

## Summary of the NORDESTE Caatinga ecosystem Soil Vegetation Atmosphere Transfer model: SEcA

### 1. Background

This document explains the structure of the output data generated by a preliminary version of the SEcA model (written in Fortran). The Shrubland Ecosystem Assessment (SEcA) model calculates the ecosystem processes for a semi-arid shrubland system, with an initial focus on the Caatinga ecosystem. The main program (in Fortran) reads in the required input data and calls the key subroutines that executes the calculation of the resistance network, fluxes (energy, water and carbon) and above-ground state variables. Currently, the model does not have a soil water balance nor a soil heat transfer model.

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Please contact Prof Anne Verhoef (The University of Reading, UK) for further information ([a.verhoef@reading.ac.uk](mailto:a.verhoef@reading.ac.uk))

### 2. THEORY

#### 2.1. SECA model description

This ecosystem model describes the component and total energy- and carbon balance fluxes of a shrubland or multi-tree ecosystem. It employs a mechanistic  $A_n-g_s$  model, and a range of plant water stress functions. The resistance network and flux partitioning approach are based on Verhoef and Allen (2000); VA2000.

Total latent heat flux,  $\lambda E$  ( $\text{W m}^{-2}$ ), from a surface consisting of  $ns+1$  components (with  $ns$  the number of vegetation components, and the final component the bare soil), each with fractional coverage  $c_i$  and  $\sum_i^{ns+1} c_i = 1$ , can be written as:

$$\lambda E = \sum_i^{ns+1} c_i PM_i Y_i \quad (1)$$

with  $\lambda$  the latent heat of vaporisation ( $\text{J kg}^{-1}$ ) and  $PM_i$  and  $Y_i$  the Penman-Monteith and resistance combination terms for surface component  $i$ , respectively.

The  $PM_i$  terms are given by

$$PM_i = \Delta A + \frac{\rho C_p D_r - \Delta r_{c,i} (A - A_i)}{r_{a,a} + r_{c,i}} / \left[ \Delta + \gamma \left( \frac{r_{a,a} + r_{a,i} + \mu r_{b,i}}{r_{a,a} + r_{c,i}} + \frac{r_{s,i}}{r_{a,a} + r_{c,i}} \right) \right] \quad (2)$$

with  $r_{a,a}$  ( $\text{s m}^{-1}$ ) the atmospheric aerodynamic resistance between the canopy source height (level of mean canopy flow) and atmospheric reference level  $z_r$  (m),  $r_{c,i}$  ( $\text{s m}^{-1}$ ) the total aerodynamic resistance between surface component  $i$  and the canopy source height,  $r_{a,i}$  the within-canopy aerodynamic resistance ( $\text{s m}^{-1}$ ),  $r_{b,i}$  the bulk boundary layer resistance ( $\text{s m}^{-1}$ ) and  $r_{s,i}$  ( $\text{s m}^{-1}$ ) the surface resistance for each component  $i$ .  $A$  ( $\text{W m}^{-2}$ ) is the available energy for the whole ecosystem, whereas  $A_i$  ( $\text{W m}^{-2}$ ) denotes the available energy for the  $i^{\text{th}}$  component, which is the difference between net radiation,  $R_{n,i}$  ( $\text{W m}^{-2}$ ) and soil heat flux  $G_i$  ( $\text{W m}^{-2}$ ).  $D_r$  (mbar) is the vapour pressure deficit at reference level.  $\Delta$  (mbar  $\text{K}^{-1}$ ) is the slope of the vapour pressure temperature curve,  $\gamma$  is the psychrometric constant (mbar  $\text{K}^{-1}$ ),  $\rho$  ( $\text{kg m}^{-3}$ ) is the density of air and  $C_p$  ( $\text{J kg}^{-1} \text{K}^{-1}$ ) is the specific heat of air at constant pressure. The constant  $\mu$  can vary between 1 (amphistomatous leaves or soil) and 2 (hypostomatous leaves).

For the Caatinga dry forest, currently nine surface components are distinguished: Eight tree/shrub species (second subscript numbered from 1-9, see Table 1) that together make up  $> 90\%$  of the vegetated surface cover, and bare soil (second subscript s, for soil). A schematic diagram of the resistance network for the model and its major variables is given in Fig. 1. Atmospheric variables at the canopy source height are denoted by subscript 0, whereas at the reference and surface level subscripts  $r$  and  $s$  have been used, respectively. The coverage areas of the nine components are not allowed to overlap. Furthermore, bare soil applies to extensive patches not overshadowed by any plants.

## Bespoke Caatinga model

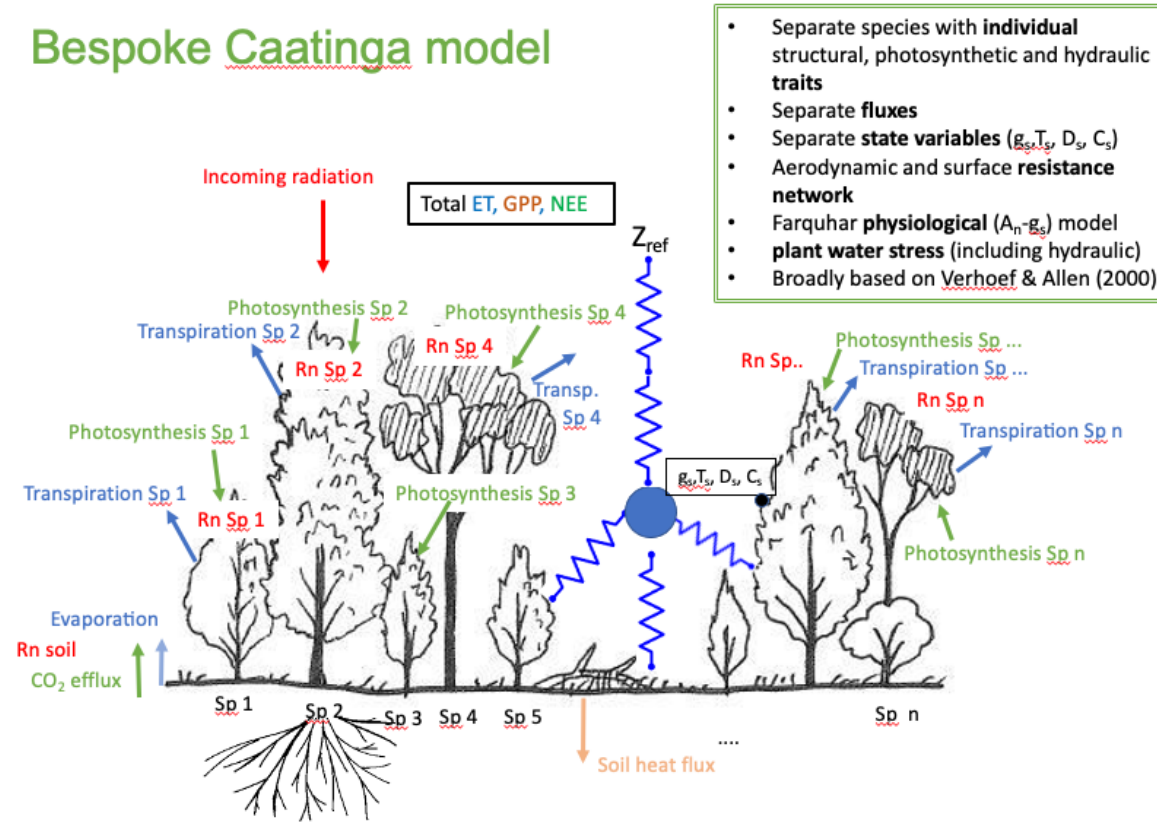


Figure 1. Schematic of the SEcA model. Sp stands for species, Rn for net radiation,  $g_s$  for stomatal conductance,  $T_s$  for surface temperature,  $D_s$  for vapour pressure deficit and  $C_s$  concentration at the leaf level. ET, GPP and NEE are evapotranspiration, gross primary productivity, and net ecosystem exchange, respectively.  $Z_{ref}$  is the reference height. For detail on the resistances, the reader is referred to Verhoef and Allen (2000).

The total aerodynamic resistances between the component surfaces and the canopy source height,  $r_{c,i}$ , are given by  $r_{a,i} + \mu r_{b,i}$ . Following Verhoef and Allen (2000),  $r_{a,i}$  for the highest species ( $r_{a,1}$ ) is set to zero. Furthermore,  $\mu r_{b,s} = 0$ , while  $r_{a,s}$  is set to a constant value of  $100 \text{ s m}^{-1}$ , following preliminary tests with the model.

These resistances, together with the atmospheric aerodynamic resistance  $r_{a,a}$ , are calculated using the parameterisations given in Huntingford *et al.* (1995), see also VA2000.

The in-canopy aerodynamic resistance is given by

$$r_{a,i} = \frac{e^n h_1}{nK(h_1)} [e^{-nz_i/h_1} - e^{-nz_1/h_1}] \quad (3)$$

with  $n$  the decay coefficient (-),  $h_1$  the canopy height of the tallest species (m), and  $K(h_1)$  the eddy diffusivity at the top of the bushes ( $\text{m}^2 \text{s}^{-1}$ ). Parameters  $z_1 (= z_{0m,1} + d_1)$  and  $z_i (= z_{0m,i} + d_i)$  are the momentum sink height (m) for the species 1 and the other species, respectively. Here,  $z_{0m,i}$  and  $d_i$  (with  $i=1, 8$ ) are the roughness lengths and displacement heights for the species (m).

The bulk boundary layer resistances are found from

$$r_{b,i} = \frac{70}{L_i^*} \left( \frac{l_i}{u_i} \right)^{0.5} \quad (4)$$

with  $L_i^*$  ( $\text{m}^2 \text{leaf m}^{-2}$  ground area) the local leaf area for component  $i$ , i.e. the leaf area index a vegetation component would have if it wholly covered the surface,  $l_i$  (m) the leaf width of species  $i$  and  $u_i$  ( $\text{m s}^{-1}$ ) is given by  $u_i = u_1 e^{n(\frac{z_i}{h_1} - 1)}$ , with  $u_1$  ( $\text{m s}^{-1}$ ) the wind speed at the canopy height of species 1. The units of the constant 70 in Eqn 4 are  $\text{s}^{1/2} \text{m}^{-1}$ .

The aerodynamic resistance between the canopy source level and the atmospheric reference level is obtained from

$$r_{a,a} = \frac{1}{\kappa u_*} \left[ \ln \frac{z_r - d}{h_1 - d} - \Psi_h(z_r) + \Psi_h(h_1) \right] + \frac{h_1}{nK(h_1)} [e^{n(1 - z_1/h_1)} - 1] \quad (5)$$

with  $u_*$  the friction velocity ( $\text{m s}^{-1}$ ),  $\kappa$  the Von Kàrmàn constant,  $d$  the zero plane displacement for the total surface (m) and  $\Psi_h(z)$  the integrated stability correction to eddy diffusivity for heat and water vapour at height  $z$ . The friction velocity is found from

$$u_* = \frac{\kappa u_r}{\ln((z_r - d)/z_{0m}) - \Psi_m(z_r - d)} \quad (6)$$

with  $\Psi_m(z_r - d)$  the integrated stability correction to eddy diffusivity for momentum at height  $(z_r - d)$ ,  $u_r$  the windspeed at reference height ( $\text{m s}^{-1}$ ) and  $z_{0m}$  (m) the roughness length for momentum for the total surface.

The canopy *surface* resistances for water vapour are calculated from  $r_{s,i} = r_{l,i}/L_i^*$ , where the calculation of the leaf stomatal resistance,  $r_{l,i}$  ( $\text{s m}^{-1}$ ), is based on a mechanistic model (Jacobs *et al.* 1996) which uses the relationship between the net photosynthetic rate of plants,  $P_{n,i}$  ( $\text{mg m}^{-2} \text{ leaf s}^{-1}$ ) and leaf stomatal resistance:

$$r_{l,i} = (C_{s,i} - C_{i,i})/1.6f_{\theta}P_{n,i} \quad (7)$$

Here,  $C_{s,i}$  and  $C_{i,i}$  ( $\text{mg m}^{-3}$ ) are the leaf surface and internal  $\text{CO}_2$  concentration for vegetation component  $i$ , respectively, and  $f_{\theta}$  is a linear multiplication factor, which is dependent on soil moisture status (see Eqn A10).  $r_{l,i}$  (and  $P_{n,i}$ ) is also dependent on absorbed PAR radiation,  $I_{a,i}$  ( $\text{W m}^{-2}$ ), surface temperature  $T_{s,i}$  ( $^{\circ} \text{C}$ ) and surface vapour pressure deficit  $D_{s,i}$  (mbar) as described in Appendix 1 of VA2000.

The soil surface resistance,  $r_{s,s}$ , is dependent on soil moisture content.

The  $Y_i$  terms in Eqn 1 are found from equations analogous to those given in VA2000:

$$Y_i = \prod W_{j \neq i} (W_i + W_a)/X \quad (8)$$

$$\text{with } W_a = (\Delta + \gamma)r_{a,a} \text{ and } W_i = (\Delta + \mu\gamma)r_{c,i} + \gamma r_{s,i}.$$

$X$  is given by:

$$X = \prod_{i=1}^{ns+1} W_i + \sum_{i=1}^{ns+1} c_i W_a \prod_{j \neq i}^{ns+1} W_j \quad (9)$$

The available energy for each component ( $A_{n,i} = R_{n,i} - G_i$ ) is found by calculating net radiation for each component  $i$  from

$$R_{n,i} = (1 - a_i)R_{s,\downarrow} + R_{l,\downarrow} - \varepsilon_i \sigma T_{s,i}^4 - (1 - \varepsilon_i)R_{l,\downarrow} \quad (10)$$

while soil heat fluxes are assumed to be zero for each vegetated component and 30% of  $R_n$  for the bare soil component. In Eqn 10,  $a_i$  and  $\varepsilon_i$  are the albedo and emissivity for component  $i$ ,  $R_{s,\downarrow}$  is the incoming solar radiation ( $\text{W m}^{-2}$ ),  $R_{l,\downarrow}$  is the incoming longwave radiation ( $\text{W m}^{-2}$ ), and  $T_{s,i}$  ( $^{\circ} \text{C}$ ) is the surface temperature for component  $i$  (for its calculation see Eqn 14a). Total net radiation and total available energy are found from

$$R_n = \sum_i^{ns+1} c_i R_{n,i} \text{ and } A = \sum_i^{ns+1} c_i A_i, \text{ respectively.}$$

With  $\lambda E$  found from Eqn 1, the vapour pressure deficit at the canopy source level (in mbar) is calculated with

$$D_0 = D_r + \{\Delta A - (\Delta + \gamma)\lambda E\}r_{a,a}/\rho C_p \quad (11)$$

with the symbols as described above. At this same level, the within-canopy source point temperature  $T_0$ (° C), and vapour pressure at that level,  $e_0$  (mbar) can be obtained from

$$T_0 = \{(A - \lambda E)r_{a,a}/\rho C_p\} + T_r \quad (12a)$$

$$e_0 = e_{sat}(T_0) - D_0 \quad (12b)$$

in which  $e_{sat}(T_0)$  is the saturated vapour pressure at canopy source level temperature (mbar) and  $T_r$  is the reference level air temperature (° C).

With knowledge of  $D_0$ , evapotranspiration from the component surfaces can be calculated from

$$\lambda E_i = \left[ \Delta A_i + \frac{\rho C_p D_0}{r_{c,i}} \right] / \left[ \Delta + \gamma \left( \left( \frac{r_{a,i} + \mu r_{b,i}}{r_{c,i}} \right) + \frac{r_{s,i}}{r_{c,i}} \right) \right] \quad (13)$$

Surface temperatures for the individual surface components are then found from

$$T_{s,i} = T_0 + \{(A_i - \lambda E_i)r_{c,i}\}/\rho C_p \quad (14a)$$

and surface values of  $D$  using

$$D_{s,i} = (e_{sat}(T_{s,i}) - e_0) / \left( 1 + \mu \frac{r_{c,i}}{r_{s,i}} \right) \quad (14b)$$

with  $e_{sat}(T_{s,i})$  the saturated vapour pressure at surface temperature (mbar).

The total net CO<sub>2</sub> flux (positive downwards) is calculated using:

$$F_c = \sum_i^{ns} c_i L_i^* P_{n,i} - R_{ns+1} \quad (15)$$

In Eqn 15,  $R_{ns+1}$  is the total respiration of soil and roots ( $\text{mg m}^{-2} \text{s}^{-1}$ ) which was kept constant at  $-0.05 \text{ mg m}^{-2} \text{s}^{-1}$  in first instance.

With  $F_c$  obtained from Eqn 15, the CO<sub>2</sub> concentration at canopy source height,  $C_0$  ( $\text{mg m}^{-3}$ ) can be calculated using

$$C_0 = C_r - 1.4r_{a,a}F_c \quad (16)$$

where the factor 1.4 accounts for the difference between boundary layer resistances for CO<sub>2</sub> and H<sub>2</sub>O. Here,  $C_r$  is the atmospheric CO<sub>2</sub> concentration ( $\text{mg m}^{-3}$ ).

Finally, the surface level values of  $C$  are given by

$$C_{s,i} = C_0 - 1.4\mu r_{c,i}c_iL_i^*P_{n,i} \quad (17)$$

These values, and values of  $T_{s,i}$  and  $D_{s,i}$ , are required in the stomatal conductance-photosynthesis parameterisation described in Appendix 1 of VA2000. We also implanted the Farquhar model in the SEcA model (as per the JULES model; Clark et al., 2011), which was invoked in the runs for which the results are presented.

The set of Eqns 1-17 and the photosynthesis model selected are solved for  $r_l$  by iteration.

### 3. Materials and methods

#### 3.1. Micrometeorological data

The data used to drive and verify the model were obtained at the Embrapa Tropical Semiarid Research Station in the state of Pernambuco, Brazil ( $9^\circ 2' 33''\text{S}$ ,  $40^\circ 19' 16''\text{W}$ ; at 350 m a.s.l.). The Caatinga vegetation in this area has an average height of 4.5 m and consists of shrubs, trees, herbaceous

plants, and Cactaceae. In this site, sensors were installed on a 16-metre meteorological tower or in its vicinity and since 2011 they record atmospheric pressure (mbar), precipitation (mm), soil water content ( $\text{m}^3/\text{m}^3$ ), incoming long- and short-wave radiation ( $\text{W m}^{-2}$ ), air temperature ( $^{\circ}\text{C}$ ) and humidity (%), and wind speed (m/s) and wind direction (degree). Only model data generated with the inputs for 2011 are provided in the output files.

### 3.2 Plant physiological data

Plant physiological parameters maximum rate of Rubisco carboxylase activity ( $V_{\text{cMAX}}$ ,  $\mu\text{mol m}^{-2} \text{s}^{-1}$ ) and maximum rate of photosynthetic electron transport ( $J_{\text{MAX}}$ ,  $\mu\text{mol m}^{-2} \text{s}^{-1}$ ) were obtained. In order to determine these parameters, one A-Ci curve and one temperature response curve were obtained for each selected plant (2 or 3 for each dominant plant species). A four-single point measurement of assimilation rates at saturating light (Photosynthetic Photon Flux Density – PPFD - equal to 2,000 ( $\mu\text{mol photons m}^{-2} \text{s}^{-1}$ ) and ambient  $\text{CO}_2$  (400 ppm) for three leaves and four-point measurements of dark respiration for three leaves, which were wrapped in aluminium foil for 30 minutes before respiration determinations. All of these measurements were taken in the study area, for most of the eight different species used in the model, with two different portable photosynthesis systems (LI-COR® 6400 and 6800).

### 3.3 Plant structural data

The plant structural data for SeCA are denoted by the Plant Area Index (PAI,  $\text{m}^2/\text{m}^2$ ) and Leaf Area Index (LAI,  $\text{m}^2/\text{m}^2$ ), and these have been estimated on a daily temporal basis. To obtain these indexes, we applied a piecewise-linear dependence of greenness (i.e. NDVI) on the soil moisture with highest values under well-watered conditions following the approach verified in the Caatinga by Souza et al. (2016). The parameters to estimate NDVI were calibrated by using Landsat-derived NDVI (Landsat 5 TM, Landsat 7 ETM+, and Landsat 8 OLI) for verification. The daily NDVI time series were then used to estimate the PAI and LAI following the equations developed by Miranda et al. (2020) for the same area of study.

The partitioning of the PAI and LAI values per plant species, as used in the SeCA model, was calculated by using plant structural information surveyed in a monitoring plot of dimensions (50 x 100 m) that is part of the Nordeste project permanent plot network described in Moonlight et al. (2020). The dominance and crown area of the dominant plant species were within the plot were used to divide the total ecosystem PAI and LAI into individual plant species, which were used as input in the SeCA model.

### 3.4 Model input parameters



The model input parameter file provides information on a range of species specific and general input parameters; a summary is given in Table 1.

Table 1 Caatinga vegetation parameters. Note that these species and their cover fraction were valid as per June 2019, but that recently (October 2020) some species have been renamed, and hence the cover fractions, etc. will have changed. Also, improved estimates of photosynthetic parameters ( $V_{c,max}$  and  $J_{max}$ ) have been provided.

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The input file also provides information on soil water retention parameters:  $\theta_r = 0.023 \text{ m}^3 \text{ m}^{-3}$ ,  $\theta_s = 0.31 \text{ m}^3 \text{ m}^{-3}$ ,  $\alpha = 0.269 \text{ cm}^{-1}$ ,  $n = 1.2662$ , which stand for residual soil moisture content, saturated soil moisture content, and Van Genuchten (VG) fitting parameters. These parameters were obtained by fitting the VG equation to measured water retention curves for the Petrolina site (personal communication, Magna Moura).

Final rows of the input file concern model choice parameters (see Egea et al. (2011) and Verhoef and Egea, 2014) for an explanation of the plant water stress models and their parameters:

- Soil water stress model, betatype (1): JULES (curvi) linear; 2 (Sinclair); 3 (Dewar) selected option
- Where is stress applied? locstress = 1 is stomatal, locstress = 2 is physiological, loc stress = 3 is mesophyl, stress = 4, is all.
- Finally we have the qs, qb and qm values in the Egea et al. (2011) approach: if these are 1.0 then the curve is linear as in JULES. These values need to be 1.0 for Sinclair and Dewar models.
- Finally, there is switchjacobs in subroutine multicompva2000. Set to 1 when using the Jacobs model, 2 for 'JULES with JULES beta', 3 for 'JULES with Dewar Beta', 4 for SOX model (not discussed here) and to 0 when using Jarvis-Stewart approach (see e.g. Verhoef and Allen (2000))

#### 4. Model outputs

The model generates 4 output files, those generating the aerodynamic and surface resistances (resistancesCaatinga.txt), state variables (variablesCaatinga.txt), energy balance fluxes (enbalCaatinga.txt), and carbon flux-related outputs (CO2Caatinga.txt). The data provided here relate to model runs with the JULES Farquhar model, with the Sinclair plant water stress switched on (for  $\Psi_{leaf} = -1 \text{ MPa}$ ).

##### Contents resistancesCaatinga.txt

Column nr	Description
1	year
2	month
3	day in year
4	decimal time within day

<b>5</b>	decimal time within year
<b>6</b>	Aerodynamic resistance between the within-canopy point and reference height [s m-1]
<b>7-15</b>	Within-canopy aerodynamic resistance between boundary layer resistance and the within-canopy point for the eight tree species (in the order as they appear in Table 1), and soil [s m-1]
<b>16-24</b>	boundary layer resistance for the eight tree species plus soil (in the order as they appear in Table 1) [s m-1]
<b>25-33</b>	surface resistances for the eight tree species plus soil (in the order as they appear in Table 1) [s m-1]
<b>34-41</b>	Stomatal conductances for the eight tree species (in the order as they appear in Table 1) [m s-1]

#### Contents VariablesCaatinga.txt

<b>Column nr</b>	<b>Description</b>
<b>1</b>	year
<b>2</b>	month
<b>3</b>	day in year
<b>4</b>	decimal time within day
<b>5</b>	decimal time within year
<b>6</b>	air temperature at reference height [deg C]
<b>7</b>	atmospheric temperature at within-canopy sink/source level [deg C]

<b>8-16</b>	Surface temperature for the 8 tree species (in the order as they appear in Table 1), and bare soil [deg C]
<b>17</b>	vapour pressure deficit at reference height [mbar]
<b>18</b>	Atmospheric vapour pressure deficit at within-canopy sink/source level [mbar]
<b>19</b>	atmospheric vapour pressure at within-canopy sink/source level [mbar]
<b>20</b>	atmospheric CO <sub>2</sub> concentration at reference height [mg m <sup>-3</sup> ]
<b>21</b>	atmospheric CO <sub>2</sub> concentration at within-canopy sink/source level [mg m <sup>-3</sup> ]
<b>22-29</b>	Vapour pressure deficit between leaf and within-canopy sink/source level, for the 8 tree species (in the order as they appear in Table 1) [mbar]
<b>30-37</b>	CO <sub>2</sub> concentration at leaf surface level for the 8 tree species (in the order as they appear in Table 1) [mg m <sup>-3</sup> ]

#### Contents enbalCaatinga.txt

Column nr	Description
<b>1</b>	year
<b>2</b>	month
<b>3</b>	day in year
<b>4</b>	decimal time within day
<b>5</b>	decimal time within year
<b>6</b>	total ecosystem net radiation [W m <sup>-2</sup> ]
<b>7</b>	total ecosystem available energy [W m <sup>-2</sup> ]

<b>8</b>	total ecosystem sensible heat flux [W m-2]
<b>9</b>	total ecosystem evapotranspiration [W m-2]
<b>10-18</b>	net radiation per surface component; for the 8 tree species (in the order as they appear in Table 1), and bare soil [W m-2]
<b>19-27</b>	available energy per surface component; for the 8 tree species (in the order as they appear in Table 1), and bare soil [W m-2]
<b>28-36</b>	soil heat flux per surface component; for the 8 tree species (in the order as they appear in Table 1), and bare soil [W m-2]
<b>37-45</b>	evapo(transpi)ration per surface component; for the 8 tree species (in the order as they appear in Table 1), and bare soil [W m-2]
<b>46-54</b>	sensible heat flux per surface component; for the 8 tree species (in the order as they appear in Table 1), and bare soil [W m-2]

### Contents Co2Caatinga.txt

<b>Column nr</b>	<b>Description</b>
<b>1</b>	year
<b>2</b>	month
<b>3</b>	day in year
<b>4</b>	decimal time within day
<b>5</b>	decimal time within year
<b>6-13</b>	Soil water stress factor (1 mean no water stress) for the 8 tree species (in the order as they appear in Table 1) [-]

<b>14-21</b>	Leaf level photosynthesis for the 8 tree species (in the order as they appear in Table 1) [mg m <sup>-2</sup> s <sup>-1</sup> ]
<b>22-29</b>	Canopy level photosynthesis for the 8 tree species (in the order as they appear in Table 1) [mg m <sup>-2</sup> s <sup>-1</sup> ]
<b>30</b>	Soil respiration [mg m <sup>-2</sup> s <sup>-1</sup> ]
<b>31</b>	net ecosystem CO <sub>2</sub> flux [mg m <sup>-2</sup> s <sup>-1</sup> ]

## 5. Researchers involved

The following researchers were involved in providing the model parameters. Model development and model runs were performed by Anne Verhoef.

Raquel Carolina Miatto, Plant physiology, University of São Paulo, Brazil

Luiza Helena Menezes Cosme, Plant physiology, University of São Paulo, Brazil

Tomas Ferreira Domingues, Plant physiology, University of São Paulo, Brazil

Magna Soelma Beserra de Moura, Micrometeorology, Brazilian Agricultural Research Corporation (EMBRAPA), Brazil

Peter Moonlight, Plant species identification, Royal Botanic Garden Edinburgh, Brazil

Rodolfo Nobrega, Plant structural indices and modelling input collation, Imperial college, UK

Colin Prentice, Modelling advice, Imperial college, UK

Anne Verhoef, Modelling, The University of Reading, UK

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