

Description of an alternative method to compute SEFs

The second method is based on Guenther et al. (1995) and Guenther (1997) as described by Gonzaga Gomez et al. (2019). For fluxes depending on light and temperature, such as isoprene, the SEF for each compound i ($\mu\text{g m}^{-2} \text{h}^{-1}$) is defined by:

$$SEF_i = \frac{E_i}{C_L C_T} \quad (7)$$

Where E_i is the measured BVOC flux per leaf surface ($\mu\text{g m}^{-2} \text{h}^{-1}$), and C_L and C_T are the temperature and light response function of the BVOC emissions, defined as:

$$C_T = (1 - \text{LDF}) * \exp(\beta(T - T_S)) + \text{LDF} * \frac{\exp\left[\frac{C_{T1}(T-T_S)}{R T_S T}\right]}{1 + \exp\left[\frac{C_{T2}(T-T_M)}{R T_S T}\right]} \quad \text{and} \quad C_L = (1 - \text{LDF}) + \text{LDF} * \frac{\alpha C_{L1} L}{\sqrt{1 + \alpha^2 L^2}} \quad (8)$$

Where $C_{T1} = 95000 \text{ J mol}^{-1}$, $C_{T2} = 230000 \text{ J mol}^{-1}$, $T_M = 314 \text{ K}$, $\alpha = 0.0027$, $\beta = 0.09 \text{ K}^{-1}$, $C_{L1} = 1.066$ are empirically derived constants, T is the leaf experimental temperature (K), T_S is the leaf temperature at standard condition (297 K), R the gas law constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), and L is the photosynthetically active radiation (PAR) flux ($\mu\text{mol photon m}^{-2} \text{s}^{-1}$).

The comparison of the SEF values obtained by both methods (the one based on Guenther et al. (2012) and the one described here above) is displayed in Table 1, along with the fitted parameters for both methods (LDF and C_{CE}). It shows that the SEF calculated by both methods are pretty close to each other.

Table 1 – Comparison of SEF values obtained by the approaches based on the equations provided by Gunether et al. (2012) (Megan2.1) and by Guenther et al. (1995) (G95). Fitted parameters for both approaches (LDF, C_{CE}) are also displayed.

	Tentative VOC identification		G95		Megan 2.1		G95		Megan 2.1						
m/z	Ion formulas	VOC names	SEF ± se [μg m ⁻² (leaf) h ⁻¹]				RMSE [μg m ⁻² (leaf) h ⁻¹]				LDF	CCE Megan		CCE G95	
<i>Oxygenated and terpenes VOC</i>			P1	P2	P1	P2	P1	P2	P1	P2		P1	P2	P1	P2
33.033	(CH4O)H+	methanol	130 ± 8	199 ± 13	123 ± 7	175 ± 11	104	305	103	304	0.8	0.42	0.34	0.21	0.18
59.049	(C3H6O)H+	acetone	3.6 ± 0.1	12 ± 1	5.1 ± 0.2	17 ± 1	1.5	17.2	1.4	16.6	0.2	0.22	0.19	0.2	0.18
69.07	(C5H8)H+	isoprene	3.4 ± 0.1	3.2 ± 0.2	2.5 ± 0.1	1.9 ± 0.1	1.7	3.5	1.9	3.8	1	0.64	0.51	0.21	0.18
87.078	(C5H10O)H+	MBO	0.5 ± 0.02	0.1 ± 0.01	0.4 ± 0.01	0.1 ± 0.004	0.2	0.1	0.3	0.1	1	0.64	0.51	0.21	0.18
137.129	(C10H16)H+	monoterpenes	10.2 ± 0.3	7.1 ± 0.2	13 ± 0.3	8 ± 0.3	4	5	3	4	0.5	0.27	0.23	0.21	0.18
205.186	(C15H24)H+	sesquiterpenes	0.86 ± 0.05	0.12 ± 0.01	0.7 ± 0.05	0.06 ± 0.01	3.2	0.2	0.7	0.2	0.5	0.39	0.32	0.21	0.18
<i>Bi-directional VOC</i>			na	45 ± 3	na	38 ± 2	6	53	6	48	0.8	0.42	0.34	0.21	0.18
31.018	(CH2O)H+	formaldehyde													
45.033	(C2H4O)H+	acetaldehyde													
<i>Stress VOC</i>			0.23 ± 0.01	0.029 ± 0.002	0.22 ± 0.01	0.02 ± 0.002	0.14	0.05	0.14	0.05	0.8	0.42	0.34	0.21	0.18
118.078	(C8H7N)H+	indole													
<i>Other VOC leaf surface compounds</i>			0.68 ± 0.03	1.2 ± 0.1	1 ± 0.04	1.5 ± 0.1	0.4	2.2	0.4	2.2	0.2	0.22	0.19	0.2	0.18
49.014	(CH4S)H+	methanethiol													
101.059	(C5H8O2)H+	4-oxopentanal (4-OPA)	0.65 ± 0.02	0.5 ± 0.02	0.9 ± 0.03	0.6 ± 0.02	0.3	0.4	0.3	0.4	0.2	0.22	0.19	0.2	0.18