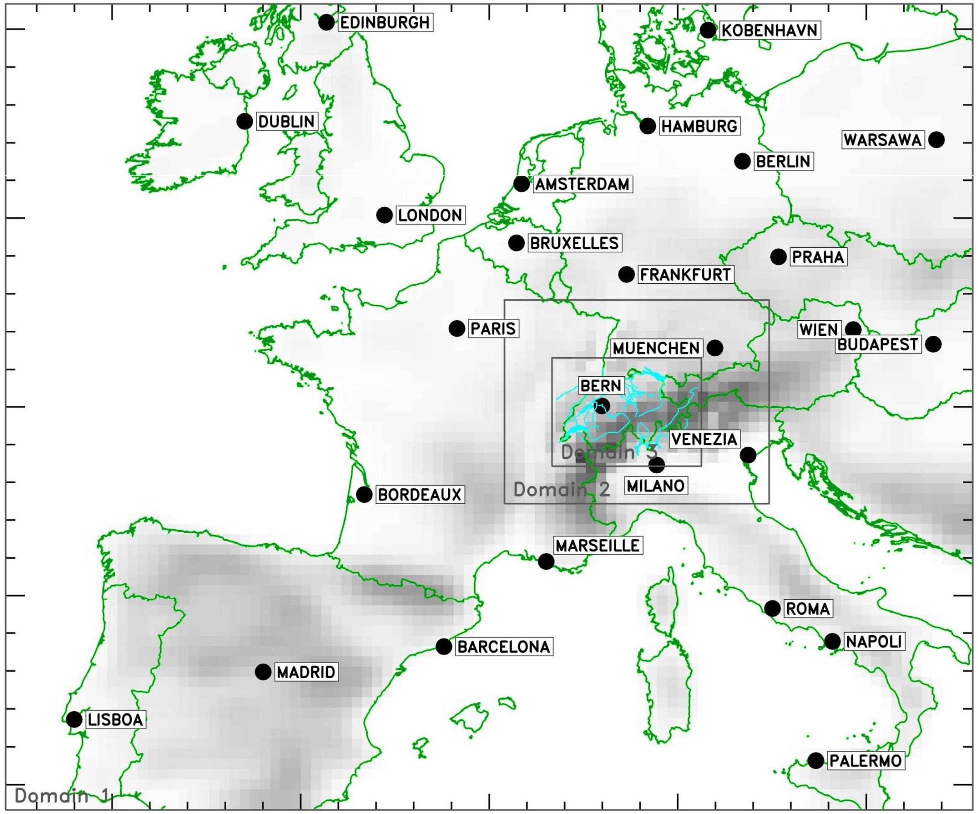
Setup

PSI Model setup (simplified)



Model Setup

- All simulations where carried out using CAMx 5.10
- 3 Nested Domains, 14 σ-Levels up to about 7000 m above ground
- Period: June 2006



Scenarios discussed

Scenario	Base	New	High
Emission Model	emCAMx	SimBioEmCAMx	SimBioEmCAMx
Canopy Correction	Yes	No	
Landuse	*Five major tree species of Switzerland: Norway spruce (Picea abies), White Fir (Abies alba), Scots pine (Pinus sylvestris), Larch (Larix decidua), Oak (Quercus robur) Plus Corn, Wheat, Grassland and general Forest*		
Isoprene (ISP)	*Andreani-Aksoyoglu & Keller,1995*	*Reference Emission data: Steinbrecher et al.,2009 Algorithms: Guenther, 1997*	Equal to "New"
Monoterpenes (TRP)			1.5 * "New"
Sesquiterpenes (SQT)	0.1 * TRP ("Base")		10 * "New"

Modelling of BVOC Emissions

Modelling of BVOC Emissions in SimBioEmCAMx

$$E_{cell} = A_i * E_{0,i} * d_i * \gamma$$

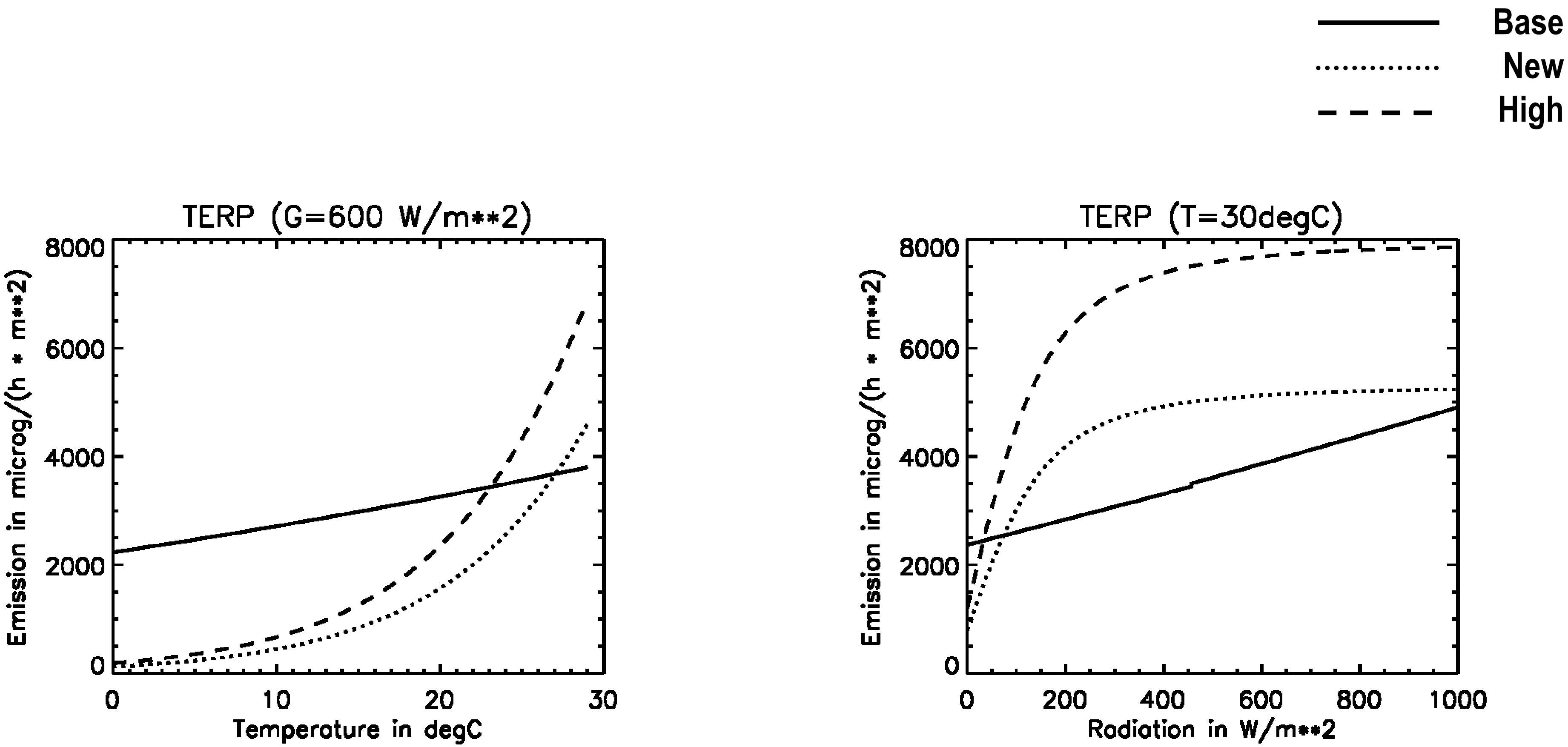
Isoprene (C_5H_8): $\gamma = f_I(T, Light)$
Monoterpenes ($C_{10}H_{16}$): $\gamma = f_M(T, Light)$
Sesquiterpenes($C_{15}H_{24}$): $\gamma = f_S(T)$

Tree Species-specific data:

- A_i **Area covered by tree species i on the grid**
- $E_{0,i}$ **Reference emission rates per gram (dry weight) of leaves**
- d_i **Leaf biomass density in gram (dry weight) per m^2**

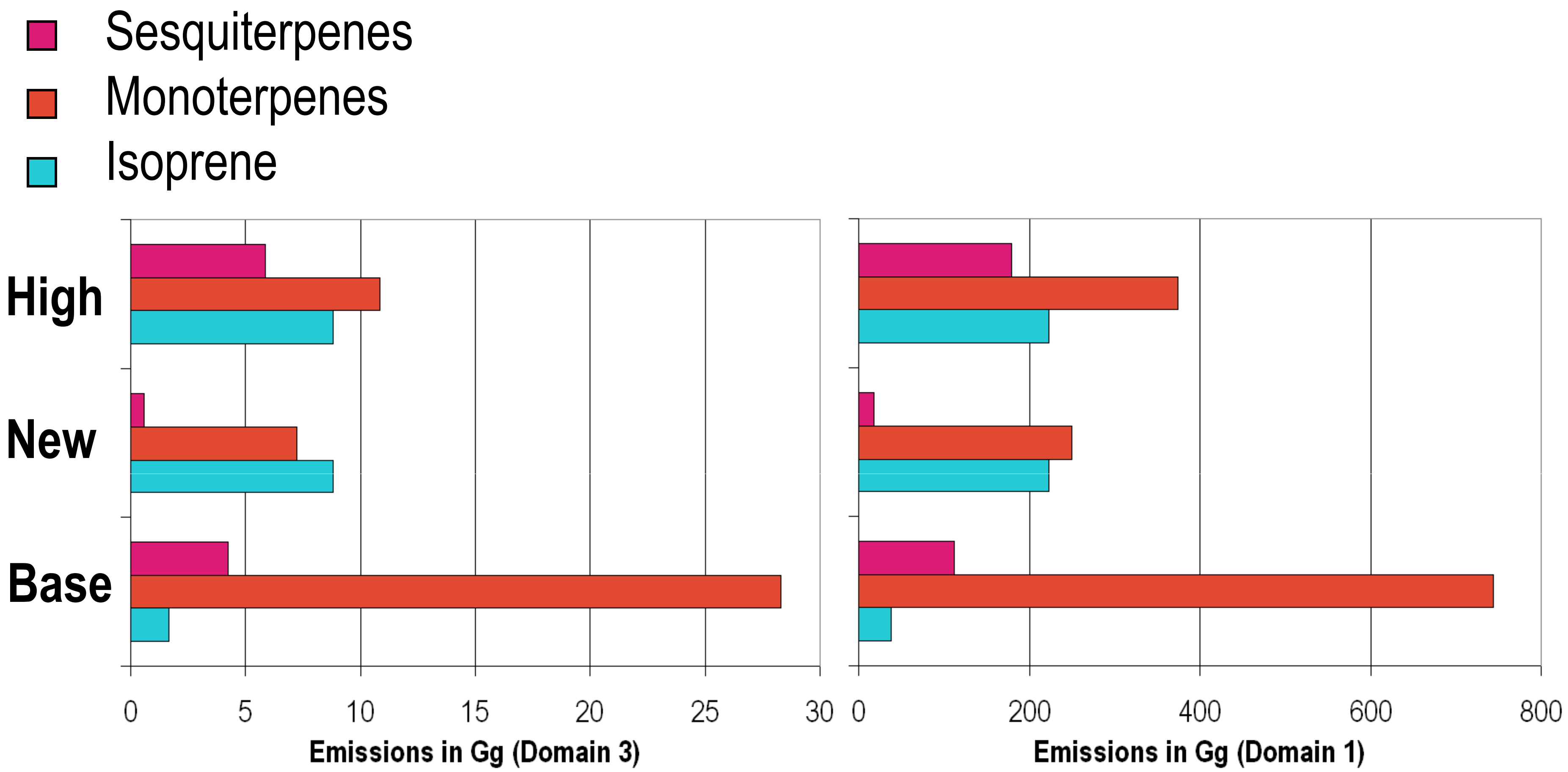
Steinbrecher, R., et al., Atmos. Environ. 2009.
Guenther, A., et al., J. Geophys. Res. D: Atmos. 1995.
Guenther, A., et al., Ecol. Appl. 1997.

Dependence on Temperature and Radiation (TERP)



Results: Emissions

Results – Total Emissions June 2006



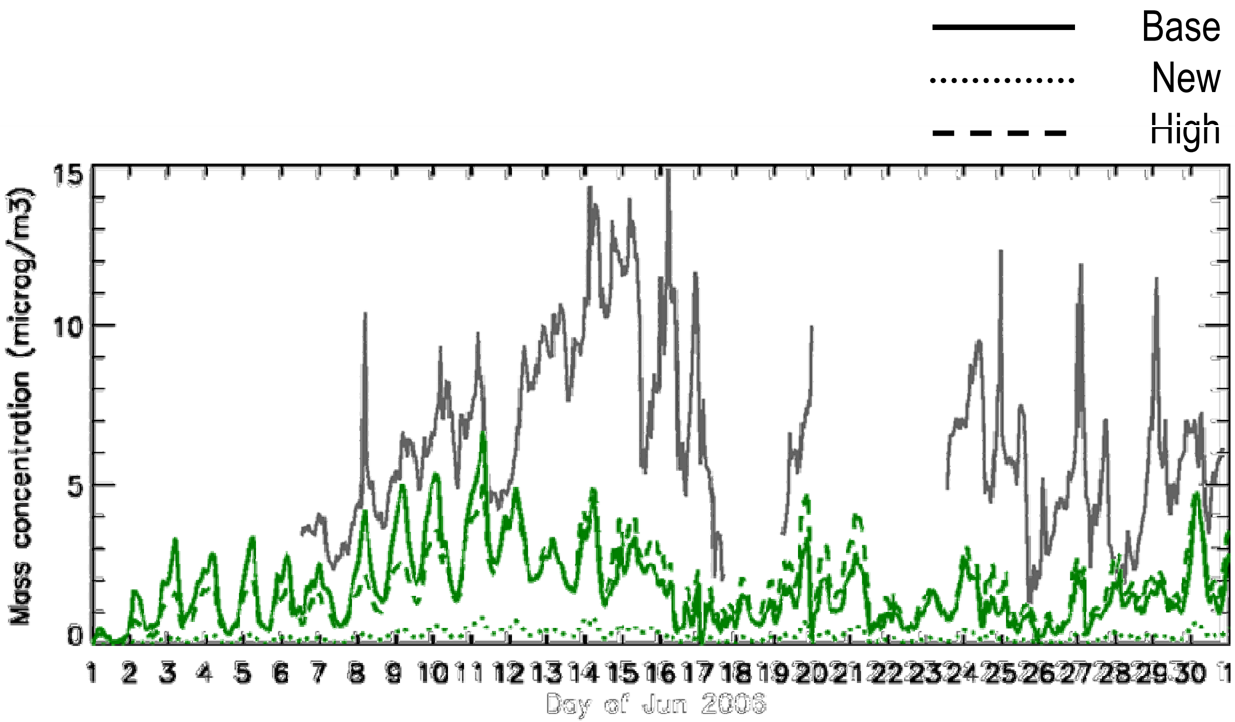
Switzerland **European Domain**

Results: Secondary Organic Aerosol

Modelling results – time series Payerne (with AMS-FA)

Measurement-Derived
SOA (AMS-FA)

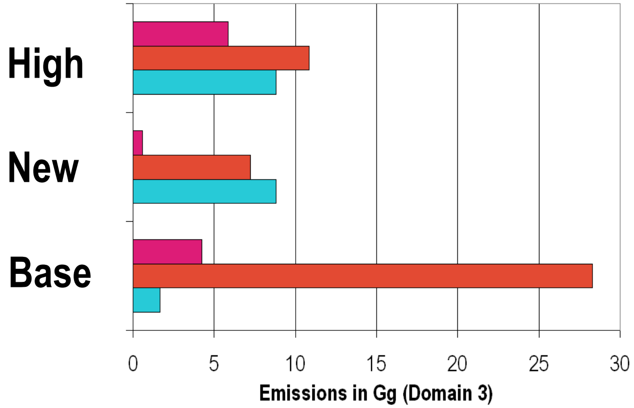
Predicted
BSOA

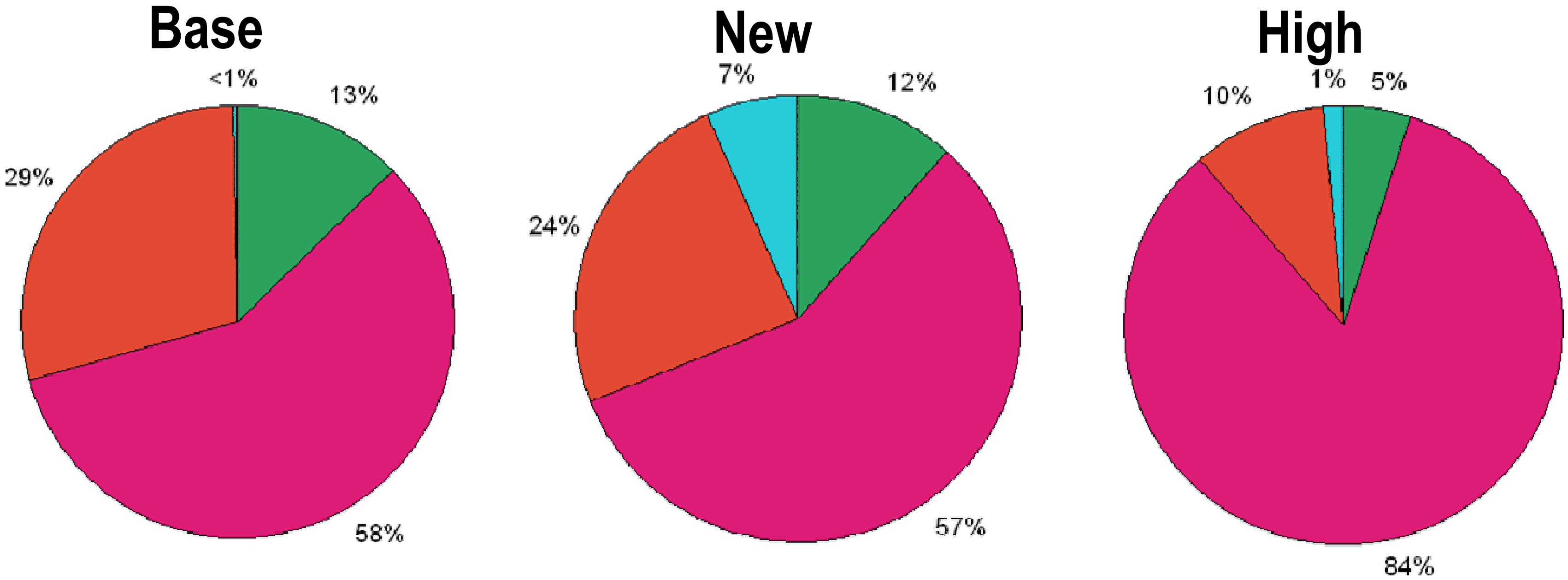


Day of June 2006

Modelling results – BSOA fractions in Payerne, June 06

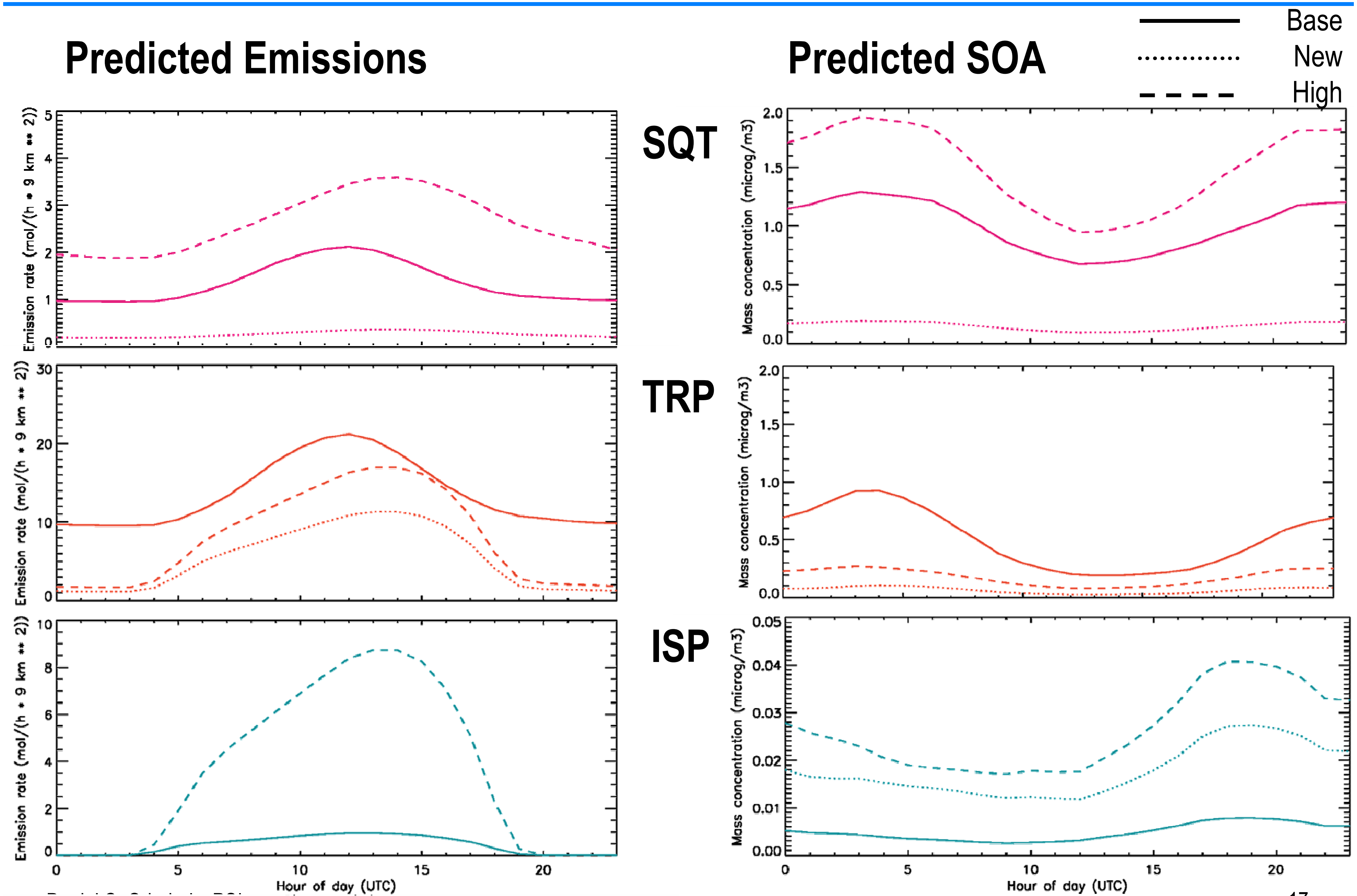
- Oligomerized Biogenic SOA
- Sesquiterpenes SOA
- Monoterpenes SOA
- Isoprene SOA





Average [BSOA]	1.74 µg/m3	0.26 µg/m3	1.79 µg/m3

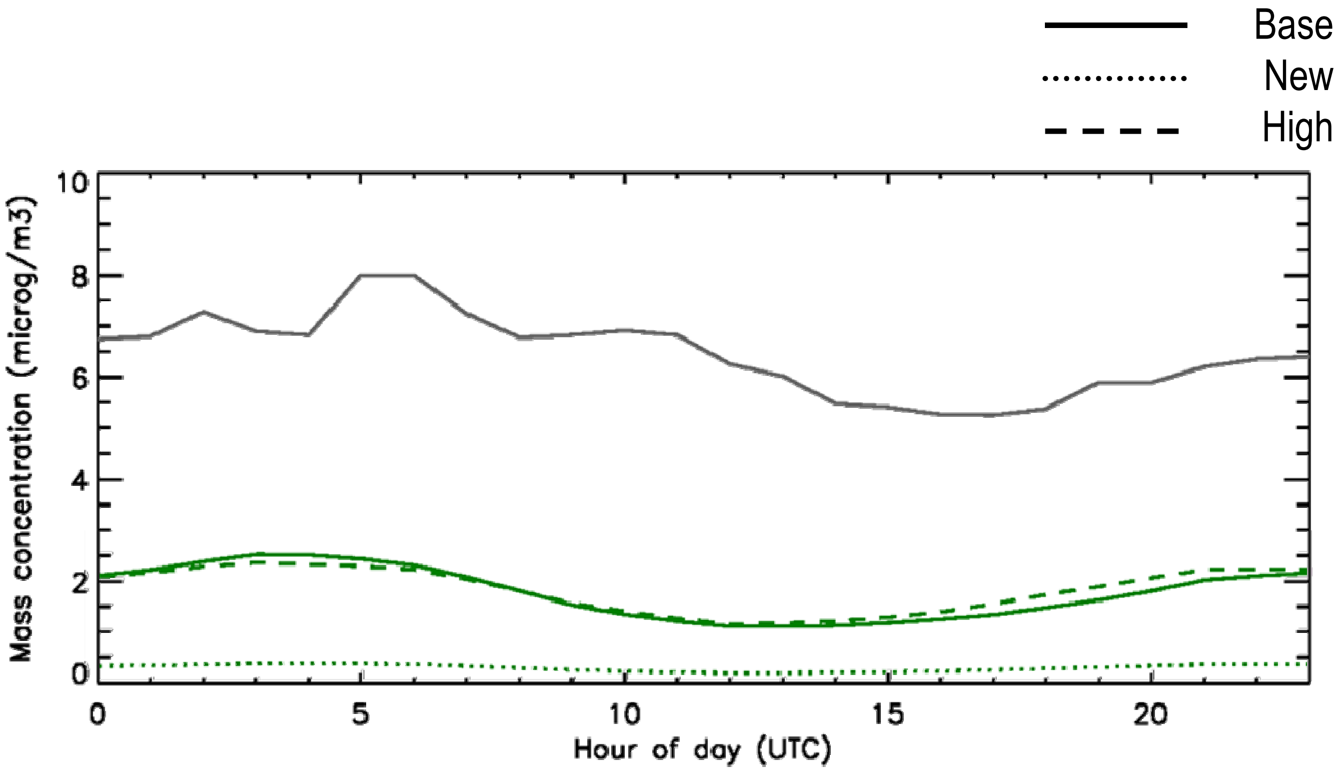
Modelling results – mean diurnal patterns Payerne



Modelling results – mean diurnal pattern AMS-FA Payerne

Measurement-Derived SOA (AMS-FA)

Predicted BSOA



Conclusions

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Conclusions

- An accurate BVOC inventory is crucial to model OA in Switzerland
- Sesquiterpene emissions may contribute to a large fraction of BSOA, especially at higher temperatures
- Uncertainty of BVOC emission factors is high
- Model results suggest that CAMx overestimates volatility of SOA
- Landcover data is crucial!

Outlook

- We will test sensitivity to the heat of evaporation
- A comparison of different landuse scenarios is under way (Köble, Skjøth)
- Robinsons Volatility Basis Set approach will be applied, however, this does not affect BSOA directly

Acknowledgements

Funding

FOEN (Swiss Federal Office of the Environment)

Emission Data

TNO, INFRAS, Meteotest

AMS Data

R. Alfarra

AMS-FA Data

Valentin A. Lanz

Global CTM Data

M. Schultz

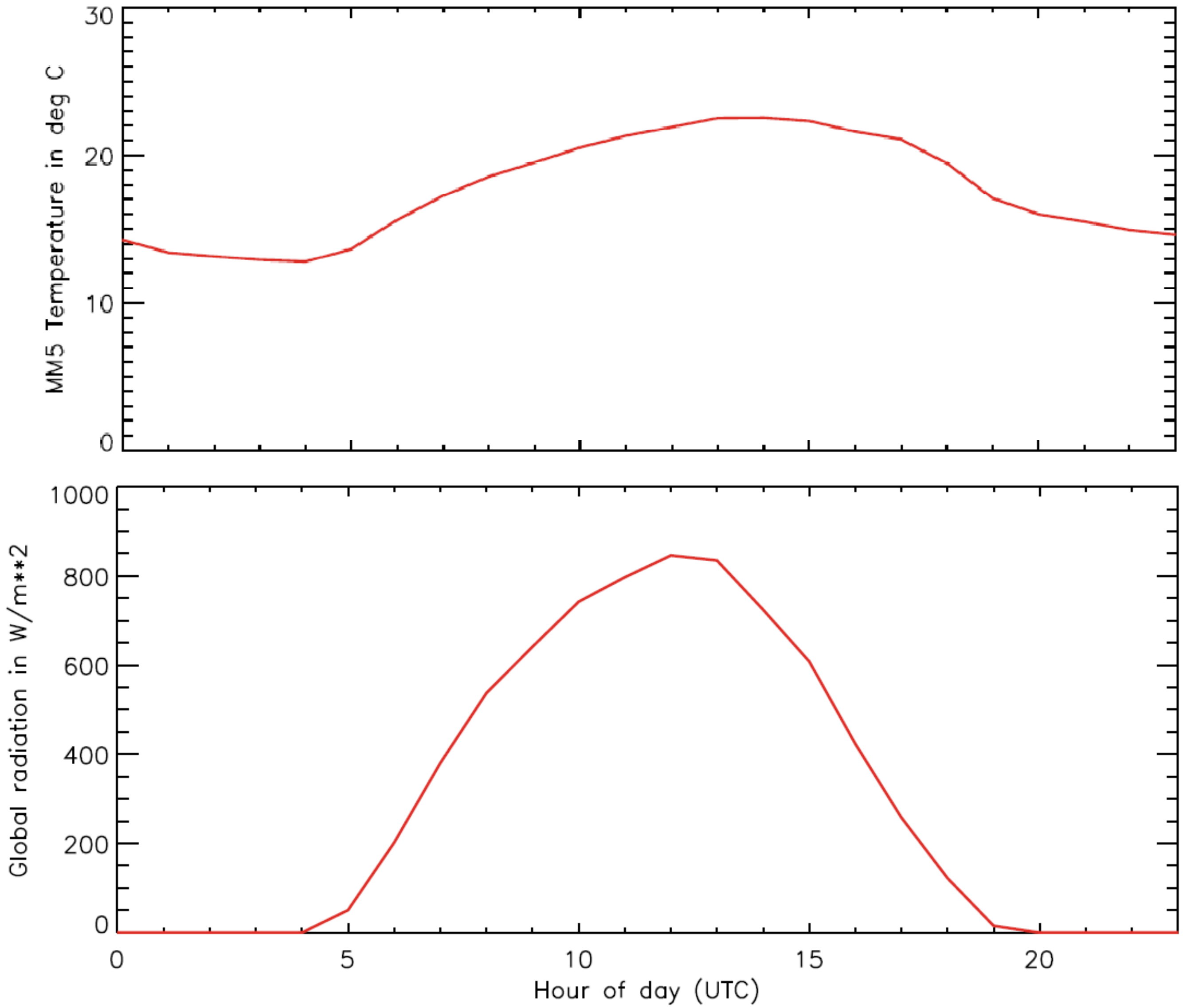
Surface-Plotting tools

M. Tinguely

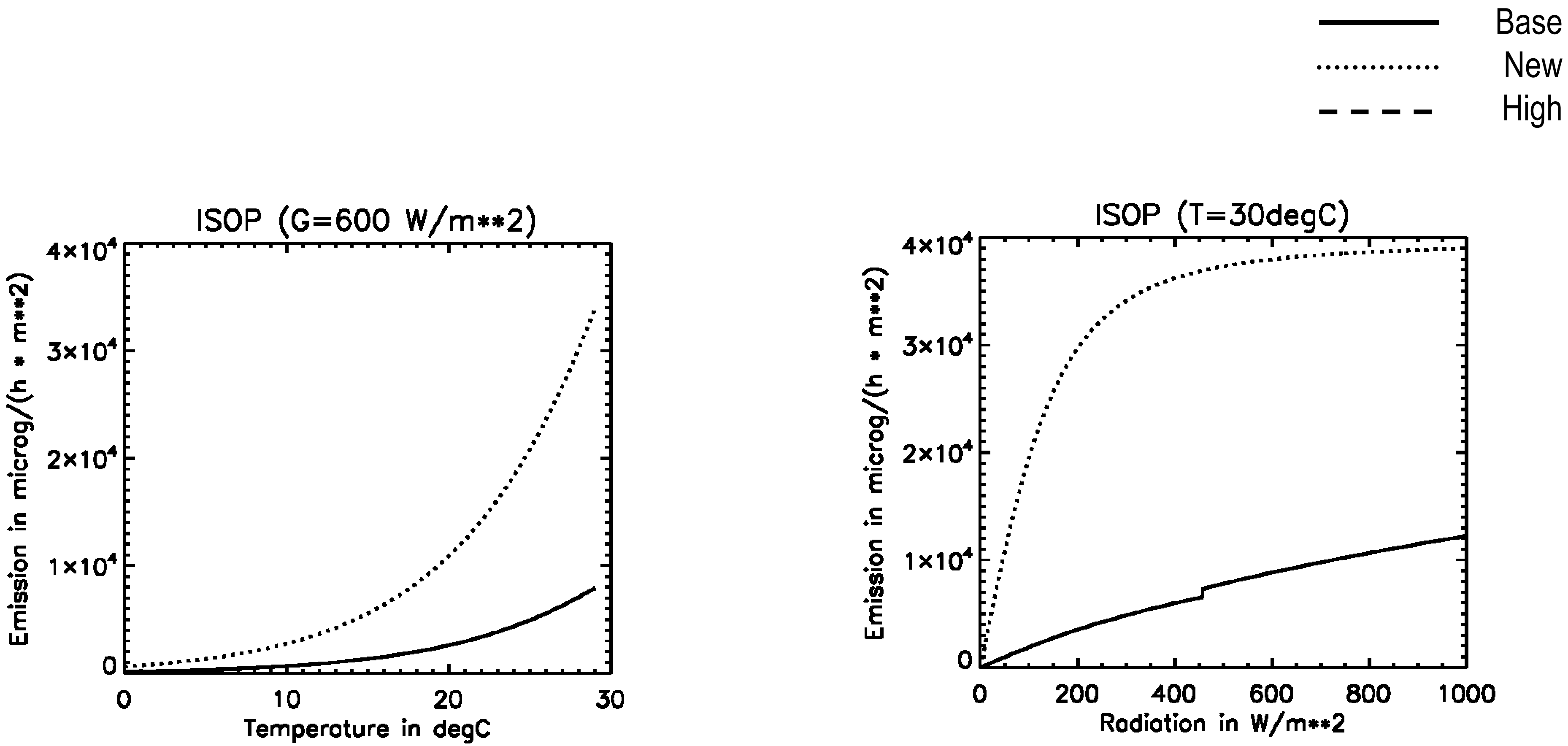
[redacted]

Modelling results – mean diurnal patterns Payerne

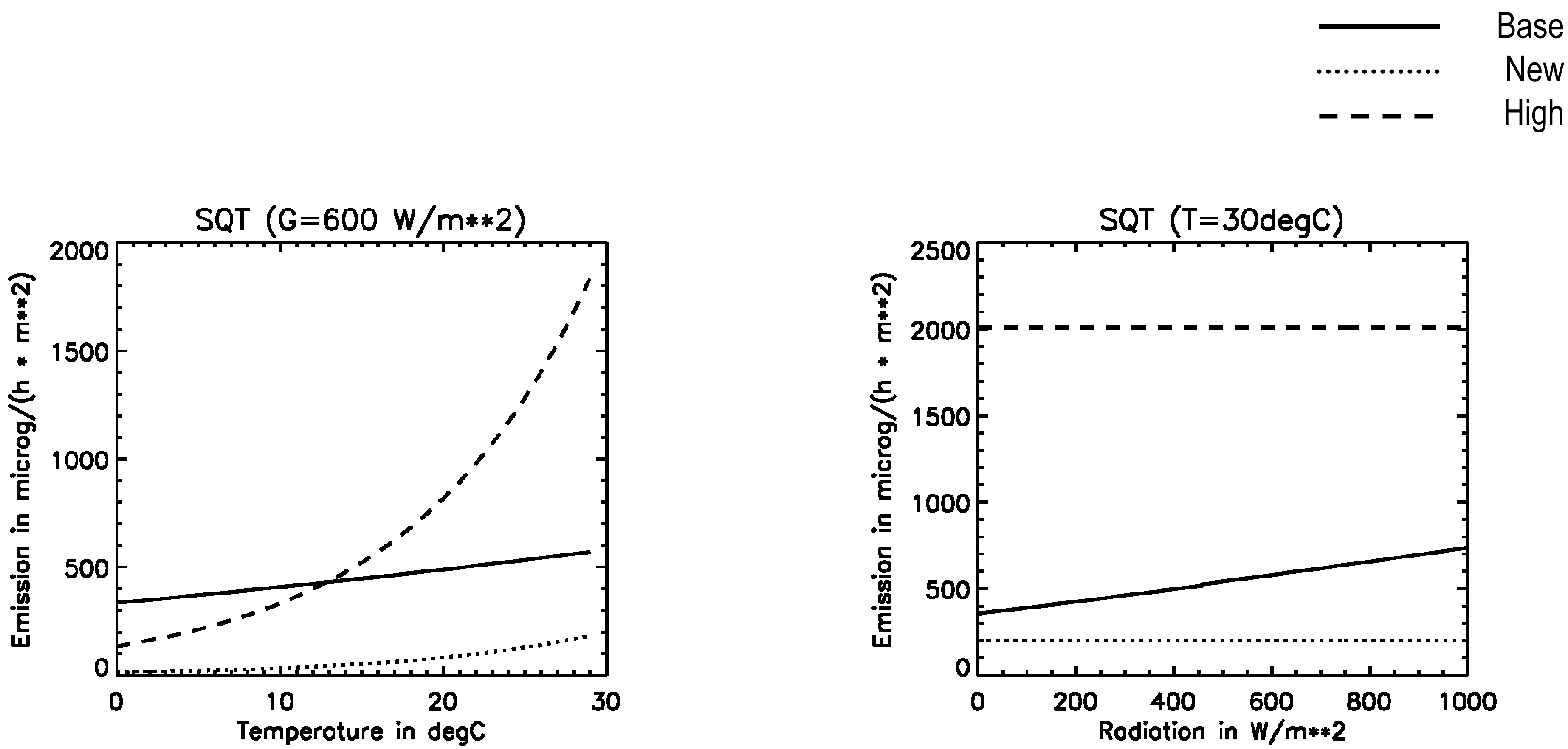
Meteo data



Dependence on Temperature and Radiation (ISOP)

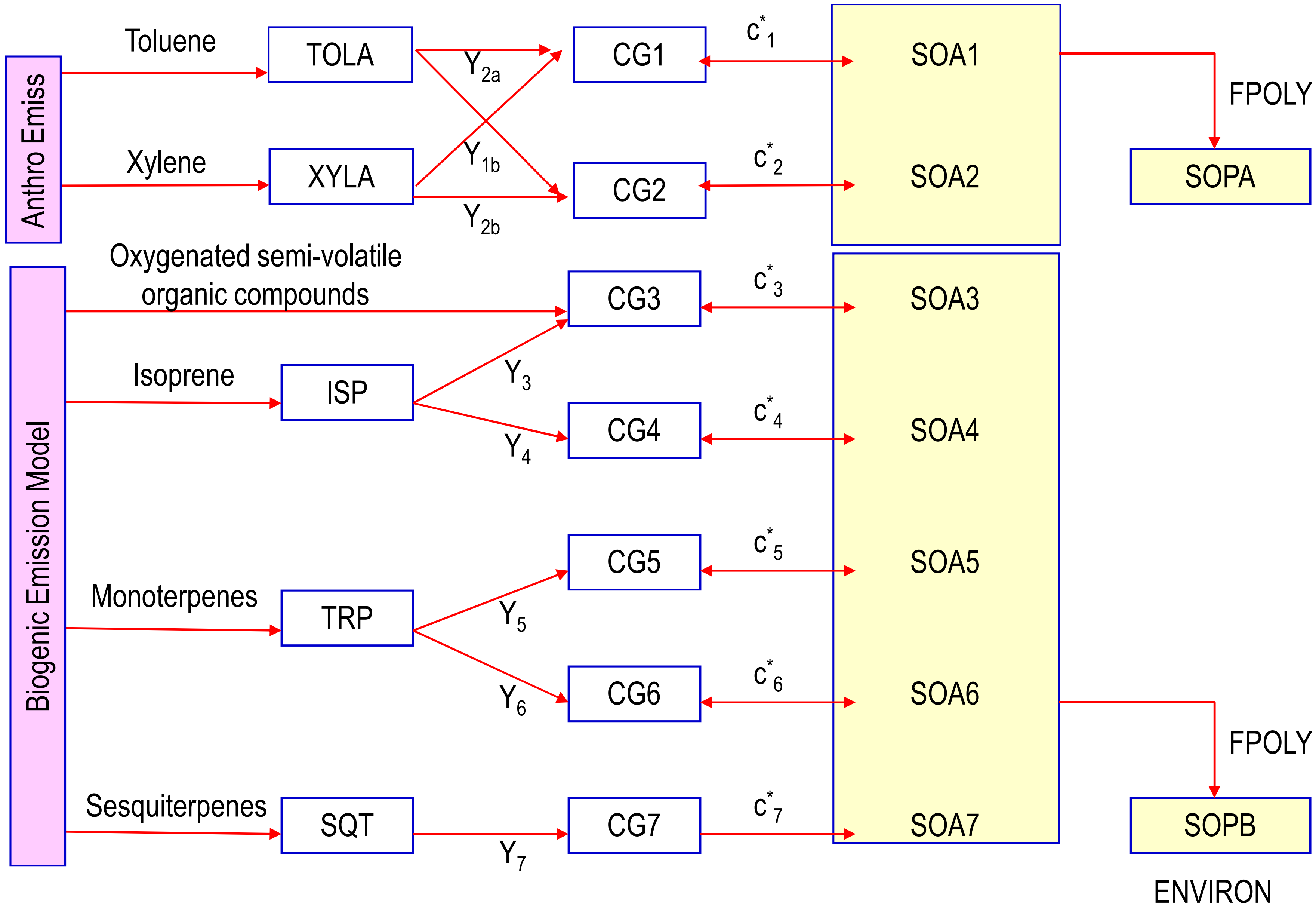


Dependence on Temperature and Radiation (SQT)



Model details

Updated Model implementation



Parameters for the updated SOA module

Species Name	Molecular Weight	Y [ppm/ppm]	c^* [µg/m3] at 298K	ΔHvap [kJ/mol]
TOLA	92			
XYLA	106			
ISP	68			
TRP	136			
SQT	204			
CG1/SOA1	150	0.044[a] / 0.027[b]	7.82	66.8
CG2/SOA2	150	0.085[a] / 0.118[b]	227	66.8
CG3/SOA3	130	0.015	0.726	42
CG4/SOA4	130	0.12	136	42
CG5/SOA5	180	0.065	3.92	75.5
CG6/SOA6	180	0.29	55.8	75.5
CG7/SOA7	210	0.85	~ 0	0
SOPA/SOPB	220			

[a] from TOLA
[b] from XYLA

ENVIRON, 2009

SOA reactions in CAMx 5.10 (same as in 4.51)

Precursor	Reaction	CG Products[1]	k_{298}[2] (ppm^{-1} min^{-1})
Anthropogenic			
Toluenes	TOLA + OH	0.044 CG1 + 0.085 CG2	8.75E+03
Xylenes	XYLA + OH	0.027 CG1 + 0.118 CG2	3.71E+04
Biogenic			
Isoprene	ISP + O	none	5.32E+04
	ISP + OH	0.015 CG3 + 0.12 CG4	1.47E+05
	ISP + O3	none	1.90E-02
	ISP + NO3	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 + O3	0.065 CG5 + 0.29 CG6	1.33E-01
	TRP + NO3	0.065 CG5 + 0.29 CG6	9.18E+03
Sesquiterpenes	SQT + OH	0.85 CG7	2.91E+05
	SQT + O3	0.85 CG7	1.71E+01
	SQT + NO3	0.85 CG7	2.81E+04

ENVIRON, 2008