Supplementary material (SM)

**SM\_A. Solving equation (5)**

Considering , , et ; the eigenvalues (λ) of matrix M (Eqn. 5) are obtained by solving ∆ = 0  as follows :

|  |  |
| --- | --- |
|  | (A.1) |

If Δ < 0, the equation does not admit a solution in R

If Δ = 0, the equation admits a double solution ()

If Δ > 0, the equation admits two distinct solutions λ1 and λ2 such that:

and

The last suggestion being the case of this study. Let P1 be the eigenvector associated with λ1. the matrix can be written as Eq. (A.2). It is the same for P2 (the eigenvector associated with λ2).

|  |  |
| --- | --- |
|  | (A.2) |

Eq. (A.4) becomes :

|  |  |
| --- | --- |
| Where  and | (A.3) |

Solving Eq. (A.3) is like solving the following form:

|  |  |
| --- | --- |
|  | (A.4) |

Thus, the raw expressions of the two compartment (L and R) fugacity are:

|  |  |
| --- | --- |
|  | (A.5) |
| Where *C1* and *C2* are constants | (A.6) |

At a giving time and considering *C1* and *C2* as function of time, Eq. (A.4) becomes:

|  |  |
| --- | --- |
|  | (A.7) |
|  | (A.8) |

Rearranging Eq. (5) gives :

|  |  |
| --- | --- |
|  | (A.9) |
|  | (A.10) |

Including values of *P1* and *P2* to Eq. (A.8) and rearranging Eq. (A.10) gives

|  |  |
| --- | --- |
|  | (A.11) |

Rearranging Eq. (A.11) gives

|  |  |
| --- | --- |
|  | (A.12) |

By simplifying the repetitive similar terms, Eq. (A.12) gives:

|  |  |
| --- | --- |
| With and | (A.13) |

Multiplying the second equation by , Eq. (A.13) becomes:

|  |  |
| --- | --- |
|  | (A.14) |

Thus, Eq. (A.14) can be written as :

|  |  |
| --- | --- |
|  | (A.15) |

The integration of Eq. (A.15) gives:

|  |  |
| --- | --- |
|  | (A.16) |

Multiplying the second equation by, Eq. (A.13) becomes:

|  |  |
| --- | --- |
|  | (A.17) |

By analogy with Eqns. (A.14) and (A.15), Eq. (A.17) can be written as follows

|  |  |
| --- | --- |
|  | (A.18) |

At the initial time (*t* = 0), fugacity is zero in all the plant compartments (*fL* = *fR* = 0); and from Eqns. (A.5) and (A.6), *fL* = 0 and *fR* = 0 means *C1 + C2* = 0 and respectively. So, Eq. (A.19) can be written as:

|  |  |
| --- | --- |
|  | (A.19) |

Rearranging the first equation in Eq. (A.19) using expressions of *C1* and *C2* gives:

|  |  |
| --- | --- |
|  | (A.20) |

Rearranging the second equation in Eq. (A.19) using expressions of *C1* and *C2* gives:

|  |  |
| --- | --- |
|  | (A.21) |

Eq. (A.20) times (-λ1) gives:

|  |  |
| --- | --- |
|  | (A.22) |

Eq. (A.21) + Eq. (A.22) gives:

|  |  |
| --- | --- |
|  | (A.23) |

Eq. (A.20) x (-λ2) + Eq. (A.21) gives:

|  |  |
| --- | --- |
|  | (A.24) |

**SM\_B. Flowrates and retention times**

Let’s consider E = leaves compartment and T = stems compartment. The air-leaves exchange can be expressed as “*GAE* = *kEA* x *a*”. Where *kEA* is the mass transfer coefficient [*kEA=* (*τEA* x *a*)*/*(*ln(2)* x *VA*)] and “*a*”isthe leaves exchange area; with *GAE* = *GEA*. All flowrates between E and T compartments are equal to *GP* or *GX* according to the flow direction. Thus, *GTE = GX* and *GET = GP*.

The xylem flow (*GX*) of each species has been calculated according to their evapotranspiration data (ETP= 1.9108E-4 mm.h-1) from the experimental study site, using the weather data [9]. Including the pot area (3.14E-2 m2), the transpiration rate of each pot is 6E-6 m3/h/pot. As this evapotranspiration is for turf plant, and therefore *Cynodon dactylon*, it has also been used as the xylem flow for *Eleusine indica* due to the fact that these two species belong to the grass family. *Cynodon dactylon* transpiration rate is then considered as potential evapotranspiration (*ETPo*). Thus, it was used to calculate the transpiration rate of *Alternanthera sessilis* (*As*) in combination with its cultural coefficient (*Kc*) as follows: *ETPAs = Kc* x *ETPo*. With *ETPo* = *GXCd* and *ETPAs* = *GXAs*. The *Kc* (0.8) of *A. sessilis* was found in the literature.

**Table S1.** Flowrates of PAHs from one compartment to another.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Air | Stem\_leaves | Root | Soil |
| Air |  | *GAL* = *GAE* + *GP* |  |  |
| Stem\_leaves | *GLA* = *GEA* + *GX* |  |  |  |
| Root |  | *GRL* = *GX* |  | *GRS* ≈ 0.05 *GX* |
| Soil |  |  | *GSR* = 1.05 *GX* |  |

**Table S2.** PAHs retention times in plant compartments.

|  |  |
| --- | --- |
| Xylem flow | Phloem flow |
| *𝜹L,X* = *VL/GLA* | *𝜹L,P* = *VL/GAL* |
| *𝜹R,X* = *VR/GSR* | *𝜹R,P* = *VR/GRS* |
| *𝜹E,X* = *VE/GEA* | *𝜹E,P* = *VE/GAE* |
| *𝜹T,X* = *VT/GX* | *𝜹T,P* = *VT/GX* |

**SM\_C. Air and leaves exchanges half-lives**

For air and leaves exchanges, the air-leaves transfer half-life (*τAE*) and the leaves-air transfer half-life (*τEA*) are the same:

|  |  |
| --- | --- |
|  | (C.1) |

Where :

* *τc,O* is the characteristic time of PAH through cuticle;
* *τc,A* is the characteristic time of PAH through air compartment;
* *KOA* is the partition coefficient of PAH between cuticle and air.

Thus, to calculate the air to stem\_leaves transfer half-life (*τAL*) and the stem\_leaves to air half-life (*τLA*), a mean half-life of the stems and leaves compartments taken separately has been expressed as shown on Eqs. (C.2) and (C.3). According to [2], *τET,T=* ln(2)*KTW𝜹T,P* ; *τET,E=* ln(2)*KEW𝜹E,P* ; *τTE,T=* ln(2)*KTW 𝜹T,X* and *τTE,E=* ln(2)*KEW 𝜹E,X*. Thus, *τAL* and *τLA* are expressed as:

|  |  |
| --- | --- |
|  | (C.2) |
|  | (C.3) |

**Table S3.** PAHs half-lives of model compartments.

|  |  |
| --- | --- |
| Downwards | Upwards |
|  |  |
|  |  |
|  |  |
|  |  |

Where *Ø* is the diffusion fraction of xylem flow.

**SM\_D. PAHs content in the air compartment**

The PAH content in the air compartment is calculated according to the Henry law constant (H) of each PAH as follows

|  |  |
| --- | --- |
|  | (D.1) |

* *CA* is the concentration of PAHs in the air compartment (kg.m-3);
* *CW*, their concentrations in water (kg.m-3)
* *KAW* is a dimensionless value of the air-water partition coefficient, expressed as *KAW* = *H* x 8.32 x 298 (with 8.32 the universal constant of perfect gases and 298 the temperature in kelvin).

Dimensionless expression of *CA* is giving according to the density of air (1.225 kg.m-3) as follows:

|  |  |
| --- | --- |
|  | (D.2) |

Expression of *CA* in mg.kg-1 gives:

|  |  |
| --- | --- |
|  | (D.3) |

**SM\_E.**

**Table S4.** example of sensitivity analysis for *E. indica.*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model parameters | Plant compartments | Variation of input parameters | PAHs | | |
| Flu | Chy | DahA |
| Phloem flow multiplying factor (α) | Stem\_leaves | 5 × 10−2 | 4.26 × 10−2 | 4.44 × 10−1 | 4.68 × 10−2 |
| 5 × 10−3 | 4.43 × 10−1 | 4.59 × 10−2 | 4.85 × 10−3 |
| 5 × 10−4 | 4.59 × 10−2 | 4.63 × 10−3 | 4.87 × 10−4 |
| 5 × 10−1 | 3.14 × 10−1 | 3.31 | 3.50 × 10−1 |
| Roots | 5 × 10−2 | 8.61 × 10−2 | 7.06 × 10−3 | 7.14 × 10−4 | |
| 5 × 10−3 | 6.69 × 10−2 | 6.74E-03 | 7.08 × 10−4 | |
| 5 × 10−4 | 6.67 × 10−2 | 6.74 × 10−3 | 7.08 × 10−4 | |
| 5 × 10−1 | 1.50 | 3.07 × 10−2 | 1.16 × 10−3 | |
| Diffusion fraction of xylem flow  (Ø) | Stem\_leaves | 5 × 10−2 | 4.26 | 4.44 × 10−1 | 4.68 × 10−2 | |
| 5 × 10−3 | 4.26 | 4.44 × 10−1 | 4.68 × 10−2 | |
| 5 × 10−4 | 4.26 | 4.44 × 10−1 | 4.68 × 10−2 | |
| 5 × 10−1 | 4.26 | 4.44 × 10−1 | 4.68 × 10−2 | |
| Roots | 5 × 10−2 | 8.61 × 10−2 | 7.06 × 10−3 | 7.14 × 10−4 | |
| 5 × 10−3 | 8.36 × 10−2 | 6.78 × 10−3 | 6.84 × 10−4 | |
| 5 × 10−4 | 8.33 × 10−2 | 6.75 × 10−3 | 6.81 × 10−4 | |
| 5 × 10−1 | 1.11 × 10−1 | 9.89 × 10−3 | 1.02 × 10−3 | |
| Characteristic time of PAH through cuticle  (τ*O*) | Stem\_leaves | 126h | 4.26 | 4.44 × 10−1 | 4.68 × 10−2 | |
| 12.6h | 3.77 | 4.47 × 10−1 | 4.82 × 10−2 | |
| 1.26h | 1.73 | 3.67 × 10−1 | 4.65 × 10−2 | |
| 1260h | 3.34 | 3.67 × 10−1 | 3.50 × 10−2 | |
| Roots | 126h | 8.61 × 10−2 | 7.06 × 10−3 | 7.14 × 10−4 | |
| 12.6h | 7.33 × 10−2 | 6.90 × 10−3 | 7.11 × 10−4 | |
| 1.26h | 2.88 × 10−2 | 5.59 × 10−3 | 6.83 × 10−4 | |
| 1260h | 8.31 × 10−2 | 7 × 10−3 | 7.13 × 10−4 | |

**SM\_F.**

**Table S5.** Sum of the square deviations (SSD) calculated between the simulated and the measured values for the 13 PAHs.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | SSD\_L | | | SSD\_R | | | |
|  | *E. indica* | *A. sessilis* | *C. dactylon* | *E. indica* | | *A. sessilis* | *C. dactylon* |
| F | 3.04 × 10−1 | 2.43 × 10−1 | 6.47 × 10−1 | 9.96 | | 22.4 | 3.82 |
| Ant | 4.69 × 10−2 | 3.85 × 10−2 | 1.22 × 10−1 | 2.40 | | 6.75 | 1.29 |
| Phe | 2.23 × 10−1 | 1.92 × 10−1 | 6.14 × 10−1 | 12.2 | | 34.6 | 6.64 |
| Flu | 1.32 × 10−5 | 3.03 × 10−7 | 5.74 × 10−5 | 1.89 × 10−3 | | 1.33 × 10−2 | 9.92 × 10−4 |
| Pyr | 5.28 × 10−6 | 3.63 × 10−6 | 1.13 × 10−5 | 1.08 × 10−3 | | 5.43 × 10−2 | 1.69 × 10−2 |
| BaA | 1.07 × 10−5 | 2.91 × 10−7 | 1.51 × 10−8 | 9.04 × 10−6 | | 8.80 × 10−5 | 2.43 × 10−6 |
| Chy | 2.36 × 10−5 | 3.22 × 10−6 | 4.13 × 10−7 | 6.02 × 10−5 | | 5.88 × 10−5 | 2.15× 10−4 |
| BbF | 1.50 × 10−5 | 2.56 × 10−6 | 2.14 × 10−7 | 9.46 × 10−6 | | 1.25 × 10−6 | 4.42 × 10−5 |
| BaP | 1.13 × 10−6 | 1.31 × 10−6 | 1.23 × 10−7 | 1.62 × 10−5 | | 4.89 × 10−6 | 4.33 × 10−5 |
| BkF | 8.01 × 10−7 | 3.72 × 10−7 | 1.24 × 10−7 | 7.81 × 10−7 | | 1.64 × 10−6 | 2.78 × 10−6 |
| DahA | 1.89 × 10−7 | 2.18 × 10−7 | 1.99 × 10−7 | 4.33 × 10−8 | | 8.34 × 10−7 | 2.09E-08 |
| BP | 3.25 × 10−7 | 1.48 × 10−6 | 2.48 × 10−7 | 9.30 × 10−5 | | 1.70 × 10−5 | 5.74 × 10−4 |
| IP | 3.45 × 10−7 | 2.44 × 10−7 | 2.40 × 10−7 | 1.04 × 10−5 | 9.64 × 10−7 | 3.16 × 10−4 |