Supplementary Information for

High temperature sensitivity of monoterpene emissions from global vegetation

by

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Supplementary Text

Monoterpene emissions in MEGAN

A detailed formulation of monoterpene emissions is provided in Guenther et al. (1). Briefly, the monoterpene emissions in MEGAN are based on a mechanistic model that considers the major processes driving variations in emissions. The activity factor for monoterpenes accounts for emission responses to temperature (γ_T), light (γ_P), leaf age (γ_A), soil moisture (γ_{SM}), leaf area index (LAI) and CO_2 (γ_C) inhibition as

$$\gamma = C_{CE} LAI \gamma_T \gamma_P \gamma_A \gamma_{SM} \gamma_C \quad (1)$$

where CCE is a factor that sets the emission activity to unity at standard conditions. The temperature activity factor (γT), that was investigated in this study, is a weighted average of a light-dependent (LDF) and a light-independent fraction (LIF = 1-LDF)

$$\gamma_T = (1 - LDF)\gamma_{T\_LIF} + LDF\gamma_{T\_LDF} \quad (2)$$

The light-dependent fraction response is calculated similar to isoprene response as

$$\gamma_{T\_LDF} = E_{opt} \times [C_{T2} \times \exp(C_{T1} \times x)/(C_{T2} - C_{T1} \times (1 - \exp(C_{T2} \times x)))] \quad (3)$$

where x = [(1/T_{opt}) – (1/T)]/0.00831, T is the leaf temperature (K), CT1 and CT2 (=230) are empirically determined coefficients.

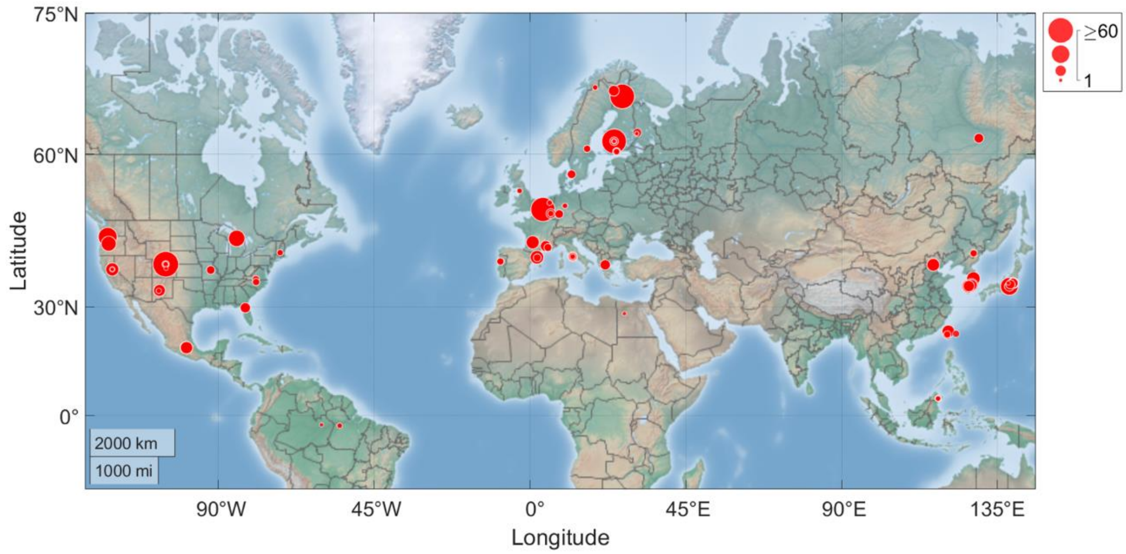
$$T_{opt} = 313 + \left(0.6 \times (T_{240} - T_S)\right) \quad (4)$$

$$E_{opt} = C_{eo} \times \exp\left(0.05 \times (T_{24} - T_S)\right) \times \exp\left(0.05 \times (T_{240} - T_S)\right) \quad (5)$$

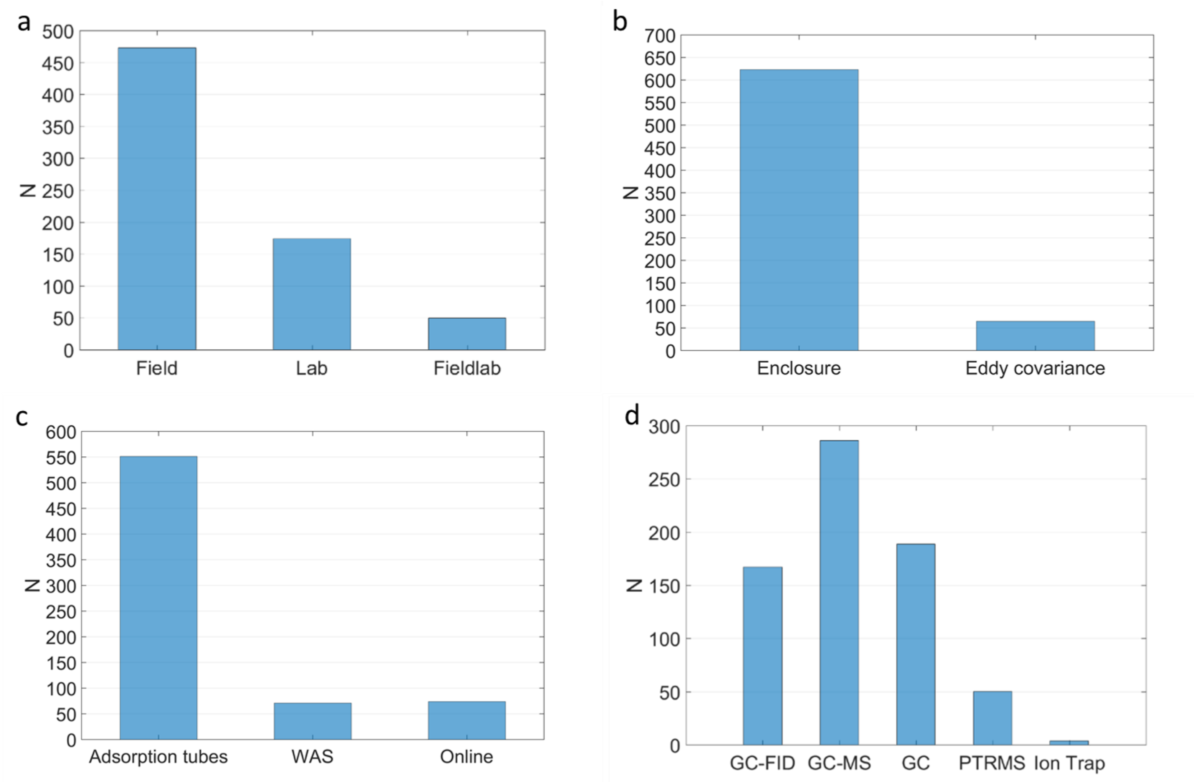
here, Ts represents the temperature for standard conditions, T24 and T240 the average temperature over the past 24 and 240 hours respectively and C_{eo} is an emission-class dependent empirical coefficient.

In our study, the light-dependent fraction was not modified. The response of the light-independent fraction follows the monoterpene function as

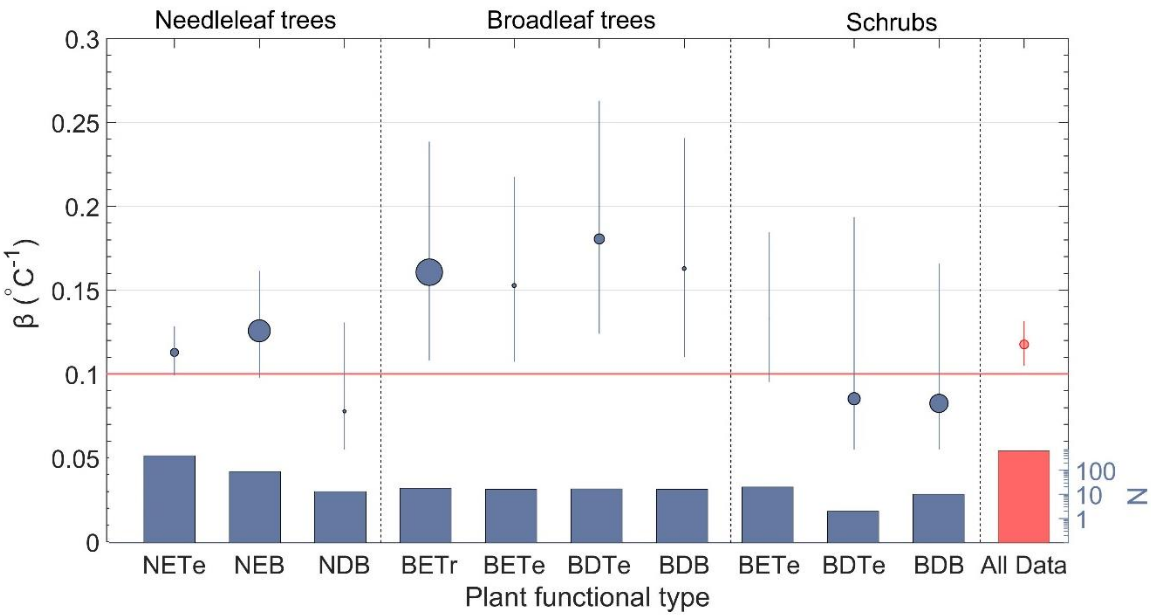
$$\gamma_{T_{LIF}} = \exp(\beta(T - T_S) \quad (6)$$



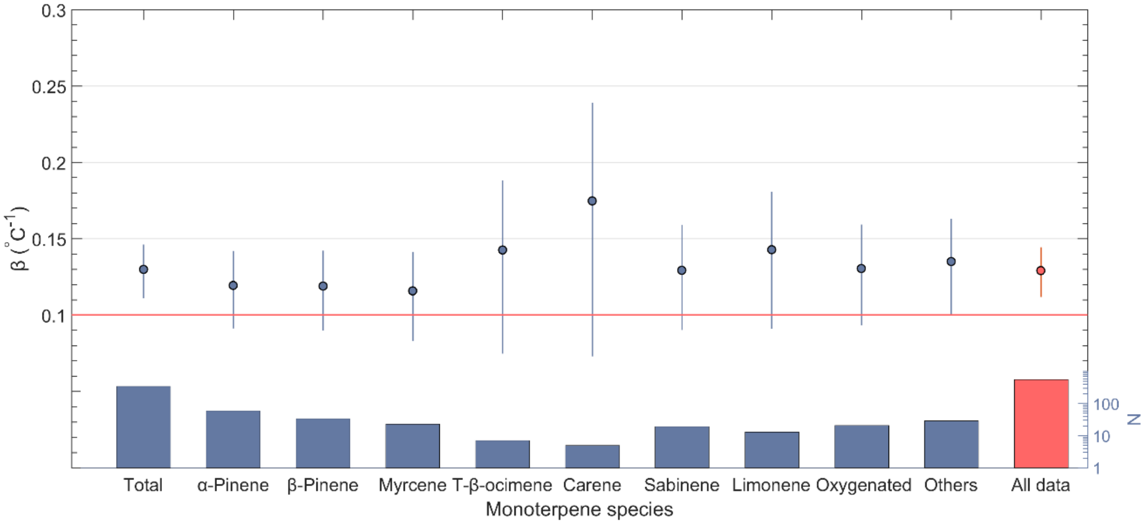
Supplementary Fig. 1. Locations of experimentally derived β. The size of the circles indicates the number of coefficients obtained from all studies[1–87].



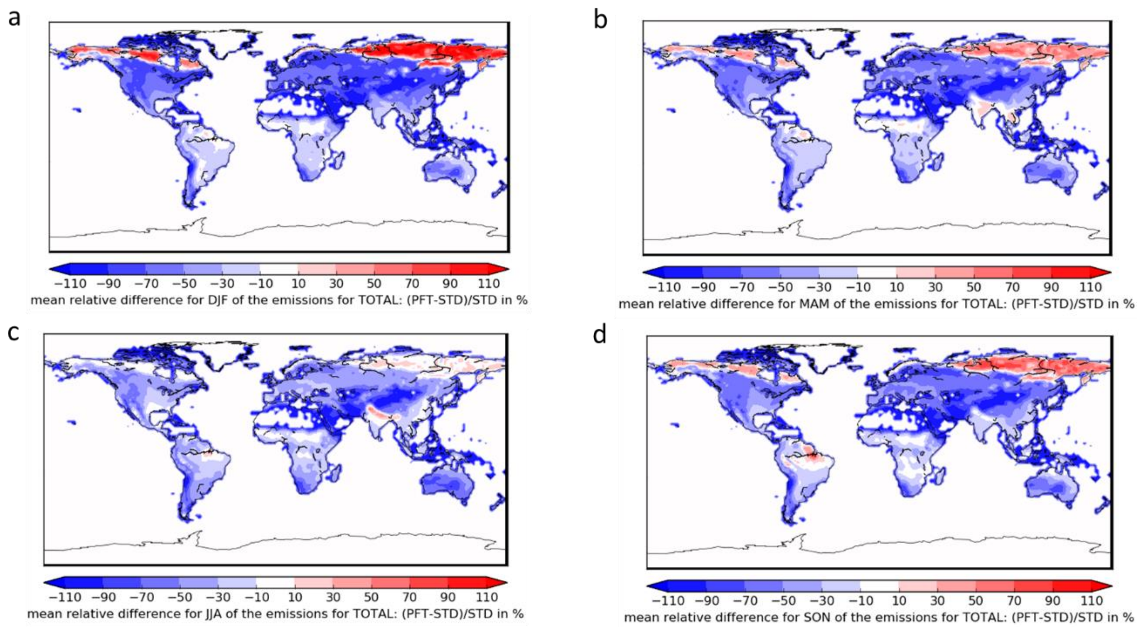
Supplementary Fig. 2. Number (N) of β coefficients collected under different experimental approaches. a. Environmental conditions (Fieldlab indicates plants re-potted in the field in an environment different than the original). b. Determination of the rate of emission. c. VOC sampling. d. VOC analysis.



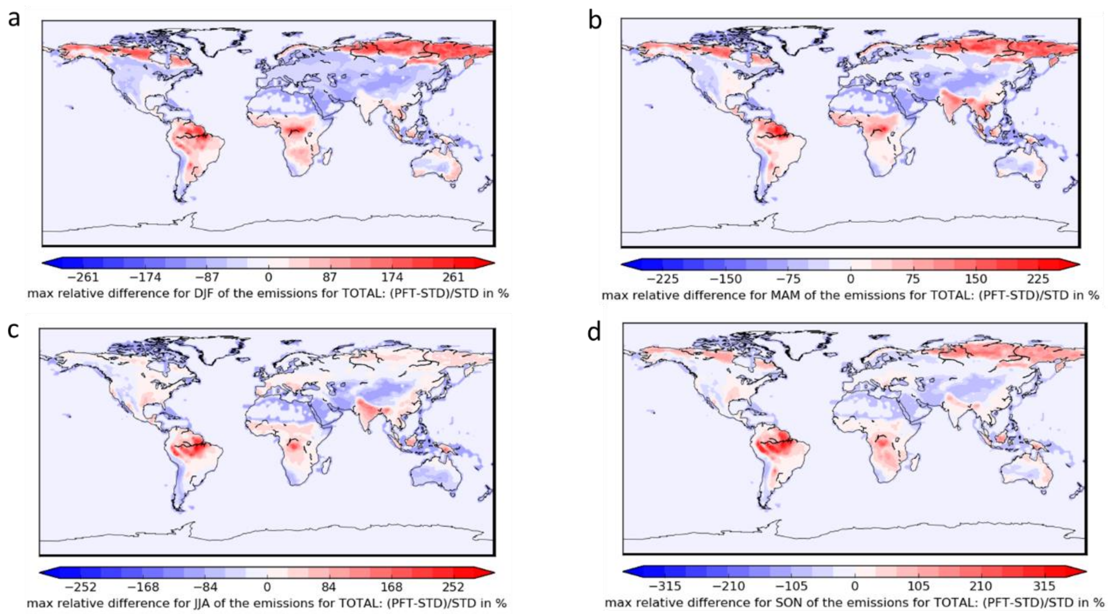
Supplementary Fig. 3. Dependence on temperature (β) for the plant functional types considering the complete dataset. The error bars in panel indicate 95% confidence intervals, and the size of the blue bullet points is proportional to the global surface area of each plant functional type. NETe, needleleaf evergreen temperate forest; NEB, needleleaf evergreen boreal forest; NDB, needleleaf deciduous boreal forest; BETr, broadleaf evergreen tropical forest; BETe, broadleaf evergreen temperate forest/shrubs; BDTe, broadleaf deciduous temperate forest/shrubs; BDB, broadleaf deciduous boreal forest/shrubs.



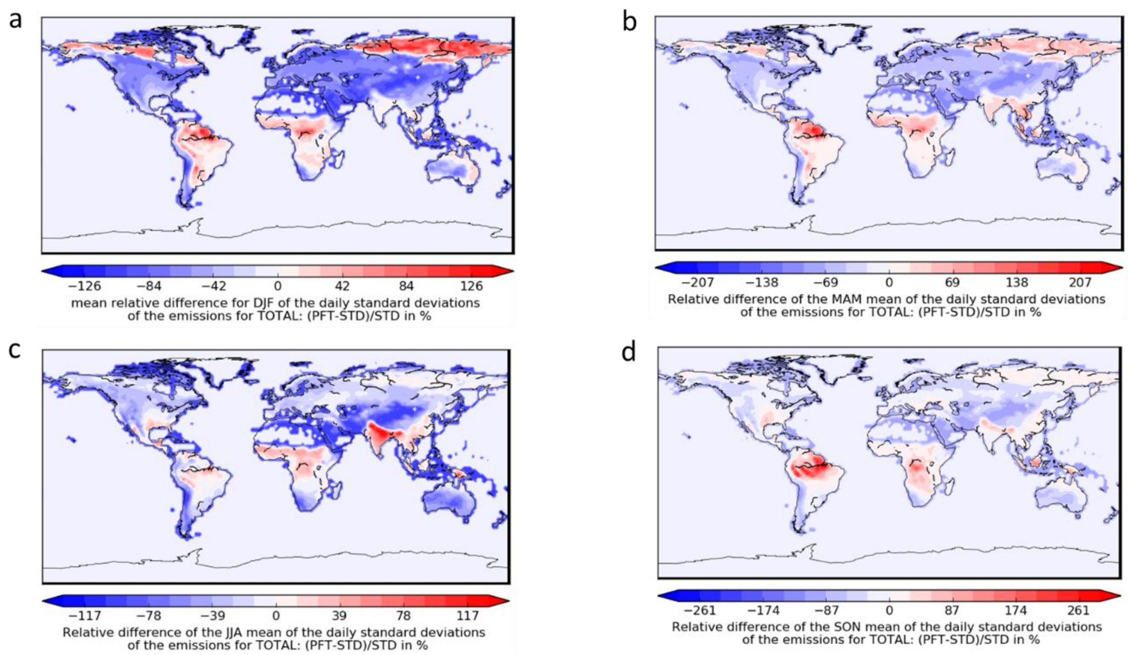
Supplementary Fig. 4. Coefficient of temperature dependency (β) for various monoterpenes.



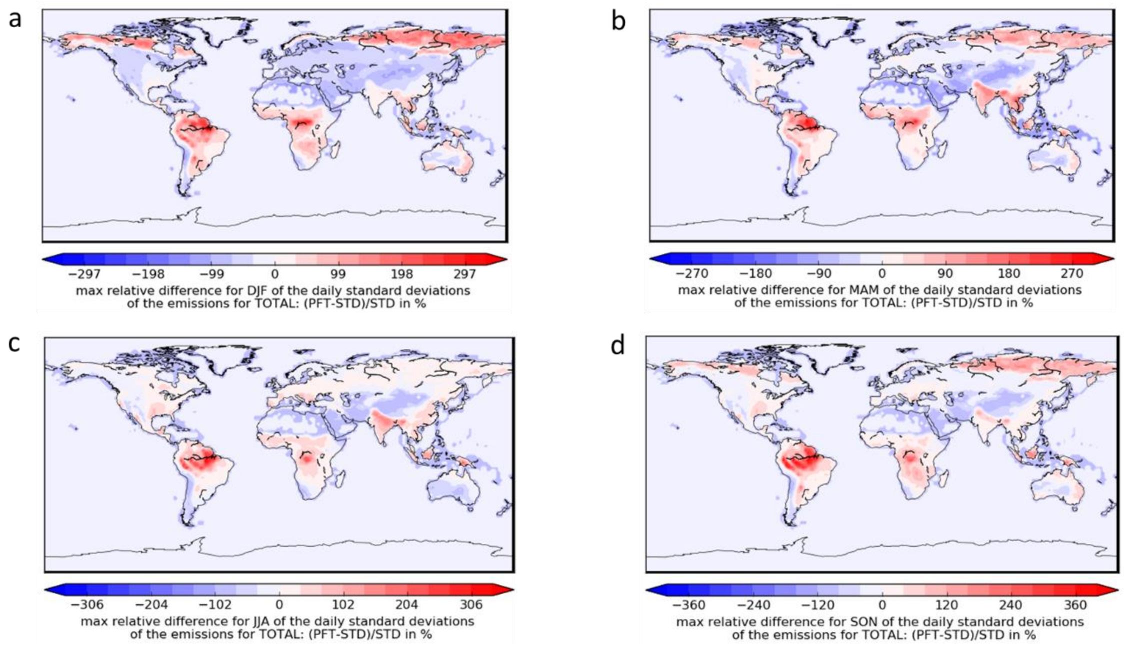
Supplementary Fig. 5. Mean relative differences between a constant β (0.1 °C^{-1}, STD) and β dependent on plant functional type (PFT) for monoterpene emissions. Northern Hemisphere (NH) a) winter, b) spring, c) summer, and d) autumn.



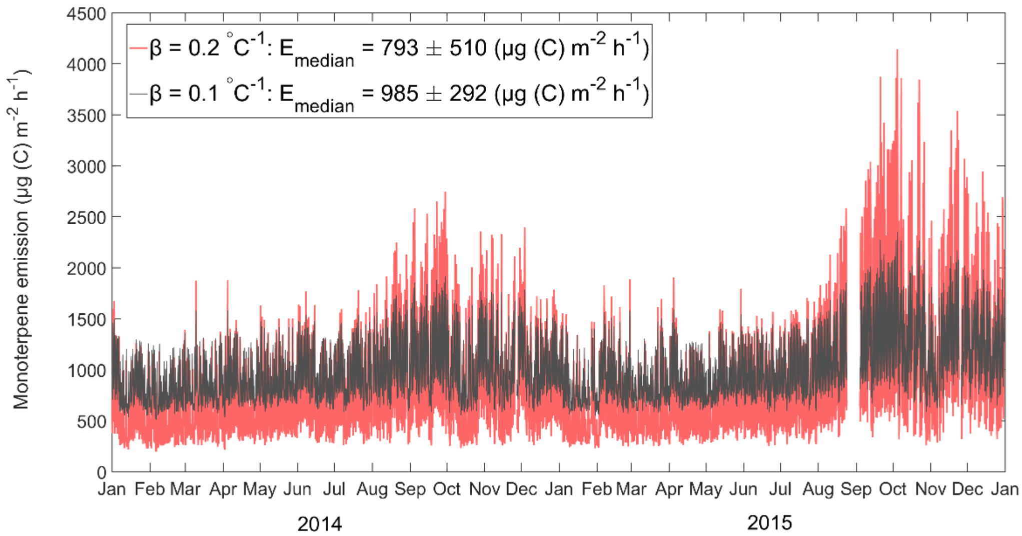
Supplementary Fig. 6. Hourly maximum relative differences between a constant β (0.1 °C^{-1}, STD) and β dependent on plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



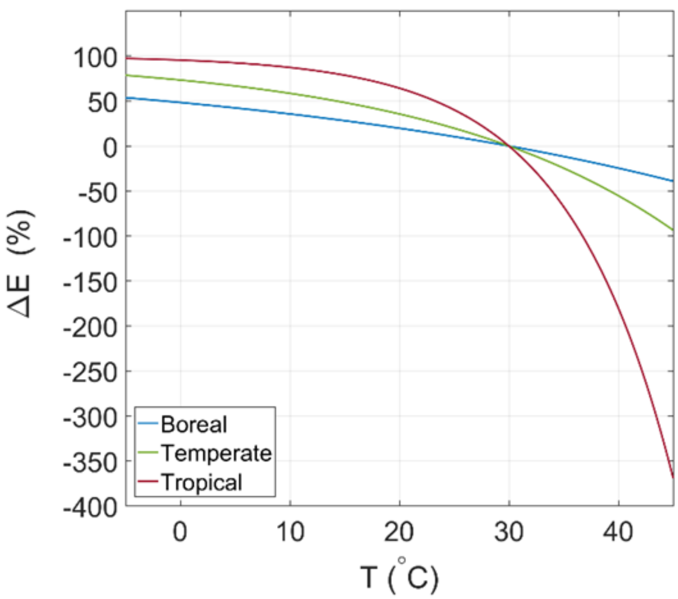
Supplementary Fig. 7. Mean relative differences of the daily standard deviation (STD) between a constant β (0.1 $°C^{-1}$) and β dependent on plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



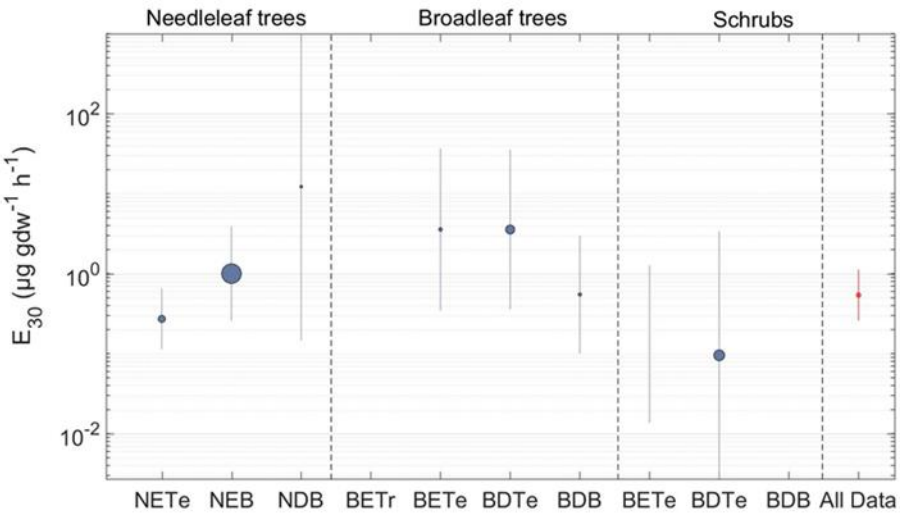
Supplementary Fig. 8. Hourly maximum relative differences of the daily standard deviation (STD) between a constant β (0.1 °C^{-1}) and β dependent on plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



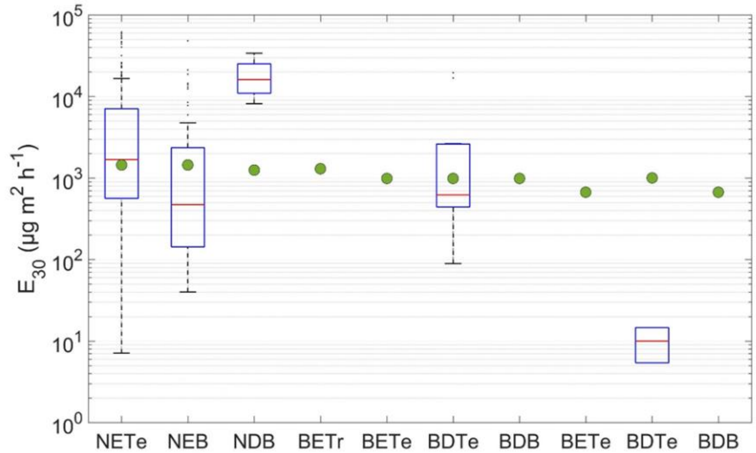
Supplementary Figure 9. Timelines of simulated (using Eq. 1) monoterpene emissions at the Amazonian Tall Tower Observatory (ATTO) using data from Bourtsoukidis *et al.*[88].



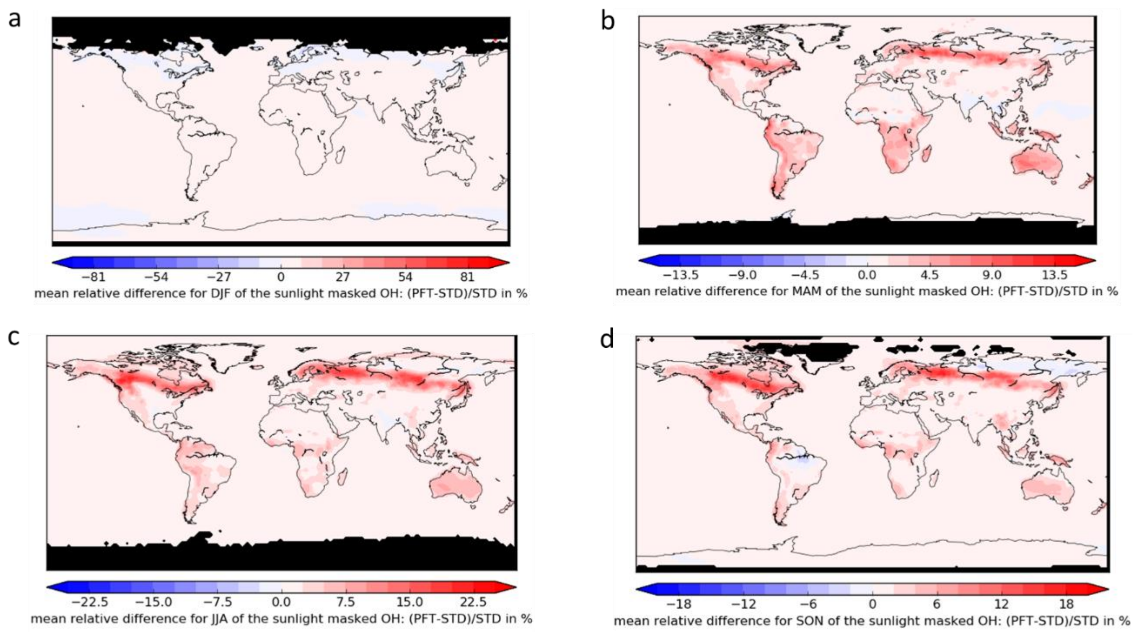
Supplementary Figure 10. Percent differences using Eq. 1 with β=0.1 °C^{-1} and with β for each ecosystem as derived in Supplementary Table 2.



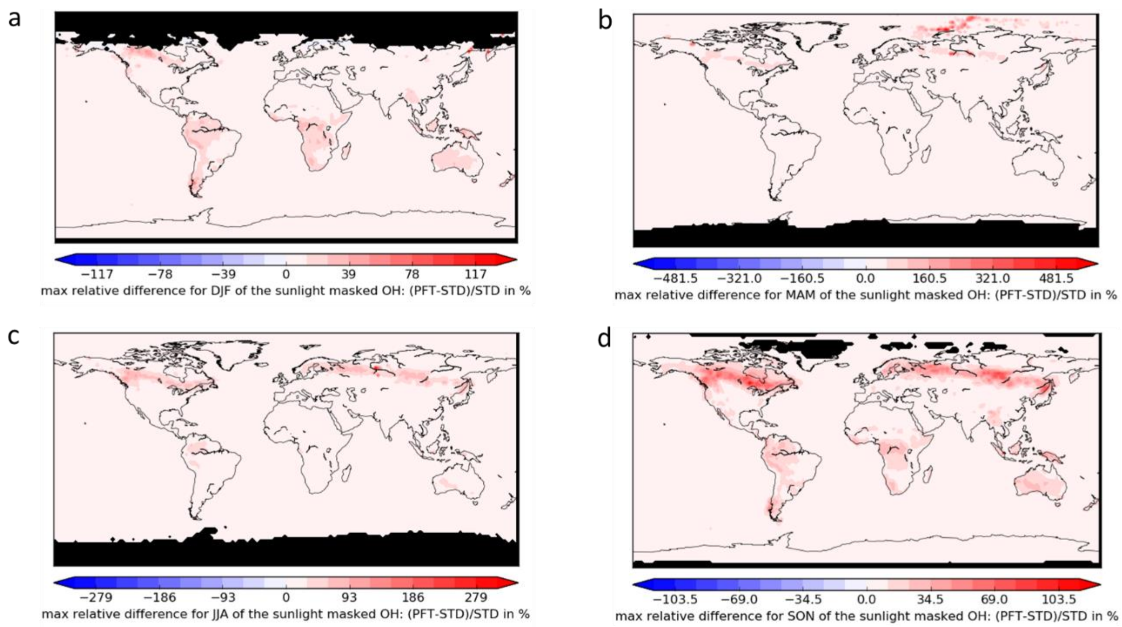
Supplementary Figure 11. Reported standardized (at 30 °C) potential emissions for different plant functional types. The error bars indicate 95% confidence intervals, and the size of the blue bullet points is proportional to the global surface area of each plant functional type. NETe, needleleaf evergreen temperate forest; NEB, needleleaf evergreen boreal forest; NDB, needleleaf deciduous boreal forest; BETr, broadleaf evergreen tropical forest; BETe, broadleaf evergreen temperate forest/shrubs; BDTe, broadleaf deciduous temperate forest/shrubs; BDB, broadleaf deciduous boreal forest/shrubs.



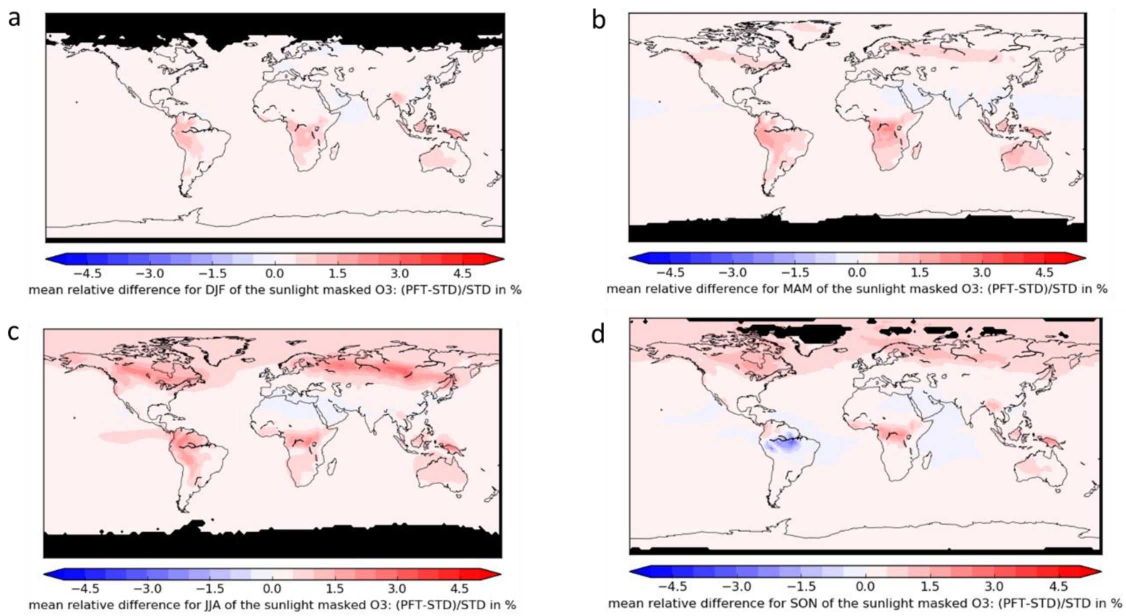
Supplementary Figure 12. Calculated standardized (at 30 °C) potential emissions for different plant functional types. NETe, needleleaf evergreen temperate forest; NEB, needleleaf evergreen boreal forest; NDB, needleleaf deciduous boreal forest; BETr, broadleaf evergreen tropical forest; BETe, broadleaf evergreen temperate forest/shrubs; BDTe, broadleaf deciduous temperate forest/shrubs; BDB, broadleaf deciduous boreal forest/shrubs. The values in MEGAN are represented with green dots.



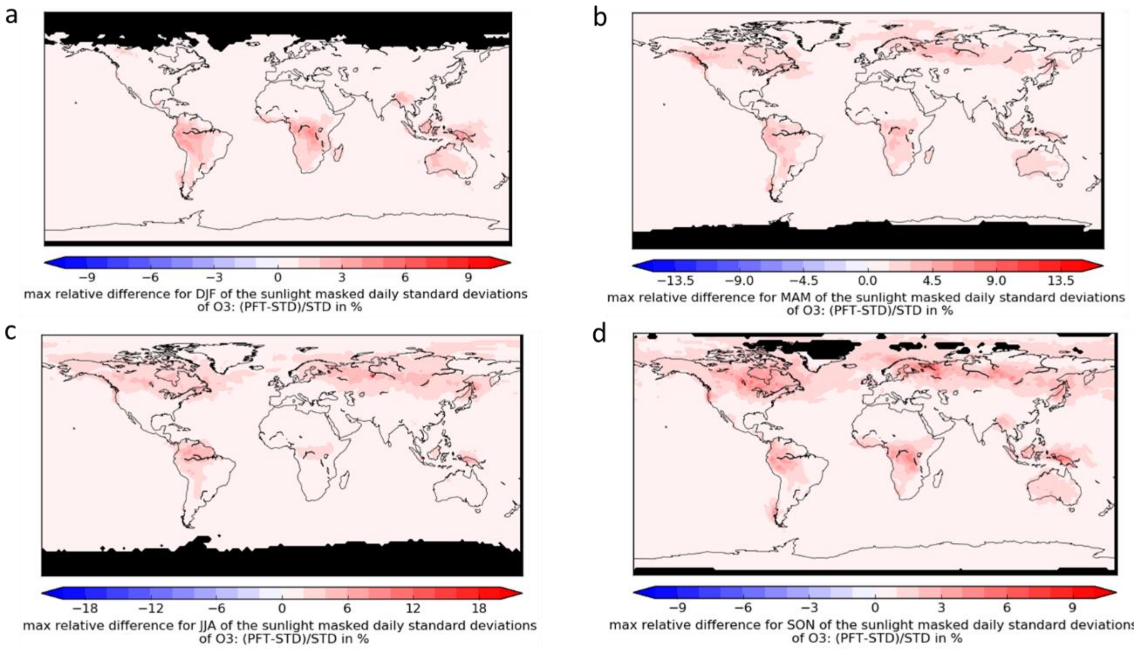
Supplementary Fig. 13. Mean relative differences for sunlight masked OH (i.e. daytime values) between a constant β (0.1 °C^{-1} (STD) and dependent on the plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



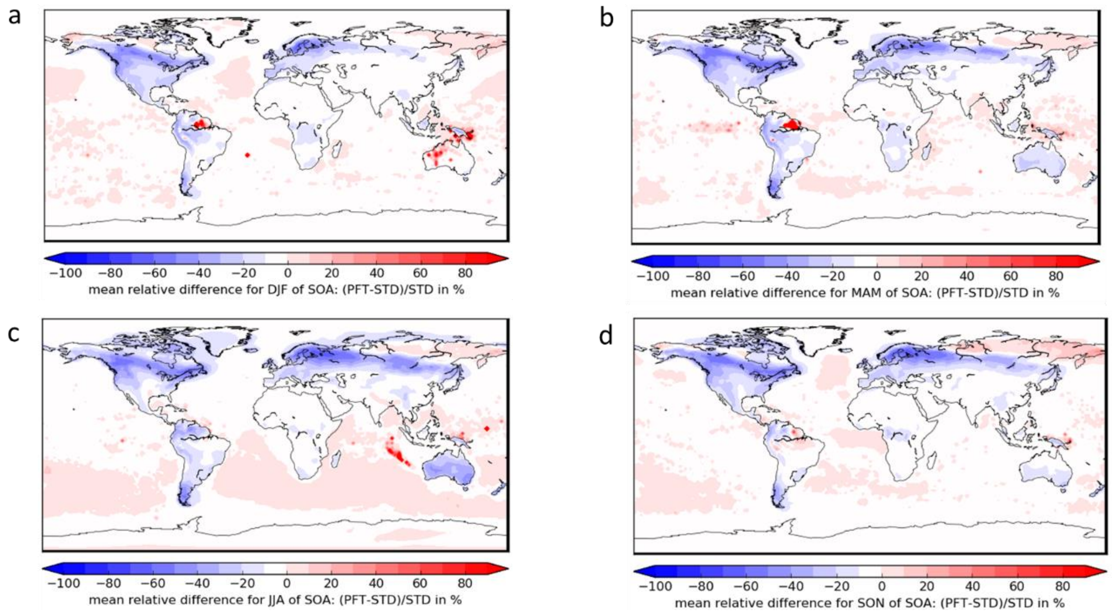
Supplementary Fig. 14. Maximum relative differences for sunlight masked OH (i.e. daytime values) between a constant β (0.1 °C^{-1} (STD) and plant functional type (PFT) dependent β coefficient for monoterpenes emissions. NH a) winter, b) spring, c) summer, and d) autumn.



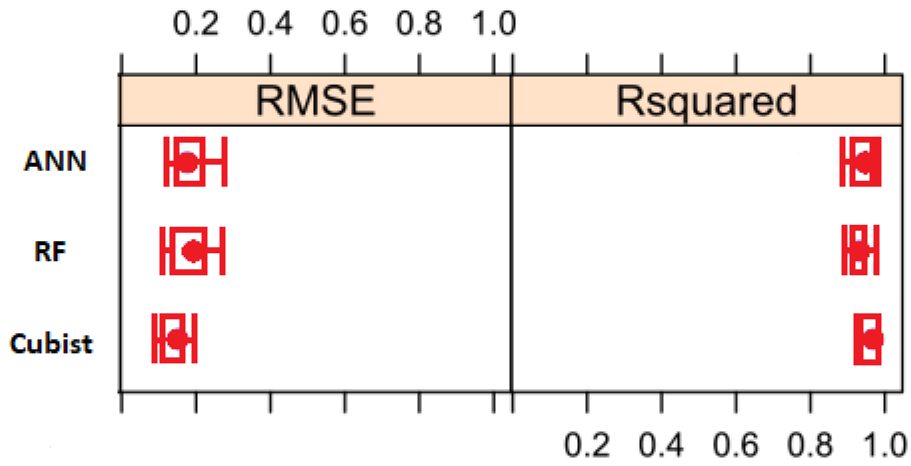
Supplementary Fig. 15. Mean relative differences for surface ozone between a constant β (0.1 °C^{-1}, STD) and β dependent on plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



Supplementary Fig. 16. Maximum relative differences for surface ozone between a constant β (0.1 °C^{-1}, STD) and β dependent on plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



Supplementary Fig. 17. Mean relative differences for secondary organic aerosols between a constant β (0.1 °C^{-1}, STD) and β dependent on plant functional type (PFT) for monoterpene emissions. NH a) winter, b) spring, c) summer, and d) autumn.



Supplementary Figure 18. RMSE and Rsquared for the ANN, RF and Cubist algorithms.

Category	Group	Parameters collected
Experimental	Conditions	Field, laboratory, controlled field
Experimental	Emission calculation	Enclosure, eddy covariance
Experimental	VOC sampling	Adsorbent tubes, whole air samples, online
Experimental	VOC analysis	Gas Chromatography (MS+FID), PTR-(ToF-)-MS, ion trap
Location	Coordinates	Latitude, longitude, meters above sea level
Seasonality	Time	Year, season, month
Vegetation	Ecosystem	Temperate, mediterranean, boreal, tropical, arctic
Vegetation	Tree type	Plant functional types (as in MEGAN)
Vegetation	Tree characteristics	Tree age, tree height, sampling height
Emissions	Conclusion	Temperature dependent, temperature and light dependent, temperature and other other environmental factor dependent
Emissions	Regression	β-factor, E_{30}, R^2
Emissions	Temperature	Minimum, maximum, average, range

Supplementary Table 1. Parameters collected from each study.

Total monoterpene emission (Tg y^{-1})			
Plant functional type	MEGAN v2.1	This study	%change
Needleleaf evergeen boreal trees	5.34	3.00	-43.8
Needleleaf deciduous boreal trees	0.57	0.54	-4.6
Broadleaf evergreen tropical trees	27.02	25.77	-4.6
Broadleaf evergreen temperate trees	1.99	1.18	-40.7
Broadleaf deciduous tropical trees	10.15	9.86	-2.9
Broadleaf deciduous temperate trees	3.92	3.13	-20.2
Broadleaf deciduous boreal trees	0.89	0.50	-43.8
Broadleaf evergreen temperate shrubs	0.03	0.02	-33.3
Broadleaf deciduous temperate shrubs	3.57	2.55	-28.6
Broadleaf deciduous boreal shrubs	1.71	1.50	-12.3
Arctic C3 grass	0.96	0.69	-28.1
Cool C3 grass	7.80	6.39	-18.1
Warm C3 grass	13.40	12.70	-5.2
Crop1	9.48	8.09	-14.7
Total (Sum of PFTs)	86.83	75.92	-12.6

Supplementary Table 2. Simulated monoterpene emissions for each plant functional type.

Boreal Ecosystems

Vegetation type	% coverage	E30	β
Needleleaf Evergreen Boreal	10.6	1450	0.15
Needleleaf Decidious Boreal	1.46	1250	0.09
Broadleaf Decidious Boreal	2.14	990	0.19
Broadleaf Decidious Boreal Schrub	9.33	670	0.08
Weighted averages :		**1086**	**0.12**

Temperate Ecosystems

Vegetation type	% coverage	E30	β
Needleleaf Evergreen Temperate	5.46	1450	0.12
Broadleaf Evergreen Temperate	2.64	990	0.15
Broadleaf Decidious Temperate	5.33	990	0.19
Broadleaf Evergreen Temperate Schrub	0.18	670	0.17
Broadleaf Decidious Temperate Schrub	4.15	1000	0.12
Weighted averages :		**1131**	**0.14**

Tropical Ecosystems

Vegetation type	% coverage	E30	β
Broadleaf Evergreen Tropical	15.6	1300	0.20
Broadleaf Decidious Tropical	12.9	1300	NaN
Weighted averages :		**1300**	**0.20**

Supplementary Table 3. Weighted β and standardized potential emissions.

```
   DO jt=1,nmegan
      !-----------------------------------------------------
      !  TEMPERATURE DEPENDENCE FACTOR (GAMMA_T)--> GAM_TMP
      !-----------------------------------------------------
      SELECT CASE (MGN_SPC(jt))
      CASE ('ISOP')
        CALL GAMMA_TISOP( TEMP(1:kproma,jrow), D_TEMP(1:kproma,jrow),
gam_tmp(jt)%ptr(1:kproma,jrow) )
!mz_ap_20210906+
!      CASE ( 'MBO','MYRC','SABI','LIMO','CAR3','OCIM','BPIN',       &
!           'APIN','FARN','BCAR','MEOH','ACTO','ACTA','FORM',       &
!            'CH4',  'NO','OMTP','OSQT',  'CO'              )
!        CALL GAMMA_TNISP( TDF_PRM(jt), TEMP(1:kproma,jrow), gam_tmp(jt)%ptr(1:kproma,jrow))
! new code, moved here for speed. Not included in the main repository as only sensitivity case
! only for Terpenes:
      CASE ( 'FARN','BCAR','MEOH','ACTO','ACTA','FORM',       &
           'CH4',  'NO','OSQT',  'CO'              )
        CALL GAMMA_TNISP( TDF_PRM(jt), TEMP(1:kproma,jrow), gam_tmp(jt)%ptr(1:kproma,jrow))
      CASE ( 'MBO','MYRC','SABI','LIMO','CAR3','OCIM','BPIN',       &
          'APIN','OMTP' )
         gam_tmp(jt)%ptr(1:kproma,jrow) =
input_NETeT(1:kproma,jrow)*exp(0.12_dp*(TEMP(1:kproma,jrow)-303.0_dp) )  &
                              +  input_NEBoT(1:kproma,jrow)*exp(0.15_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_NDBoT(1:kproma,jrow)*exp(0.09_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BETrT(1:kproma,jrow)*exp(0.20_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BETeT(1:kproma,jrow)*exp(0.15_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BDTrT(1:kproma,jrow)*exp(0.13_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BDTeT(1:kproma,jrow)*exp(0.19_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BDBoT(1:kproma,jrow)*exp(0.19_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BETeS(1:kproma,jrow)*exp(0.17_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BDTeS(1:kproma,jrow)*exp(0.12_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_BDBoS(1:kproma,jrow)*exp(0.08_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_ArC3G(1:kproma,jrow)*exp(0.13_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_CoC3G(1:kproma,jrow)*exp(0.13_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_WaC3G(1:kproma,jrow)*exp(0.13_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
&
                              +  input_Crop1(1:kproma,jrow)*exp(0.13_dp*(TEMP(1:kproma,jrow)-303.0_dp) )
!mz_ap_20210906-

      CASE DEFAULT
!        CALL FINISH(substr,'Error: GAMMA_T, invalid variable:'//MGN_SPC(jt))
```

```
      CALL error_bi('Error: GAMMA_T, invalid variable:'//MGN_SPC(jt),substr)
    ENDSELECT
    !----------------------------------------------------
    !  LAI CORRECTION FACTOR (GAMMA_LAI) --> GAM_LHT
    !----------------------------------------------------
    CALL GAMMA_LAI(input_lai(1:kproma,jrow),gam_lht(jt)%ptr(1:kproma,jrow))
    !----------------------------------------------------
    !  LIGHT CORRECTION FACTOR (GAMMA_P) --> GAM_PHO
    !----------------------------------------------------
    ! NB: cossza_2d : COS(zenith angle)
    CALL GAMMA_P(DAY, cossza_2d(1:kproma,jrow), PPFD(1:kproma,jrow), D_PPFD(1:kproma,jrow), &
             gam_pho(jt)%ptr(1:kproma,jrow) )
    !----------------------------------------------------
    !  AGE CORRECTION FACTOR (GAMMA_A) --> GAM_AGE
    !----------------------------------------------------
    nday_month = JulianMonthLength(YEAR, MONTH)
    CALL GAMMA_A(MGN_SPC(jt),input_laip(1:kproma,jrow),input_lai(1:kproma,jrow),nday_month, &
             D_TEMP(1:kproma,jrow), gam_age(jt)%ptr(1:kproma,jrow) )
    !----------------------------------------------------
    !  SOIL MOSTURE DEPENDENCE FACTOR (GAMMA_S) --> GAM_SMT
    !----------------------------------------------------
     CALL GAMMA_S(gam_smt(jt)%ptr(1:kproma,jrow))
    !----------------------------------------------------
    ! ADDITIONAL TERMS IN THE EQUATIONS (FROM NAMELIST)
    !----------------------------------------------------
    !----------------------------------------------------
    !  PRODUCTION AND LOSSES WITHIN THE CANOPY (RHO_FCT)--> RHO
    !----------------------------------------------------
    ! in this case is always equal to 1 (see namelist)
    RHO = RHO_FCT(jt)
    !----------------------------------------------------
    !  light dependent fraction (LDF_FCT)--> LDF
    !----------------------------------------------------
    LDF = LDF_FCT(jt)
    ! final emissions ER = ( EF * GAM_TMP * GAM_AGE * GAM_LHT * GAM_SMT * RHO ) *  &
    !                 ( (1-LDF) + (GAM_PHO*LDF) )
    ! which is equivalent to : ER =  EF * (GAM_TMP * GAM_AGE * GAM_LHT * GAM_SMT * RHO ) *  &
    !                   ( (1-LDF) + (GAM_PHO*LDF) )
    ! which is equivalent to : ER =  EF * (GAM_TOTAL)
    ! with GAM_TOTAL = (GAM_TMP * GAM_AGE * GAM_LHT * GAM_SMT * RHO ) * ( (1-LDF) +
(GAM_PHO*LDF) )
    gam_total(jt)%ptr(1:kproma,jrow) = ( gam_tmp(jt)%ptr(1:kproma,jrow)                  &
                         * gam_age(jt)%ptr(1:kproma,jrow)                   &
                         * gam_lht(jt)%ptr(1:kproma,jrow)                   &
                         * gam_smt(jt)%ptr(1:kproma,jrow) * RHO )           &
                         * ((1-LDF)+(gam_pho(jt)%ptr(1:kproma,jrow) *LDF))
    WHERE (gam_total(jt)%ptr(1:kproma,jrow) < 0.0_dp) gam_total(jt)%ptr(1:kproma,jrow) = 0.0_dp
  END DO !jt loop (nmegan)
```

Supplementary Code 1. Code used for including β for each PFT in MEGAN.

Supplementary References

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