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Implementation of the MEGAN (v2.1) biogenic emission model in the ECHAM6-HAMMOZ chemistry climate model

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S1 Emission activity factor parameterizations

The activity factor for LAI, γ_{LAI}, is calculated as

$$\gamma_{LAI} = \frac{0.49LAI}{(1+0.2LAI^2)^{0.5}} \tag{S1}$$

where LAI is the leaf area index (m^2 m^{-2}) computed by JSBACH and averaged over the vegetated part of the grid cell.

The activity factor for light γ_P is calculated as follows

$$\gamma_P = 0 \qquad a < 0, a > 180 \tag{S2}$$

$$\gamma_P = \sin(a)\left[2.46(1+0.0005(P_{24}-400))\Phi - 0.9\Phi^2\right] \qquad 0 < a < 180 \tag{S3}$$

where P_{24} is the average surface PPFD over the last 24 hours (μmol of photons in 400-700 nm range m^{-2} s^{-1}), a is the solar angle (degrees) and Φ is the above canopy PPFD transmission (non-dimensional) estimated as $\Phi = P/P_{toa}$, with P the surface PPFD at current time step and P_{toa} the PPFD at the top of the atmosphere adjusted for solar angle.

The light dependent activity factor for temperature γ_T is estimated as

$$\gamma_T = \frac{E_{opt} C_{T2} \exp(C_{T1}x)}{(C_{T2} - C_{T1}(1-\exp(C_{T2}x)))} \tag{S4}$$

where

$$x = [(1/T_{opt}) - (1/T)]/0.00831 \tag{S5}$$

$$T_{opt} = 313 + 0.6(T_{24} - T_S) \tag{S6}$$

$$E_{opt} = C_{eo}\exp(0.08(T_{24} - T_S)) \tag{S7}$$

$$\tag{S8}$$

with T the lowest atmospheric model level temperature at the current time step (K), T_{24} the average temperature at the same level over the last 24 hours (K) and T_S the leaf temperature in standard condition (= 297 K). C_{T1} and C_{eo} are emission-class empirical coefficients given for each compound in Table S1 in Section S2. C_{T2} is an empirical coefficient (= 200).

The light independent activity factor for temperature γ_{TLI} is estimated as

$$\gamma_{TLI} = \exp(\beta(T - T_S)) \tag{S9}$$

where β is an empirical coefficient specific of each compound class (see Table S1) and T_S the leaf temperature in standard condition (= 297 K).

The soil moisture activity factor γ_{SM} is calculated as

$$\gamma_{SM} = 1 \qquad W > W_1 \tag{S10}$$

$$\gamma_{SM} = (W - W_W)/\Delta W_1 \qquad W_W < W < W_1 \tag{S11}$$

$$\gamma_{SM} = 0 \qquad W < W_W \tag{S12}$$

$$\tag{S13}$$

where W is the relative water content (m m^{-1}), W_W is wilting point (i. e., the soil moisture limit below which plants cannot extract water from soil, m m^{-1}), W_1 is defined as $W_W + \Delta W_1$ with the empirical parameter ΔW_1=0.04 (Guenther et al., 2006, 2012).

S2 Compound specific parameters

Table S1. Compound-class specific model parameters for the calculation of light and temperature activity factor

Compound Classes	LDF	C_{T1}	C_{eo}	β
isoprene	1	95	2	-
myrcene	0.6	80	1.83	0.1
sabinene	0.6	80	1.83	0.1
limonene	0.2	80	1.83	0.1
3-carene	0.2	80	1.83	0.1
t-β-ocimene	0.8	80	1.83	0.1
α-pinene	0.6	80	1.83	0.1
β-pinene	0.2	80	1.83	0.1
β-caryophyllene	0.5	130	2.37	0.17
232-MBO	1	95	2	-
methanol	0.8	60	1.6	0.08
acetone	0.2	80	1.83	0.1
carbon monoxide	1	60	1.6	-
nitric oxide	0	-	-	0.1
bidirectional VOCs	0.8	95	2	0.13
stress VOCs	0.8	80	1.83	0.1
other VOCs	0.2	80	1.83	0.1

S3 Compound specific emission factor for the MEGAN2.1-CLM4 15-PFTs

Table S2. Compound specific emission factor for each of the 15 PFTs of the MEGANv2.1-CLM4 scheme (μg m^{-2} h^{-1}).

Compound Names	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_6	ϵ_7	ϵ_8	ϵ_9	ϵ_{10}	ϵ_{11}	ϵ_{12}	ϵ_{13}	ϵ_{14}	ϵ_{15}
isoprene	600	3000	1	7000	10000	7000	10000	11000	2000	4000	4000	1600	800	200	1
myrcene	70	70	60	80	30	80	30	30	30	50	30	0.3	0.3	0.3	0.3
sabinene	70	70	40	80	50	80	50	50	50	70	50	0.7	0.7	0.7	0.7
limonene	100	100	130	80	80	80	80	80	60	100	60	0.7	0.7	0.7	0.7
3-carene	160	160	80	40	30	40	30	30	30	100	30	0.3	0.3	0.3	0.3
t-β-ocimene	70	70	60	150	120	150	120	120	90	150	90	2	2	2	2
α-pinene	500	500	510	600	400	600	400	400	200	300	200	2	2	2	2
β-pinene	300	300	200	120	130	120	130	130	100	150	100	1.5	1.5	1.5	1.5
β-caryophyllene	80	80	80	60	40	60	40	40	50	50	50	1	1	1	4
232-MBO	700	60	0.01	0.01	0.01	0.01	2	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
methanol	900	900	900	500	900	500	900	900	900	900	900	500	500	500	900
acetone	240	240	240	240	240	240	240	240	240	240	240	80	80	80	80
carbon monoxide	600	600	600	600	600	600	600	600	600	600	600	600	600	600	600
nitric oxide	0	-	-	0.1											
ethanol	200	200	200	200	200	200	200	200	200	200	20	20	20	20	20
acetaldehyde	200	200	200	200	200	200	200	200	200	200	20	20	20	20	20
formaldehyde	40	40	40	40	40	40	40	40	40	40	16	16	16	16	16
acetic acid	30	30	30	30	30	30	30	30	30	30	12	12	12	12	12
formic acid	30	30	30	30	30	30	30	30	30	30	12	12	12	12	12
ethene	174	174	174	174	174	174	174	174	174	174	174	174	174	174	174
hydrogen cyanide	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	4.5	
toluene	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9
methyl bromide	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8	2.8
methyl chloride	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4
methyl ioide	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14
dimethyl sulfide	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42
methane	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7	0.7
ethane	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4	1.4
propane	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14
butene	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2	67.2
propene	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6	33.6
benzaldehyde	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14	0.14

S4 Global annual emission totals of the reference and sensitivity simulations for the 32 compounds

Table S3. Global annual emission totals (Tg C yr^{-1}) of the 32 compounds averaged over the 12 years (2000-2012) for the reference CTRL, PFT-CLM4, PFT-JSBACH and TEST-NUDG simulations.

Compounds	CTRL	PFT-CLM4	PFT-JSBACH	TEST-NUDG
isoprene	417	381.7	304	409.3
methanol	43.9	43.9	36.3	42.4
α-pinene	26.1	45.7	37.1	25.3
acetone	22.9	22.9	18.8	21.6
ethene	22.9	22.9	19.9	22
β-pinene	15.8	15.6	12.5	15
t-β-ocimene	14	10.5	8.4	13.8
propene	12.7	12.7	10.9	11.8
ethanol	8.8	8.8	7	8.5
acetaldehyde	9.2	9.2	7.3	8.9
limonene	8.4	9.5	7.4	8
butene	6.3	6.3	5.5	5.9
3-carene	6	6.1	5.1	5.7
sabinene	5.7	6.3	5.2	5.5
β-caryophyllene	4.3	4.3	3.4	4
myrcene	2.3	5.9	4.9	2.2
232-MBO	2	1.7	1.3	1.9
formaldehyde	1.7	1.7	1.4	1.6
acetic acid	1.3	1.3	1	1.2
toluene	1.3	1.3	1.1	1.2
formic acid	0.8	0.8	0.7	0.8
hydrogen cyanide	0.3	0.3	0.3	0.3
ethane	0.3	0.3	0.2	0.2
methane	0.12	0.12	0.1	0.1
methyl chloride	0.07	0.07	0.06	0.07
dimethyl sulfide	0.04	0.04	0.03	0.03
propane	0.03	0.03	0.02	0.02
benzaldehyde	0.02	0.02	0.02	0.02
methyl bromide	0.01	0.01	0.01	0.01
methyl ioide	0.003	0.003	0.002	0.002
carbon monoxide	41.1	41.1	35.7	40.4
nitric oxide	5.9	3.6	3.4	5.4

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