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Challenges in modelling isoprene and monoterpene emission dynamics of Arctic plants: a case study from a subarctic tundra heath

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Supplementary material

S1 PFTs simulated for the study area

Table S1 Detailed descriptions of the PFT parameters for the study area (Abisko, tundra heath). LSE: low shrubs evergreen; SLSS: *Salix*, low shrubs summergreen; NSLSS: non-*Salix*, low shrubs summergreen; EPDS: evergreen prostrate dwarf shrubs; SPDS: summergreen prostrate dwarf shrubs; GRT: graminoid tundra; CLM: cushion forbs, lichens and mosses tundra; S: shrub; G: grass; NL: needleleaf; BL: broadleaf; Max.: maximum; Min.: minimum; EG: evergreen; SG: summergreen; GDD5: growing degree days above 5 ^{o}C; GDD0: growing degree days above 0 ^{o}C.

Parameters	LSE	SLSS	NSLSS	EPDS	SPDS	GRT	CLM
Growth form	S	S	S	S	S	G	G
Leaf physiognomy	NL	BL	BL	NL	BL	BL	BL
Fraction of roots in the upper (0.5 m)/lower (1 m) soil layer	0.8/0.2	0.8/0.2	0.8/0.2	0.8/0.2	0.8/0.2	0.9/0.1	0.9/0.1
Max. leaf:root carbon mass ratio	1	1	1	0.5	0.5	0.2	0.2
Min. canopy conductance (mm/s)	0.3	0.5	0.5	0.5	0.5	0.5	0.5
Phenology types	EG	SG	SG	EG	SG	any	any
Longevity of leaves (years)	3	0.5	0.5	3	0.5	1	1
Leaf turnover rate (year^{-1})	0.33	1	1	0.5	1	1	0.6
Root turnover rate (year^{-1})	0.7	0.7	0.7	0.7	0.7	0.5	
Sapwood turnover rate (year^{-1})	0.01	0.01	0.01	0.01	0.01	-	-
Fire resistance (0-1)	0.12	0.12	0.12	0.12	0.12	0.5	0.5
Min. forest floor PAR establishment (KJ m^{-2} day^{-1})	1000	1000	1000	1250	1250	1250	1250
Interception coefficient[€]	0.06	0.02	0.02	0.04	0.02	0.01	0.01
Parameter for relationship between crown area and stem diameter	10	10	10	10	10	-	-
Allometry parameter (k_allom2) related vegetation height and stem diameter	4	4	4	1	1	-	-
Allometry parameter (k_allom3) related vegetation height and stem diameter	0.67	0.67	0.67	0.67	0.67	-	-
Constant in crown area and stem diameter relationship	1.6	1.6	1.6	1.6	1.6	-	-
Max. tree crown area (m^2)	1	1	1	1	1	-	-
Tree leaf to sapwood area ratio	125	125	125	100	100	-	-
Sapwood and heartwood density (kg C m^{-3})	200	200	200	200	200	-	-

Growth efficiency threshold (kg C m^{-2} leaf yr^{-1})	0.012	0.012	0.012	0.01	0.01	-	-
Max. establishment rate (samplings m^{-2} yr^{-1})[*]	0.6	0.8	1	0.8	0.8	-	-
Recruitment shape parameter[Γ]	10	10	7	10	10	-	-
Mean non-stress longevity (yr)	25	25	25	30	30	-	-
GDD5 required to obtain full leave cover	0	50	50	0	50	50	1
Photosynthesis min. temperature (^{o}C)	-4	-4	-4	-4	-4	-4	-4
Approximate lower range of temperature optimum for photosynthesis	10	10	10	10	10	10	10
Approximate upper range of temperature optimum for photosynthesis	30	30	30	25	25	25	25
Photosynthesis max temperature (^{o}C)	38	38	38	38	38	38	38
Min. temperature of coldest month for survival	-32.5	-40	-40	-1000	-1000	-1000	-1000
Min. temperature of coldest month for establishment	-32.5	-32.5	-32.5	-1000	-1000	-1000	-1000
Max. temperature of coldest month for establishment	1000	1000	1000	1000	1000	1000	1000
Min. temperature of warmest month for establishment	-1000	-1000	-1000	-1000	-1000	-1000	-1000
Min. GDD5 for establishment	100	100	100	0	0	0	0
Min. GDD0 for reproduction	300	300	300	150	150	150	50
Max. GDD0 for reproduction[ξ]	-	-	-	1500	-	1400	-
Min. snow cover (mm)	-	-	-	20	20	-	50
Maintenance respiration coefficient	1	1	1	1	1	1	1
Min. fraction of available soil water in upper soil layer during growing season	0.1	0.1	0.1	0.01	0.01	0.01	0.01
Max. evapotranspiration rate	5	5	5	5	5	5	5
Litter moisture flammability threshold (fraction of available water holding capacity)	0.3	0.3	0.3	0.3	0.3	0.2	
Sapwood C:N mass ratio	330	330	330	330	330	-	-
Fine root C:N mass ratio	29	29	29	29	29	29	29
Maximum nitrogen uptake per fine root (kg N kg C^{-1} day^{-1})	0.0028	0.0028	0.0028	0.0028	0.0028	0.00551	0.00551
Half-saturation concentration for N uptake (kg N l^{-1})	1.477E-06	1.477E-06	1.477E-06	1.477E-06	1.477E-06	1.886E-06	1.886E-06
Fraction of sapwood or root for N long-term storage	0.3	0.3	0.3	0.3	0.3	0.3	0.3
Specific leaf area (m^2 kg C^{-1})	12.56	24.25	24.25	12.56	24.25	19.75	25.8
Isoprene emission capacity (µg C g^{-1} h^{-1}) E_{IS20}	1.751/1.737	11.305/11.213	2.512/2.492	1.411/1.400	14.117/14.003	9.898/9.818	1.198/1.188
Isoprene emissions show a seasonality (1) or not (0)	0	1	1	0	1	1	0
Monoterpene emission capacity (µg C g^{-1} h^{-1}) E_{MS20}	0.089/0.088	0.300/0.297	1.208/1.199	1.312/1.301	0.428/0.425	0.000/0.000	0.030/0.029

Fraction of monoterpene production that go into storage pool	0.5	0.5	0.5	0.5	0.5	0.5	0
Aerodynamic conductance (m s^{-1})	0.04	0.04	0.04	0.03	0.03	0.03	0.03

*, ξ: the values were adjusted based on the point intercepted-based observations to increase/decrease relative abundance;

[€]: a dimensionless biome-dependent proxy for rainfall region (Gerten et al., 2004).

[Γ]: relates to life history class of plant functional types. High values of this parameter represent a steeper decline in establishment rate as shading reduces potential seedling growth.

Table S2 Detailed description of literature values used for parameterizing PFT emission capacities, isoprene (I_S, μg C gdw^{-1} h^{-1}) and monoterpene (M_S, μg C gdw^{-1} h^{-1}) emissions at 20 °C and 30 °C. For some PFTs, the multiple data values from the same study are from different sampling dates in the original publications.

Plant funtional types (PFTs)	Species name	Emission potentials (μg C gdw^{-1} h^{-1})		Reference	Emission potentials (μg C gdw^{-1} h^{-1})		Reference
		E_{IS30}†	E_{IS20}Γ		E_{MS30}†	E_{MS20}Γ	
Low Shrub evergreen (LSE)	*Empetrum hermaphroditum*	8.050	7.985	(Schollert et al., 2015)	0.029	0.029	(Schollert et al., 2015)
		0.700	0.694		0.066	0.065	
		0.000	0.000	(Vedel-Petersen et al., 2015)	0.020	0.020	(Vedel-Petersen et al., 2015)
		0.004	0.004		0.110	0.109	
		0.003	0.003		0.198	0.218	
	Average	**1.751**	**1.737**		**0.089**	**0.088**	
***Salix*, Low Shrubs Summergreen (SLSS)**	*Salix phylicifolia*	14.160	14.045	(Rinnan et al., 2011)	0.910	0.903	(Rinnan et al., 2014)
	Salix glauca	2.050	2.033	(Vedel-Petersen et al., 2015)	0.048	0.048	(Vedel-Petersen et al., 2015)
		12.670	12.567		0.130	0.129	
		16.340	16.207		0.110	0.109	
	Average	**11.305**	**11.213**		**0.300**	**0.297**	
Non-*Salix* group of summergreen shrubs (NSLSS)	*Vaccinium uliginosum*	0.000	0.000	Schollert unpublished data			
		0.000	0.000	(Rinnan et al., 2011)	1.070	1.061	(Rinnan et al., 2011)
		19.480	19.322	(Schollert et al., 2015)	1.730	1.716	(Schollert et al., 2015)
		1.870	1.855		0.680	0.674	
	Betula nana	0.000	0.000	Schollert unpublished data			
		0.000	0.000				
		0.000	0.000	(Vedel-Petersen et al., 2015)	2.400	2.381	(Vedel-Petersen et al., 2015)
		0.990	0.982		0.840	0.833	
		0.267	0.265		0.530	0.526	
	Average	**2.512**	**2.492**		**1.208**	**1.199**	
Evergreen Prostrate Dwarf Shrub (EPDS)	*Cassiope tetragona*	0.132	0.131	(Schollert et al., 2015)	1.800	1.785	(Schollert et al., 2015)
		7.315	7.255		0.110	0.109	
		0.000	0.000		0.033	0.033	
		2.430	2.410		0.190	0.188	
		0.000	0.000		0.029	0.029	
		0.000	0.000	(Rinnan et al., 2011)	3.160	3.134	(Rinnan et al., 2011)
		0.000	0.000		3.860	3.829	
	Average	**1.411**	**1.400**		**1.312**	**1.301**	
Summergreen Prostrate Dwarf Shrub (SPDS)	*Salix arctica*	27.350	27.128	(Rinnan et al., 2014)			
		2.240	2.222	(Schollert et al., 2015)	0.330	0.327	(Schollert et al., 2015)
		21.960	21.782		0.930	0.922	
		6.030	5.981		0.025	0.025	

	Salix arctophila	4.640	4.602	(Vedel-Petersen et al., 2015)	0.430	0.427	(Vedel-Petersen et al., 2015)
		13.260	13.152		0.720	0.714	
		23.340	23.151		1.700	1.686	
	Average	**14.117**	**14.003**		**0.428**	**0.425**	
Graminoid (GRT)	*Eriophorum angustifolium*	20.240	20.076	(Ekberg et al., 2009)	0.000	0.000	(Ekberg et al., 2009)
		10.001	9.920				
		0.735	0.729				
		3.463	3.435				
		27.359	27.137				
		26.432	26.217				
		14.832	14.712				
	Carex rostrata	0.080	0.080				
		0.266	0.264				
		1.704	1.690				
		6.150	6.100				
		7.521	7.460				
	Average	**9.898**	**9.818**		**0.000**	**0.000**	
Cushion forbs, lichens, and moss tundra (CLM)	*Sphagnum cuspidatum*	1.160	1.151	Tiiva unpublished data			
	Sphagnum fuscum	0.864	0.857	(Hanson et al., 1999)			
	Sphagnum balticum	2.034	2.017	(Ekberg et al., 2011)			
		2.108	2.091				
		3.216	3.190				
		1.703	1.689				
	Warnstorfia exannulata	0.132	0.131	(Tiiva et al., 2007)	0.010	0.009	(Faubert et al., 2010)
	Aulacomnium palustre	2.860	2.837	Tiiva unpublished data			
	Dicranum polysetum	0.043	0.043	(Hanson et al., 1999)			
	Hylocomium splendens	0.011	0.011				
	Ptilidium ciliare	0.024	0.024				
	*Sphagnum**	0.220	0.218	(Janson and De Serves, 1998)	0.050	0.050	(Janson et al., 1999)
	Average	**1.198**	**1.188**		**0.030**	**0.029**	

*There is no species name in the original publication. †: These values from original publications were standardized to 30 °C using the Guenther's algorithm (Guenther et al., 1993); $^{\Gamma}$: There values were standardized to 20 °C using Eq. 3 (α_{τ} = 0.23, T_S = 20 °C).

S2 Sensitivity testing of α_{c3}

A uniform sampling of the parameter α_{c3} (1000 times, under the range of 0.02 to 0.125 µmol CO_2 µmol photons^{-1}) was implemented and the model simulations with different α_{c3} values were conducted to investigate how the modelled GPP, ER and LAI are influenced by the parameter α_{c3}. Closed-chamber based CO_2 fluxes and point intercepted-based plant coverage in the control plots were compared with the simulated outputs. Modelled GPP, ER, NEP and LAI were largely influenced by the parameter value of α_{c3} (Fig. S1). The root mean square error (RMSE) values of the four investigated variables showed a slight decrease, followed by a sharp increase with increasing α_{c3}. For the RMSE of GPP, ER and NEP, the first quantile occurs at the lowest value range of α_{c3}, with the RMSE of LAI spreading between 0.03 and 0.07. The parameter values with the lowest RMSE (Best) for GPP, ER, LAI are 0.034, 0.037 and 0.051 µmol CO_2 µmol photons^{-1}, respectively.

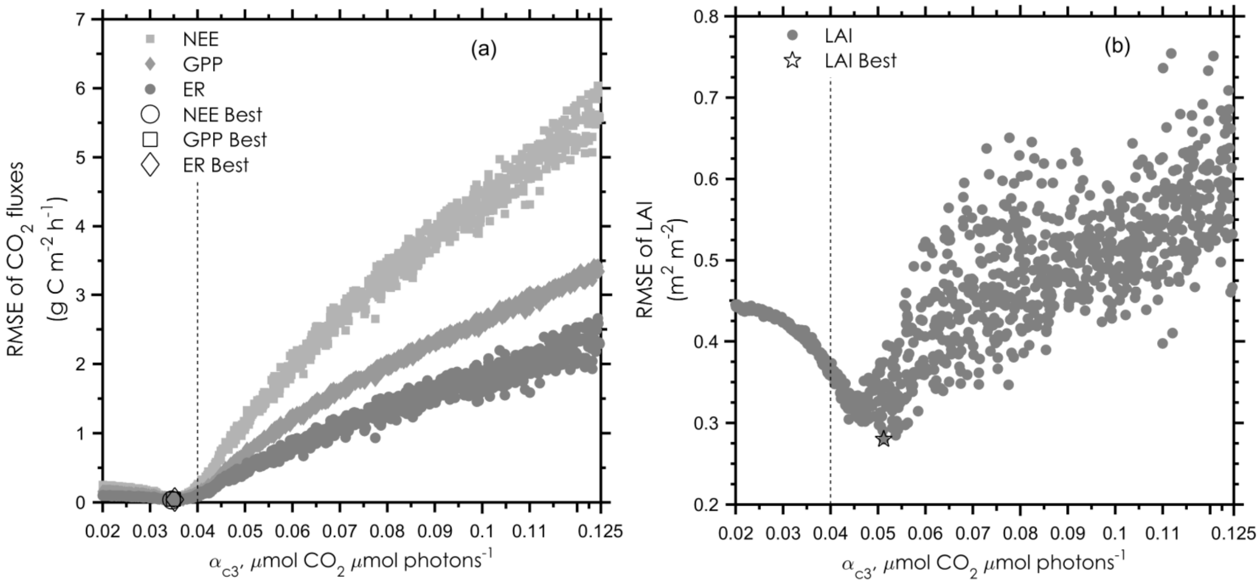

Figure S1 The root mean square error (RMSE) of the modelled net ecosystem production (NEP), gross primary production (GPP), ecosystem respiration (ER), (a) and leaf area index (LAI), (b) related to the observations for the years 2006 and 2007. The parameter values with the lowest RMSE (Best, in the legend) are marked. The dashed lines point out the α_{c3} selected for this study.

S3 Seasonal variation of BVOC emissions

The span of the BVOC measurements covered the main growing seasons over three years. The modelled daily average emission rates in the C plots showed pronounced day-to-day and seasonal variations (Fig. S2). The modelled emissions of isoprene and monoterpenes were low in Spring and Autumn, and peaked on warm days during the Summer. The day-to-day variations in the emissions agreed well with the variations of T and PAR. When both T and PAR were high, the peaks of both isoprene and monoterpene emissions occurred. The observed magnitude of isoprene emissions during daytime showed large spatial variation between the blocks for the days with the observed high average emission rates (blue error bars in Fig. S2. with low emissions, . The emission of monoterpenes remained more constant than that of isoprene towards the end of the growing season (not fully presented here).

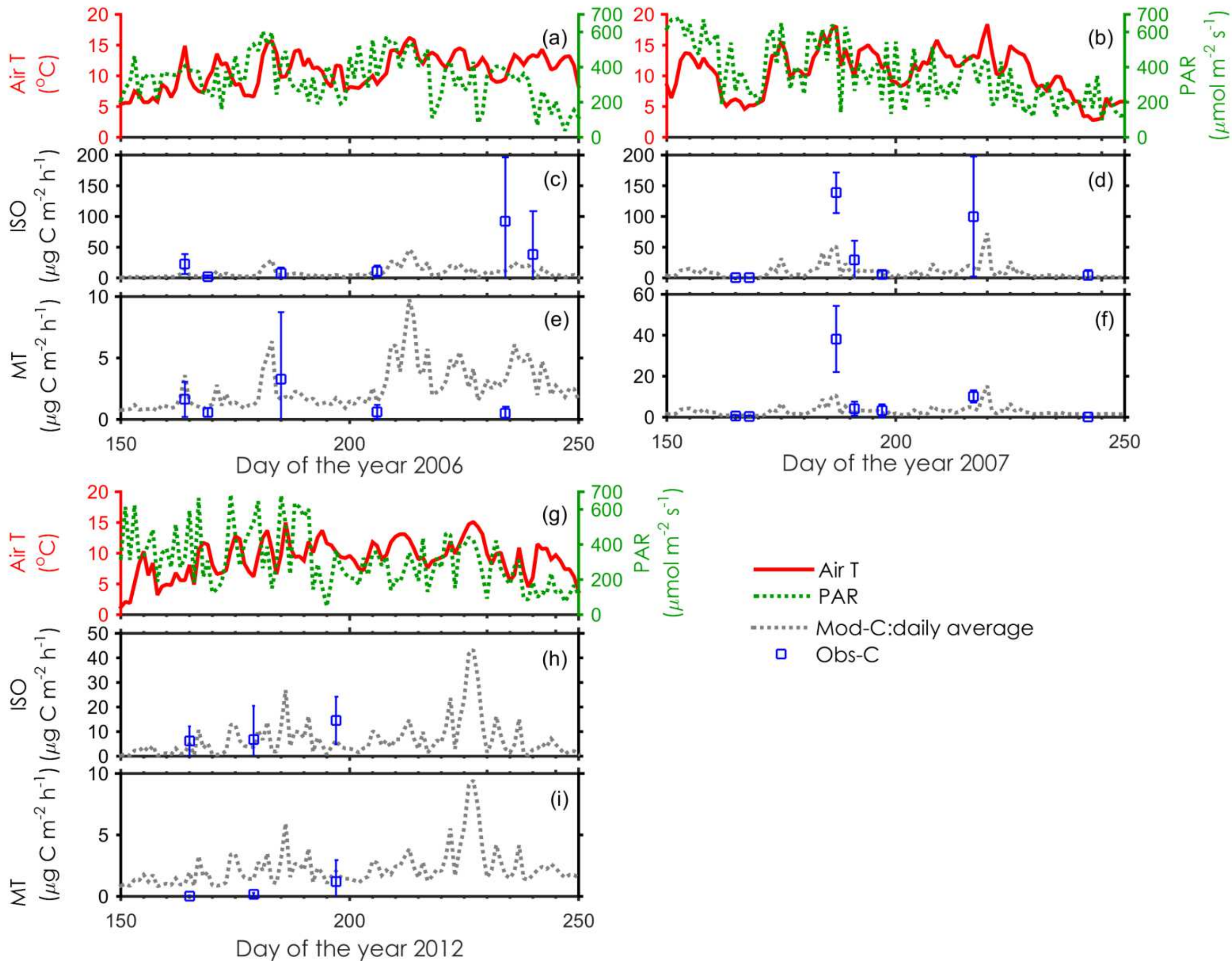

Figure S2 Time-series of the air temperature (Air T) at 2 m height, photosynthetically active radiation (PAR), the modelled isoprene (ISO) and monoterpene emissions (MT) for the days 150-250 in 2006, 2007and 2012 in the Abisko tundra heath. Both modelled and observed fluxes are from the control (C) conditions. Error bars indicate the standard deviation for the six replicates.

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