Supplementary Material 3 for

Growth and actual leaf temperature modulate CO2-responsiveness of monoterpene emissions from Holm oak in opposite ways

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**Description of the simulation approach** to assess the potential effect of high-CO2-inhibition on total annual monoterpene emission from QI leaves under a future warmer climate with double [CO2]

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**Table S4.** Results from non-linear fitting of the relative monoterpene emission rates (ECO2 E400-1) measured during CO2-ramping experiments to the MEGAN algorithm accounting for CO2-effects on isoprene emissions (Eq. (1), **Fig. 4**). Values shows best-fit coefficients ± Standard Error performed on the merged data sets of the four growth populations (All), and on two subsets differing in growth temperature (400/20+800/20 and 400/25+800/25). For comparison, coefficients are given from the MEGAN model used to predict the short-term effects of CO2 on isoprene emissions from plants growing under current atmospheric [CO2]. The estimation of the coefficients was carried out using least squares method (Marquardt-Levenberg algorithm, SigmaStat 2.0 Jandel Scientific Software). R is the correlation coefficient and P the probability value of the fits.

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| --- | --- | --- | --- | --- |
| **Data set** | **Emax ± SE** | ***h* ± SE** | **C\*± SE** | **R (P)** |
| **All** | **1.041 ± 0.027** | **1.68 ± 0.29** | **1241 ± 97** | **0.70 (<0.001)** |
| **400/20+800/20** | **0.985 ± 0.028** | **1.71 ± 0.62** | **1933 ± 522** | **0.54 (<0.001)** |
| **400/25+800/25** | **1.109 ± 0.046** | **1.57 ± 0.30** | **938 ± 78** | **0.80 (<0.001)** |
| **MEGAN** | **1.072** | **1.70** | **1218** |  |

**Description of the simulation approach**

To better understand the relative importance of CO2 inhibition in interaction with other co-determinants of leaf MT-emissions from QI, we computed annual emissions by combining eight high-CO2-inhibition scenarios differing in their maximum high-CO2 inhibition with four warming scenarios (1-4 °C warming) and three scenarios of EF seasonality (seasonality without and with summer drought, no seasonality) according the following approach:

where E(EF,CO2,L,T) is the actual emission rate (ng m-2 s-1) as a function of the emission factor EF, atmospheric [CO2], light (PPFD) and temperature. EF(season) is the leaf’s emission factor as a function of season, CCO2(T) is the percent inhibition at double [CO2] as a function of temperature, and CT and CT are correction factors accounting for the short-term effects of light (PPFD) and temperature (°C) on emissions.

Concerning CT and CT we applied the well-known algorithms of MEGAN in their original forms with coefficient values adjusted for monoterpene emissions from QI as described in Staudt and Bertin (1998). As input data we used the temperature and PPFD data (30 min averages) of the years 2019, 2020 and 2021 (annual mean temperatures: 14.7, 14.8 and 14.0 °C) recorded on the flux tower of the experimental station of Puechabon located in a Holm oak forest 24 km north-west of our institute (see <https://puechabon.cefe.cnrs.fr/>). To simulate climate warming, temperature data were increased by 1, 2, 3 and 4 °C. These increments encompass the range of warming predicted to occur with doubling [CO2] by the end of the century (IPCC 2021 scenario SSP3-7.0: 2.8-4.6 °C relative to the 1850-1900 period).

The high-CO2-inhibition of emissions at double CO2 (CCO2(T)) was calculated according our results (10 % inhibition at 30 °C and 0 % at 35°C) and literature review (see main text) as:

**CCO2(T) = -2T + 70 for Tt<T≤35,**

**CCO2(T) = 0 for T>35,**

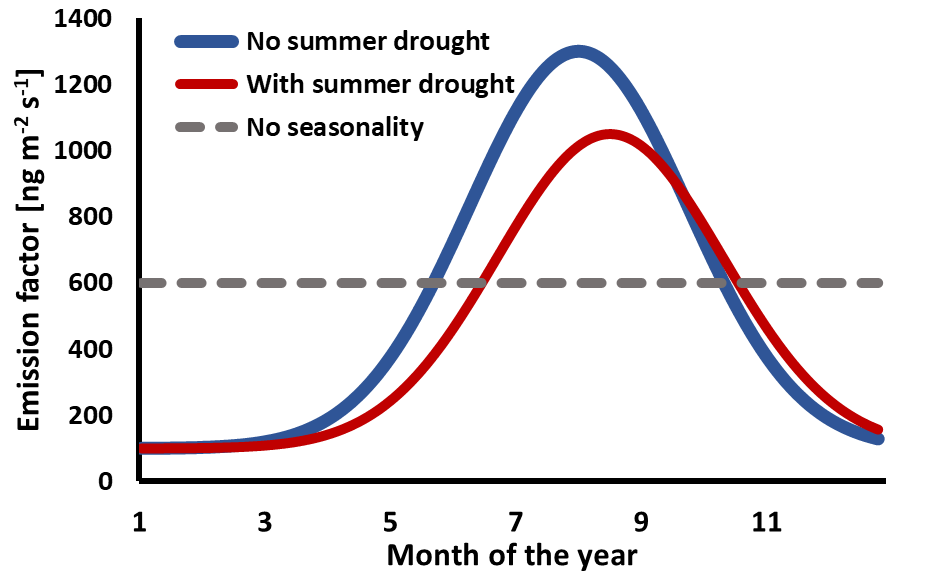
**CCO2(T) = -2 Tt + 70 for T≤ Tt .**

This approach assumes that inhibition is 0 % at a temperature T ≥ 35 °C and progressively increases at lower temperatures by 2 % per 1°C temperature decrease until a maximum inhibition at the temperature threshold Tt. Since the maximum inhibition is not known, we adjusted Tt.to reach eight different maximum inhibitions of 10, 15, 20, 25, 30, 40, 60 and 100 % (e.g. Tt = 25 and 15 °C for respectively maximum inhibitions of 20 % and 40 %).

The seasonal variation of EF (EF(season)) is driven by several factors including leaf age and phenology, prevailing meteorological conditions and summer drought (Staudt et al., 2002, 2003). The exact relationships of these factors to the EF of QI are not yet know. Therefore, we used the algorithm described in Staudt et al. (2000), which simulates a bell-shaped seasonal variation of EF as a function of a time variable, here the day of year (D):

where EFmax is the maximum EF in the year, *A* the annual EF amplitude (= EFmax - EFmin), Do the day of EFmax and *T* a coefficient describing the length (duration) of the EF amplitude (‘peak width’). The seasonal variations of QI EF described in Staudt et al. (2002) were fitted on this algorithm. In that study, emissions were measured on mature QI trees near the institute in two plots, one with trees exposed to summer drought and one with irrigated trees. In addition to the EF variations deduced from these two plots, we run simulations without EF seasonality (constant EF throughout the year). The three EF seasonal courses applied in the simulations are shown in Fig. S9 below.

On the whole, 96 scenario combinations were run (4 warming x 8 maximum CO2-inhibition x 3 EF seasonality). For each scenario the outputs of three simulations were compared to estimate the relative importance of high-CO2-inhibition: warming with CO2-inhibition versus warming without CO2-inhibition versus current climate (no warming and no CO2-inhibition). The results are summarized in Table S5 below (see also Fig. 5 in the main text). Fig. S10 (below) shows an example of the diurnal and annual emission courses resulting from a simulation (scenario: 3°C-warming x 25% maximum CO2-inhibition x EF seasonality without drought stress).



**Figure S9.** Seasonal variations of the emission factor (EF) of *Quercus ilex* leaves assumed in the simulations. Dark blue and red lines assume an EF seasonality without and with summer drought as observed in Staudt et al. (2002). The grey dotted line assumes that EF is constant throughout the year (no seasonality). The algorithm used to calculate EF seasonality is described above.

**Table S5.** Assessment of the potential effect of high-CO2-inhibition on total annual monoterpene emission from QI leaves under a future warmer climate with double [CO2] combining different warming, high-CO2-inhibition and emission seasonality scenarios (for details see above). Simulations were made using the temperature and PPFD values (30-min values) recorded at the forest station of Puechabon during the years 2019, 2020 and 2021 (annual mean temperatures: 14.7, 14.8 and 14.0 °C). Numbers in the table present the ranges of the three years. %Total-Increase is the percentage increase of the total annual emission under future climate relative to the actual climate including both temperature enhancement and high-CO2-inhibition of emissions. %CO2-Inhibition reports the percentage overestimation of emission when high-CO2-inhibition is ignored in the simulations. Colors denote simulations based on different seasonal variations of the emission factor: blue/red: seasonality without/with summer drought; grey: no seasonality at all (constant mean EF).

The short-term effects of temperature and PPFD on emissions were computed using the algorithm and coefficients described in Staudt and Bertin (1998). See Fig. S7 below for examples of diurnal and annual emission evolution, and assumed EF seasonality.

To account for the high-CO2-inhibition of emissions at double CO2, we assumed that inhibition is 0 % at ≥ 35 °C and progressively increases at lower temperatures by 2 % per 1°C decrease to reach maximum inhibitions of either 10, 15, 20, 25, 30, 40, 60 or 100%. This assumption is based on our results and a literature survey suggesting that temperature modulates the short-term, high-CO2-inhibition on isoprenoid emissions in a proxy linear way (Rasulov et al., 2010; Potosnak et al., 2014; Sharkey and Monson, 2014). The temperature enhancements (1-4 °C) encompass the range predicted to occur with doubling [CO2] by the end of the century (2.8-4.6 °C relative to the 1850-1900 period, scenario SSP3-7.0; IPCC 2021).

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Max CO2-inhibition**  **(%)** | **1°C warming** | | **2°C warming** | | **3°C warming** | | **4°C warming** | |
| **%Total Increase** | **%CO2-Inhibition** | **%Total Increase** | **%CO2-Inhibition** | **%Total Increase** | **%CO2-Inhibition** | **%Total Increase** | **%CO2-Inhibition** |
| **10** | **2.6-2.0 2.5-2.0 2.5-2.0** | **8.0-8.9 8.1-9.0 8.4-9.2** | **15.0-14.5 14.9-14.5 15.0-14.7** | **7.2-8.5 7.3-8.6 7.8-8.8** | **28.5-28.3 28.6-28.4 28.9-28.8** | **6.4-8.0 6.5-8.1 7.1-8.4** | **43.2-43.9 43.4-44.0 44.0-44.6** | **5.6-7.4 5.8-7.5 6.5-8.0** |
| **15** | **-0.1--1.9 -0.3--1.9 -0.8--2.2** | **10.4-12.4 10.6-12.4 11.3-12.9** | **12.4-10.7 12.3-10.7 11.7-10.4** | **9.3-11.5 9.5-11.6 10.4-12.3** | **26.1-24.7 26.1-24.7 25.5-24.5** | **8.2-10.6 8.4-10.7 9.6-11.5** | **41.4-40.2 41.4-40.2 41.0-40.2** | **7.2-9.6 7.4-9.7 8.7-10.7** |
| **20** | **-1.9--4.5 -2.1--4.6 -3.3--5.5** | **12.0-14.7 12.2-14.8 13.5-15.8** | **10.7-8.3 10.5-8.2 9.2-7.2** | **10.7-13.4 10.9-13.6 12.4-14.8** | **24.5-22.5 24.4-22.4 23.0-21.4** | **9.3-12.2 9.6-12.4 11.4-13.8** | **39.9-38.2 39.8-38.1 38.4-37.1** | **8.1-10.9 8.4-11.1 10.4-12.7** |
| **25** | **-3.0--6.0 -3.3--6.2 -5.2--7.7** | **13.0-16.1 13.3-16.3 15.2-17.8** | **9.7-6.9 9.4-6.7 7.3-5.0** | **11.5-14.6 11.8-14.8 13.9-16.6** | **23.6-21.3 23.4-21.0 21.1-19.1** | **10.0-13.1 10.3-13.3 12.7-15.3** | **39.0-37.1 38.9-36.9 36.6-34.9** | **8.6-11.6 9.0-11.9 11.6-14.1** |
| **30** | **-3.7--6.9 -4.0--7.1 -6.5--9.3** | **13.6-16.8 13.9-17.1 16.4-19.2** | **9.1-6.2 8.8-5.9 6.0-3.4** | **11.9-15.2 12.3-15.4 15.0-17.8** | **23.1-20.6 22.9-20.3 19.8-17.7** | **10.4-13.5 10.7-13.8 13.7-16.4** | **38.6-36.6 38.3-36.3 35.4-33.5** | **8.9-11.9 9.3-12.2 12.4-15.0** |
| **40** | **-4.1--7.5 -4.6--7.8 -8.0--11.0** | **14.0-17.4 14.4-17.7 17.7-20.8** | **8.7-5.7 8.2-5.1 4.6-1.8** | **12.3-15.6 12.8-16.0 16.2-19.1** | **22.7-20.2 22.4-19.8 18.5-16.2** | **10.6-13.8 11.0-14.2 14.6-17.4** | **38.2-36.3 37.9-35.9 34.3-32.2** | **9.1-12.2 9.5-12.5 13.2-13.8** |
| **60** | **-4.3--7.6 -4.7--8.0 -8.6--11.7** | **14.1-17.5 14.5-17.9 18.2-21.3** | **8.6-5.5 8.2-5.1 4.1-1.3** | **12.3-15.7 12.8-16.0 16.5-19.5** | **22.7-20.1 22.3-19.7 18.1-15.7** | **10.7-13.9 11.1-14.3 14.9-17.7** | **37.9-36.2 37.9-35.8 34.0-31.8** | **9.2-12.2 9.5-12.6 13.3-16.0** |
| **100** | **-4.3--7.6 -4.7--8.0 -8.6--11.7** | **14.1-17.5 14.5-17.9 18.3-21.4** | **8.6-5.5 8.2-5.1 4.1-1.3** | **12.3-15.7 12.8-16.0 16.5-19.5** | **22.7-20.1 22.3-19.7 18.1-15.7** | **10.7-13.9 11.1-14.3 14.9-17.7** | **37.9-36.2 37.9-35.8 34.0-31.8** | **9.2-12.2 9.5-12.6 13.3-16.0** |
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**Figure S10.** Example of simulations to assess the potential effects of high-CO2-inhibition on annual (a) and diel (b-g) emission courses from QI leaves under a future warmer climate with 800 ppm [CO2]. In this example we combined a temperature increase of 3°C with an EF seasonality without water stress (dark blue line in Fig. S9 above) and maximum CO2-inhibition of 25 % at temperatures ≤ 22.5 °C. The simulation uses the temperature and PPFD data recorded in a Holm oak forest (see <https://puechabon.cefe.cnrs.fr/>) for the years 2019 to 2021, Figure (a) shows the variation of the daily emissions over these years based on three simulations: current climate (light blue), 3°C warmer climate without CO2-inhibition of emissions (green), and 3 °C warmer climate with CO2-inhibition of emissions (purple). Figures (e)-(g) show examples of diel emission variations during different seasons of the year 2019 (note the different y-scales) and (b)-(d) the corresponding current climate PPFD and temperature values used for the simulation. The color numbers inserted inside the graphs report the total annual ((a)) and total daily ((e)-(g)) emissions, respectively. The results of other simulations are summarized in Table S5 above and Fig. 6 in the main text.