APPENDIX I

**Table I** List of symbols and abbreviations

|  |  |  |  |
| --- | --- | --- | --- |
| **Symbol / abbreviation** | **Description** | **Unit** | **Comment** |
| esat | Saturated water vapour pressure | kPa or Pa | Used in gsto and PEt / AEt calculation and Rn derivation |
| eact | Actual water vapour pressure | kPa or Pa | Used in PEt / AEt calculation and Rn derivation |
| VPD | Water vapour pressure deficit | kPa or Pa | Used in gsto and PEt / AEt calculation and Rn derivation |
| Ts\_c | Temperature | Degrees Celcius | Ts\_c = Ts\_k – 273.16 |
| Ts\_k | Temperature | Kelvin | Ts\_k = Ts\_c + 273.16 |
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APPENDIX I List of variables

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| Variable | Unit | Equation |
| **O3 deposition** |  |  |
| Total O3 deposition, *FO3* in text as fO3 | nmol/m2/s |  |
| O3 deposition velocity, *Vg in text as Vg* | mmol/m2/s | 1, 2 |
| O3 concentration, *O3* | nmol/mol | 1 |
| Reference height at which variable measured, *zRef* | m | 1, 2 |
|  |  |  |
| **Atmospheric (Ra) and boundary layer (Rb) resistances** |  |  |
| Atmospheric resistance, *Ra* not always in italic in the text | s/m | (2, 3, 18, 22) |
| Friction velocity, *u\** not always in italic in the text | m/s | (3a, 3d, 4, 6) |
| Monin-Obukhov length, *L* not always in italic in the text | - | (3a, 3b, 3c, 3f) |
| Displacement height, *d* | m | (3a, 3b, 3c) |
| Roughness length, *zo* not in italic in the text | m | (3a, 3b, 3c) |
| Plant canopy height, *h* | m | (3a, 6) |
| Turbulent surface stress, τ | kg / m / s-2 | (3d) |
| Surface density of dry air, *ρ* | kg/m3 | (3d) |
| Surface temperature, *Tk* in text as Tk | kelvin | (3e) |
| Specific heat capacity of dry air, c*p* in text as both cp and Cp | ? | (3f) |
| Sensible heat flux, *H* not in the text | W/m2 | (3f) |
|  |  |  |
| **Surface resistance (Rsur)** |  |  |
| Surface resistance, *Rsur* written in the text as both Rsur and Rsur | s/m | (2, 5) |
| Leaf Area Index, *LAI* not written in italic in the text | m2/m2 | (5, 7a, 7b, 8a, 8b) |
| Surface Area Index, *SAI* not written in italic in the text | m2/m2 | (5, 6) |
| Leaf level stomatal resistance to O3, *rsto* not always in italic, sometimes written as rsto/Rsto | m/s | (5) |
| Leaf level plant external resistance, *rext* not always in italic in the text | m/s | (5) |
| In-canopy resistance to O3, *Rinc* not always in italic in the text, sometimes written as rinc | m/s | (5) |
| Soil surface resistance to O3, Rgs not always in italics, sometimes written as Rgs | m/s | (5) |
| Year day, dd | day | (7a, 7b, 10) |
| Leaf level stomatal conductance to O3, *gsto* | mmol/m2/s | (9) |
| Maximum stomatal conductance to O3 (*gmax*) not always in italic, sometimes written as gmax | mmol/m2/s | (9) |
| Minimum daytime stomatal conductance to O3 (*fmin*) not always in italic | - | (9) |
| Maximum potential conductance to O3 over a species growth period (*fphen*) not always in italic in the text | - | (9, 10) |
| Stomatal conductance response function for irradiance (*flight*) not always in italics | - | (9, 11) |
| Stomatal conductance response function for air temperature (*ftemp*) not always in italics | - | (9, 12) |
| Stomatal conductance response function for air vapour pressure deficit (*fVPD*) not always in italic | - | (9, 13) |
| Stomatal conductance response function for soil moisture (*fSWP*) not always in italic in the text | - | (9, 14) |
|  |  |  |
| **Soil Water Balance (*Sn*)** |  |  |
| Species-specific maximum root depth, *Rz* not always in italic | m | (16) |
| Root zone soil water storage capacity, *Sn\** not in italic in the text | m3/m3 | (15) |
| Root zone soil water storage, *Sn* not always in italic | mm | (16) |
| Plant available soil water, *ASW* same as text | m3/m3 | (15, 19) |
| Field Capacity, *FC* same as text | m3/m3 | (19) |
| Root zone soil water storage at the end of the preceding day, *Sn-1* same as in text | mm | (16) |
| Daily precipitation, *P* written as p in the text | mm | (16) |
| Daily interception water loss, *Ei* written as *Ei* in the text | mm | (16, 17) |
| Soil water potential, Ψ same as in text | MPa | (14, 18) |
| Soil water potential at air entry, Ψe in italic in the text | MPa | (18) |
| Soil water content, *θ* is in | m3/m3 | (18) |
| Saturated water content, *θ*sat not in the text | m3/m3 | (18) |
| Soil water co-efficient, b not in the text | - | (18) |
| Soil water potential at plant specific permanent wilting point, Ψmin in italic in the text | MPa | (20) |
|  |  |  |
| **Plant transpiration (*Eat*)** |  |  |
| Daily actual transpiration, *Eat* not always in italics in the text | mm | (16, 21) |
| Net radiation, *Rn* not always in italics in the text | MJ m2/h | (17, 21) |
| Soil heat flux, *G* | MJ/m2/h | (17, 21) |
| Mean air density, ρa not in text | Kg/m3 | (17, 21) |
| Specific heat capacity of dry, *Cp* sometimes Cp and sometimes cp in text | MJ/kg/oC | (17, 21) |
| Vapour pressure deficit, *es-ea* | kPa | (17, 21) |
| Latent heat of vaporisation, λ | MJ/kg | (17, 21) |
| Psychrometric constant, γ not always in italic | kPa/oC | (17, 21) |
| Boundary layer resistance to water vapour, *RbH2O* same as in text | s/m | (17, 21) |
| Canopy stomatal resistance to water vapour, *RstoH2O* same as in text | s/m | (21) |
| Zr |  |  |
| Zl |  |  |
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Appendix II List of constants

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| --- | --- | --- |
| Constants | Unit | Equation |
|  |  |  |
| Von Karmans constant | 0.41 | (3a, 3f, 4) |
| Mass gas constant for dry air, *Rmass* in text as Rmass, not in italic | X J / Kg / K | (3e) |
| Gravitational acceleration, *g* | 9.81 m / s2 | (3f) |
| Kinetic viscosity of air, *v* | 0.15 cm-2 s-1 at 20°C | (4) |
| Molecular diffusivity of O3, *Di* |  | (4) |
| Prandtl number, *Pr* | 0.72 | (4) |
| In canopy resistance empirical constant, *b* | 14 s-1 | (6) |
| External plant surface resistance, *Rext* | 2500 s / m | (5) |
| Soil surface resistance, *Rsoi* in text as Rsoil, not always in italic | 200 s / m | (5) |
| Saturated water content, *θ*sat | m3/m3 | (18) |
| Sandy loam | 0.4 |  |
| Silt loam | 0.4 |  |
| Loam | 0.4 |  |
| Clay loam | 0.4 |  |
| Soil water potential at air entry, Ψe | m3/m3 | (18) |
| Sandy loam | -9.10 x 10-4 |  |
| Silt loam | -1.58 x 10-3 |  |
| Loam | -1.88 x 10-3 |  |
| Clay loam | -5.88 x 10-3 |  |
| Soil water release curve co-efficient, b | - | (18) |
| Sandy loam | 3.31 |  |
| Silt loam | 4.38 |  |
| Loam | 6.58 |  |
| Clay loam | 7 |  |
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\* all variables are defined on a projected leaf area basis

Appendix III List of inputs for the interfaced version of the DO3SE model.

|  |  |  |  |
| --- | --- | --- | --- |
| **Essential Site data** | **units** | **Comments** |  |
| Vegetation species/type |  |  |  |
| Soil texture |  |  |  |
| Longitude | ° |  |  |
| Latitude | ° |  |  |
| Elevation | m |  |  |
| Canopy height | m |  |  |
| Measurement height – O3 | m |  |  |
| Windspeed | m |  |  |
| Other meteorology | m |  |  |
|  |  |  |  |
| **Essential Hourly data** |  |  |  |
| Year |  |  |  |
| Month |  |  |  |
| Day of Month |  |  |  |
| Day of Year |  |  |  |
| Hour (time) |  |  |  |
|  |  |  |  |
| Temperature | °C |  |  |
| VPD | kPa |  |  |
| Wind speed | m s-1 |  |  |
| Precipitation | mm |  |  |
| Atmospheric pressure | kPa |  |  |
| O3 Concentration | ppb |  |  |
| LAI | m2 m-2 |  |  |
| Sensible heat flux HD | mol m-2 s-1 |  |  |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |
| **Desirable Hourly data** | These data are required by the DO3SE model and can be estimated from Essential variables |  |  |
| Global radiation | Wh m-2 | Both R and PAR are required by the DO3SE model. Where only one is entered this will be used to derive the other. |  |
| PAR | mol m-2 s-1 |  |
| Net radiation | Wh m-2 h-1 | Rn is derived from R, Td, Temp, VPD, elev, Lon, Lat |  |
| Soil heat flux | Wh m-2 h-1 | G is derived from Rn |  |
| ustar | m s-1 |  | when ustar is not entered conditions of neutral stability are assumed |

APPENDIX III Conversions and derivations

## AIII.1 Unit conversions

## AIII.!.!. Radiation

Both global radiation (R Wh m-2) and photosynthetically active radiation (PAR mol m-2 h-1) are required by the DO3SE model. If only one of these variable is entered, the model will derive the other using the conversion,

PAR = R\*0.45\*4.57

R = PAR/0.45/4.57

Radiation data are entered in Wh m-2 and can be converted from other units (eg. MJ m-h-1) using Table X. Where the DO3SE model converts energy terms from Wh m-2 these conversions are also used

Table X. Conversion factors for radiation units

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Wh m-2 | J m-2 h-1 | MJ m-2 h-1 | MJ m-2 d-1 |
| 1 Wh m-2 | 1 | 3600 | 0.0036 | 0.0864 |
| 1 J m-2 h-1 | 0.000278 |  | | |
| 1 MJ m-2 h-1 | 277..8 |
| 1 MJ m-2 d-1 | 11.6 |

## AIII.1.2 Temperature

Temperature in Kelvin = Temperature in degrees Celcius + 273.16

## AIII.1.3 Water Vapour Pressure

esat (Pa) = 611 \* exp((17.27\*Ts\_c)/(Ts\_c+237.3))

## AIII.1.4 Ozone concentration

Estimation of the specific molar volume of an ideal gas (**Vn**) (incorporating variation in T and P in concentration derivation)

**Vn** = R \* 

T is the temperature in Kelvin [equal to oC + 273.15]

P is the surface air pressure in kPa Pa

e.g. 24.46554 = 8.314510 \* 

is the **Vn** at standard Pressure (101.325 kPa or 1 atm and 25oC)

22.4141 = 8.314510 \* 

is **Vn** at standard Pressure (101.325 kPa and 0oC)

**μg / m3 to ppb**

ppb = Vn \* 

M is the molecular weight of the gas (i.e. for O3 = 48g)

e.g. if concentration = 60 μg/m3 then ppb = 22.4141 \*  = 30 ppb at standard temperature (25oC) and pressure.

This is where the 0.5 conversion factor from μg / m3 to ppb comes from.

**ppb to μg / m3**

μg / m3 = 

M is the molecular weight of the gas (i.e. for O3 = 48g)

e.g. if concentration = 30 ppb then μg/m3 =  = 60 μg / m3

**μg / m3 to nmol / m3**

48 g of O3 = 1 mol O3

1 g of O3 = 0.020833 mol O3

1 mg O3 = 0.000 020833 mol O3

1 μg O3 = 0.000 000 020833 mol O3

1 μg O3 = 20.83 nmol O3

1 μg / m3 O3 = 20.83 nmol /m3 O3

Therefore to convert ppb to nmol / m3

nmol / m3 = 

AIII.2 Derivation of net radiation (Rn)

If possible, net radiation (Rn) should be entered into the DO3SE model as input data. However, where these data are not available Rn will be estimated within the DO3SE model using derivations described in FAO (19??).

Global radiation (R) is entered into the DO3SE model as Wh m-2 and is converted into MJ m-2 h-1 using the conversion factor given in Appendix X.

Rn = R­ns – Rnl

Where Rns is net shortwave radiation (MJ m-2 h-1) and Rnl is net longwave radiation (MJ m-2 h-1).

Rns = (1-)R

Where  is a landcover specific constant representing albedo

Rnl =  Tk4 (0.34-0.14 √ea) (1.35 (R/pR)-0.35

Where s is the Stefan-Boltzman constant (4.903 10-9 MJ K-4 m-2 h-1, Tk is air temperature (°K), ea is the actual vapour pressure (kPa), R is the actual global radiation (MJ m-2 h-1) and pR is the potential global radiation (MJ m-2 h-1).

Tk = Tc + 273.16

Where Tc is air temperature (°C)

ea = esat – VPD

where esat is the saturated vapour pressure (kPa) and VPD is the vapour pressure deficit (kPa)

esat = 0.611exp(17.27Tc/(Tc+237.3))

pR = (0.75 + 2 10-5z)Rext

Where z is site elevation (m) and Rext is extraterrestrial radiation (MJ m-2 h-1)

Rext = (12(60)/) Gsc dr sin

Where Gsc is solar constant (0.0820 MJ m-2 min-1), d­r is the inverse relative distance Earth-Sun and sin is the solar elevation (see Irradiance, section XX)

dr = 1 + 0.033cos ((2/365)J)

where J is the Julian day.