

# NOMENCLATURE

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## LATIN SYMBOLS

|               |  |  |
|---------------|--|--|
| $a$           | leaf area density                                | $\text{m}^2 \text{m}^{-3}$               |
| $A$           | area   | $\text{m}^2$                             |
| $A_f$         | frontal area                                     | $\text{m}^2$                             |
| $A_L$         | net leaf area                                    | $\text{m}^2$                             |
| $A_n$         | assimilation rate                                | $\text{mol m}^{-2} \text{s}^{-1}$        |
| $b$           | Vogel exponent                                   | -  |
| $c_d$         | leaf drag coefficient                            | -  |
| $C_d$         | drag coefficient                                 | -  |
| $c_p$         | specific heat (at constant pressure)             | $\text{J kg}^{-1} \text{K}^{-1}$         |
| $c_a^*$       | reference $\text{CO}_2$ concentration            | $\text{mol mol}^{-1}$                    |
| $C$           | aerodynamic resistance coefficient               | $\text{s}^{0.5} \text{m}^{-1}$           |
| $C_{o,a}$     | oxygen concentration                             | $\text{mol mol}^{-1}$                    |
| $D$           | diameter   | $\text{m}$                               |
| $D$           | vapor pressure deficit                           | $\text{kPa}$                             |
| $D$           | vapor pressure deficit                           | $\text{Pa Pa}^{-1}, \text{mol mol}^{-1}$ |
| $e_m$         | maximum quantum efficiency of the leaf           | -  |
| $E$           | leaf transpiration flux                          | $\text{kg s}^{-1}$                       |
| $f_c$         | $\text{CO}_2$ assimilation (photosynthesis) rate | $\text{mol m}^{-2} \text{s}^{-1}$        |
| $f_v$         | transpiration rate                               | $\text{mol m}^{-2} \text{s}^{-1}$        |
| $F$           | force  | $\text{N}$                               |
| $F_d$         | drag force                                       | $\text{N}$                               |
| $g$           | gravitational acceleration                       | $\text{m}^2 \text{s}^{-1}$               |
| $g_l$         | liquid water flux                                | $\text{kg m}^{-2} \text{s}^{-1}$         |
| $g_v$         | water vapor flux                                 | $\text{kg m}^{-2} \text{s}^{-1}$         |
| $g_{v,leaf}$  | water vapor mass flux                            | $\text{kg m}^{-2} \text{s}^{-1}$         |
| $g_{v,root}$  | root water uptake                                | $\text{kg m}^{-2} \text{s}^{-1}$         |
| $G_{v,root}$  | net root water uptake                            | $\text{kg s}^{-1}$                       |
| $G_{v,xylem}$ | net xylem water flux                             | $\text{kg s}^{-1}$                       |
| $h$           | enthalpy   | $\text{J kg}^{-1}$                       |
| $h_{c,h}$     | convective heat transfer coefficient             | $\text{W m}^{-2} \text{K}^{-1}$          |

|               |   |                                   |
|---------------|---|-----------------------------------|
| $h_{c,m}$     | convective mass transfer coefficient                          | $\text{m s}^{-1}$                 |
| $H$           | height  | m                                 |
| $HU$          | Hounsfield units  | -                                 |
| $I$           | turbulence intensity  | %                                 |
| $k$           | turbulent kinetic energy                                      | $\text{m}^2 \text{s}^{-2}$        |
| $k_{st}$      | stomatal conductance  | $\text{mol m}^{-2} \text{s}^{-1}$ |
| $k_{st}^*$    | effective stomatal conductance                                | $\text{mol m}^{-2} \text{s}^{-1}$ |
| $K$           | permeability  | $\text{m}^2$                      |
| $K$           | hydraulic conductivity  | $\text{m s}^{-1}$                 |
| $K_{lp}$      | liquid water permeability                                     | s                                 |
| $K_{vp}$      | water vapor permeability                                      | s                                 |
| $K_{vT}$      | water vapor permeability due to temperature                   | s                                 |
| $K_c$         | Michaelis constant for $\text{CO}_2$                          | ???                               |
| $K_o$         | Michaelis constant for $\text{O}_2$                           | ???                               |
| $l$           | length  | m                                 |
| $l$           | characteristic leaf size                                      | m                                 |
| $\mathcal{L}$ | Lagrangian  | -                                 |
| $L_v$         | latent heat of vaporization for water ( $= 2.5 \times 10^6$ ) | $\text{J kg}^{-1}$                |
| $m$           | mass  | kg                                |
| $M$           | molar mass  | $\text{kg mol}^{-1}$              |
| $M_a$         | molar mass of dry air ( $= 0.028\,966$ )                      | $\text{kg mol}^{-1}$              |
| $M_v$         | molar mass of water vapor ( $= 0.018\,015\,34$ )              | $\text{kg mol}^{-1}$              |
| $n$           | Van Genuchten parameter                                       | -                                 |
| $p_c$         | capillary pressure  | Pa                                |
| $p_l$         | liquid pressure   | Pa                                |
| $p_l$         | gas phase pressure  | Pa                                |
| $p_v$         | partial vapor pressure  | Pa                                |
| $p_{v,i}$     | intercellular vapor pressure                                  | Pa                                |
| $p_{v,sat}$   | saturation vapor pressure                                     | Pa                                |
| $P$           | pressure  | Pa                                |
| $Pr$          | Prandtl number  | -                                 |
| $Pr_t$        | turbulent Prandtl number                                      | -                                 |
| $q$           | heat flux   | $\text{W m}^{-2}$                 |
| $q_{lat,lat}$ | latent heat flux from leaf                                    | $\text{W m}^{-2}$                 |
| $q_r$         | net radiative heat flux                                       | $\text{W m}^{-2}$                 |
| $q_{r,sw}$    | short-wave radiative heat flux                                | $\text{W m}^{-2}$                 |
| $q_{r,lw}$    | long-wave radiative heat flux                                 | $\text{W m}^{-2}$                 |

|               |  |                     |
|---------------|--|---------------------|
| $q_{rad,lat}$ | radiative heat flux into leaf                    | $W m^{-2}$          |
| $q_{sen,lat}$ | sensible heat flux from leaf                     | $W m^{-2}$          |
| $Q_p$         | flux of incoming PAR                             | ???                 |
| $r$           | root area density                                | $m^2 m^{-3}$        |
| $r_a$         | aerodynamic resistance                           | $s m^{-1}$          |
| $r_s$         | stomatal resistance                              | $s m^{-1}$          |
| $R$           | universal gas constant (= 8.314 459 8)           | $J mol^{-1} K^{-1}$ |
| $RAI$         | root area index                                  | $m^2 m^{-2}$        |
| $Re$          | Reynolds number                                  | -                   |
| $R_v$         | specific gas constant of dry air (= 287.042)     | $J kg^{-1} K^{-1}$  |
| $R_v$         | specific gas constant of water vapor (= 461.524) | $J kg^{-1} K^{-1}$  |
| $Sc_t$        | turbulent Schmidt number                         | -                   |
| $s_\epsilon$  | volumetric TDR source                            | $W m^{-3} s^{-1}$   |
| $s_\rho$      | volumetric mass source                           | $kg m^{-3} s^{-1}$  |
| $s_k$         | volumetric TKE source                            | $W m^{-3}$          |
| $s_{q,r}$     | volumetric radiative source                      | $W m^{-3}$          |
| $s_r$         | volumetric root water uptake source              | $kg m^{-3} s^{-1}$  |
| $s_T$         | volumetric temperature source                    | $K m^{-3}$          |
| $s_u$         | volumetric momentum source                       | $N m^{-3}$          |
| $s_w$         | volumetric humidity source                       | $kg kg^{-1} s^{-1}$ |
| $S_l$         | liquid saturation                                | -                   |
| $t$           | time   | s                   |
| $T$           | temperature                                      | K                   |
| $T_g$         | ground temperature                               | K                   |
| $T_L$         | leaf temperature                                 | K                   |
| $T_{sky}$     | sky temperature                                  | K                   |
| $TR$          | net hourly transpiration rate                    | $g h^{-1}$          |
| $u$           | velocity   | $m s^{-1}$          |
| $u_*$         | friction velocity                                | $m s^{-1}$          |
| $U$           | mean wind speed                                  | $m s^{-1}$          |
| $U_{ref}$     | reference velocity                               | $m s^{-1}$          |
| $UTCI$        | universal thermal climate index                  | $^{\circ}C$         |
| $V_{cmax}$    | maximum carboxylation capacity                   | ???                 |
| $w$           | moisture content                                 | $kg m^{-3}$         |
| $w_a$         | dry air content                                  | $kg m^{-3}$         |
| $w_{cap}$     | capillary moisture content                       | $kg m^{-3}$         |
| $w_l$         | liquid water content                             | $kg m^{-3}$         |

|       |                              |                    |
|-------|------------------------------|--------------------|
| $w_s$ | solid matrix water content   | $\text{kg m}^{-3}$ |
| $w_v$ | water vapor content          | $\text{kg m}^{-3}$ |
| $z$   | vertical height              | m                  |
| $z_0$ | aerodynamic roughness height | m                  |

## GREEK SYMBOLS

|                |   |                                  |
|----------------|---|----------------------------------|
| $\alpha$       | aerodynamic porosity                      | -                                |
| $\alpha^{2D}$  | 2D aerodynamic porosity                   | -                                |
| $\alpha_p$     | leaf absorptivity of PAR                  | -                                |
| $\beta$        | optical porosity                          | -                                |
| $\beta$        | volumetric thermal expansion coefficient  | $\text{K}^{-1}$                  |
| $\beta_p$      | fraction of MKE converted to TKE          | -                                |
| $\beta_d$      | fraction of TKE shortcut to TDR           | -                                |
| $\gamma$       | apparent quantum yield                    | -                                |
| $\delta_v$     | water vapor diffusion coefficient         | s                                |
| $\varepsilon$  | turbulent kinetic energy dissipation rate | $\text{m}^2 \text{s}^{-3}$       |
| $\kappa$       | von Kármán constant (= 0.41)              | -                                |
| $\lambda$      | thermal conductivity                      | $\text{W m}^{-1} \text{K}^{-1}$  |
| $\lambda$      | Lagrange multiplier                       | $\text{mol mol}^{-1}$            |
| $\mu$          | attenuation coefficient                   | $\text{m}^{-1}$                  |
| $\mu$          | chemical potential                        | $\text{J mol}^{-1}$              |
| $\mu$          | dynamic viscosity                         | $\text{kg m}^{-1} \text{s}^{-1}$ |
| $\nu$          | kinematic viscosity                       | $\text{m}^2 \text{s}^{-1}$       |
| $\nu_t$        | turbulent viscosity                       | $\text{m}^2 \text{s}^{-1}$       |
| $\rho$         | density                                   | $\text{kg m}^{-3}$               |
| $\rho_a$       | density of air                            | $\text{kg m}^{-3}$               |
| $\rho_l$       | density of liquid water (= 1000)          | $\text{kg m}^{-3}$               |
| $\rho_s$       | density of solid matrix                   | $\text{kg m}^{-3}$               |
| $\sigma_v$     | Schmidt number                            | -                                |
| $\sigma_{v_t}$ | turbulent Schmidt number                  | -                                |
| $\phi_0$       | open porosity                             | $\text{m}^3 \text{m}^{-3}$       |
| $\psi$         | shelter parameter                         | -                                |
| $\psi_g$       | gravitational potential                   | Pa                               |
| $\psi_L$       | leaf water potential                      | Pa                               |
| $\psi_R$       | root water potential                      | Pa                               |

|            |                      |    |
|------------|----------------------|----|
| $\psi_s$   | soil water potential | Pa |
| $\Omega$   | domain               | -  |
| $\Omega_a$ | air domain           | -  |
| $\Omega_s$ | soil domain          | -  |

## SUBSCRIPTS

|              |                |
|--------------|----------------|
| <i>eff</i>   | effective      |
| <i>g</i>     | gas            |
| <i>g</i>     | ground         |
| <i>i</i>     | intercellular  |
| <i>l</i>     | liquid (water) |
| <i>lw</i>    | long-wave      |
| <i>L</i>     | leaf           |
| <i>o</i>     | open           |
| <i>pore</i>  | pore           |
| <i>ref</i>   | reference      |
| <i>root</i>  | root           |
| <i>sat</i>   | saturated      |
| <i>R</i>     | root           |
| <i>s</i>     | solid          |
| <i>s</i>     | soil           |
| <i>sky</i>   | sky            |
| <i>sw</i>    | short-wave     |
| <i>t</i>     | time           |
| <i>v</i>     | vapor          |
| <i>xylem</i> | xylem          |

## ACRONYMS

|      |                                      |
|------|--------------------------------------|
| ABL  | atmospheric boundary layer           |
| CFD  | computational fluid dynamics         |
| CHTC | convective heat transfer coefficient |
| CMTC | convective mass transfer coefficient |

|      |   |
|------|---|
| CT   | computational tomography                    |
| DEHS | Di-Ethyl-Hexyl-Sebacat                      |
| DIG  | diagonal-based incomplete Cholesky          |
| DNS  | direct numerical simulation                 |
| ETHZ | Eidgenössische Technische Hochschule Zürich |
| FOV  | field of view                               |
| FFT  | fast Fourier transformation                 |
| FVM  | finite volume method                        |
| HPC  | high performance computing                  |
| LAI  | leaf area index                             |
| LAI  | leaf area density                           |
| LDPE | low-density Polyethylene                    |
| LES  | large eddy simulation                       |
| LHS  | left hand side                              |
| MOE  | modulus of elasticity                       |
| PAR  | photosynthetically active radiation         |
| PCG  | preconditioned conjugate gradient           |
| PIV  | particle image velocimetry                  |
| PPM  | parts per million                           |
| RAI  | root area index                             |
| REV  | representative elementary volume            |
| RANS | Reynolds-averaged Navier-Stokes             |
| RHS  | right hand side                             |
| ROI  | region of interest                          |
| SPIV | stereoscopic particle image velocimetry     |
| TDR  | turbulent dissipation rate                  |
| TKE  | turbulent kinetic energy                    |
| UHI  | urban heat island                           |

|      |                                 |
|------|---------------------------------|
| UTCI | universal thermal climate index |
| WUE  | water use efficiency            |





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# NUMERICAL MODEL FOR VEGETATION IN URBAN AREAS

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## 1.1 INTRODUCTION

The simplified vegetation model is described in ?? introduction the governing equation for moist flow vegetation. The vegetation model provides the necessary source/sink terms for heat, mass and momentum exchanges between vegetation and air as described in ?. Furthermore, radiation transfer within vegetation is also described in ?. For reader, a detailed derivation of the thermodynamic of the moist air is given in ? and a detailed derivation of the governing equation of moist flow is given in ?.

In this chapter, the numerical method for modeling vegetation inside an urban area is described. The chapter focuses on coupling of the vegetation model with the of heat (incl. radiation) and mass fluxes of the urban surfaces. The governing equation for the the coupled heat and moisture transport in the porous material is first described.

## 1.2 GOVERNING EQUATIONS OF COUPLED HEAT AND MOISTURE TRANSPORT

### 1.2.1 *Composition of the porous material*

The building materials and the soil is considered as a porous material consisting of three phases: solid phase (denoted with  $s$ ), liquid phase referring to liquid water ( $l$ ) and the air phase which is split into dry air ( $a$ ) and water vapor  $v$  (Janssen 2002; Carmeliet 2005; Defraeye 2011; Saneinejad 2013). The open porosity  $\phi_o$  ( $\text{m}^3 \text{m}^{-3}$ ) of the porous material is defined as:

$$\phi_o = \frac{V_{pore}}{V} \quad (1.1)$$

where  $V_{pore}$  ( $\text{m}^3$ ) is the volume of open pores and  $V$  ( $\text{m}^3$ ) is the total volume of the porous material  $S$ . The solid material content  $w_s$  ( $\text{kg m}^{-3}$ ) is defined as:

$$w_s = (1 - \phi_o) \rho_s \quad (1.2)$$

where  $\rho_s$  ( $\text{kg m}^{-3}$ ) is the solid material matrix density. Similarly the dry air  $w_a$ , water vapor  $w_v$ , liquid water  $w_l$  contents are defined as:

$$w_l = \phi_o S_l \rho_l \quad (1.3)$$

$$w_a = \phi_o (1 - S_l) \rho_a \quad (1.4)$$

$$w_v = \phi_o (1 - S_l) \rho_v \quad (1.5)$$

where they are related to the degree of liquid saturation  $S_l$  of the porous open pores:

$$S_l = \frac{\phi_{o,l}}{\phi_o} \quad (1.6)$$

with  $\phi_{o,l}$  being the amount of liquid water occupied inside the open pores and  $\rho_a, \rho_l$  being the air and liquid water densities, respectively. The total moisture content  $w$  ( $\text{kg m}^{-3}$ ) inside the porous material is simply the sum of liquid water and water vapor:

$$w = w_l + w_v \quad (1.7)$$

### 1.2.2 Water potential

Water potential is a universal parameter to determine the *water status* in any medium (Nobel 2009). In the thesis, we use it to define the water status of multiple domains such as solid porous materials (soil and building facades), plant xylem, and air. The water potential  $\psi$  (Pa) describes the chemical potential of water  $\mu$  ( $\text{J mol}^{-1}$ ) with respect to chemical potential of pure water  $\mu^{o,l}$  ( $\text{J mol}^{-1}$ ) at the same temperature, standard atmosphere and at zero level:

$$\psi = \frac{\mu - \mu^{o,l}}{V_l^o} \quad (1.8)$$

where  $V_l^o = 18.0510^{-3} \text{ m}^3 \text{ mol}^{-1}$  is the molar volume of pure water in liquid phase. The water potential for pure water at standard atmosphere is  $\psi = 0$  Pa. The water tends to move towards a region where  $\mu - \mu^{o,w}$  is lower, i.e. in the direction of  $-\nabla\psi$ . The water potential is related to pressure potential, osmotic potential, matrix potential, and gravitational potential. In our study, we assume that the pressure potential gradient is negligible in the solid and we ignore the influence of osmotic potential  $\psi_o$  (Pa) as we assume we have a non-saline porous material. Therefore, only the matrix potential and gravitation potential influences the water transport:

$$\psi = \underbrace{p_c}_{\psi_c} + \underbrace{\rho_l g z}_{\psi_g} \quad (1.9)$$

where  $\psi_c = p_c$  (Pa) is the capillary potential due to capillary pressure, which represents the contribution of the matrix potential, and  $\psi_g = \rho_l g h$  (Pa) is the gravitational potential with  $g = |g|$  ( $\text{m s}^{-2}$ ) where  $g$  is the gravitational acceleration. The capillary

pressure  $p_c$  is defined as the difference between liquid and gas phase pressure,  $p_l$  and  $p_g$ , respectively:

$$p_c = p_l - p_g \quad (1.10)$$

and is related to relative humidity  $\phi$  by the Kelvin's law:

$$p_c = \rho_l R_v T \ln(\phi) \quad (1.11)$$

The gravitational potential  $\psi_g$  (Pa) is defined as:

$$\psi_g = -\rho g \cdot \mathbf{x} = \rho g z \quad (1.12)$$

where  $g = |\mathbf{g}|$  with  $z$  oriented upward. Thus, by taking the capillary and gravitational water potentials into account, the transport of water can be described in building materials and, more importantly, soil where the plant roots are present.

### 1.2.3 Coupled transport of heat and mass

The conservation of mass in the solid domain is defined as:

$$\frac{\partial w_s}{\partial t} = 0 \quad (1.13)$$

$$\frac{\partial w_a}{\partial t} + \nabla \cdot (w_a \mathbf{u}_a) = 0 \quad (1.14)$$

$$\frac{\partial w_l + w_v}{\partial t} + \nabla \cdot (w_l \mathbf{u}_l + w_v \mathbf{u}_v) = 0 \quad (1.15)$$

assuming that solid matrix does not move, mass of different phases only change due to evaporation or condensation. Other phenomena such as melting, freezing, sublimation and deposition are neglected. As we are only interested in the rate of change of moisture content  $w = w_l + w_g$ , we are only interested in Eq. (1.15) and conservation of mass simplifies to:

$$\frac{\partial w}{\partial t} = -\nabla \cdot (\mathbf{g}_l + \mathbf{g}_v) \quad (1.16)$$

where  $\mathbf{g}_l \equiv w_l \mathbf{u}_l$  ( $\text{kg m}^{-2} \text{s}^{-1}$ ) and  $\mathbf{g}_v \equiv w_v \mathbf{u}_v$  ( $\text{kg m}^{-2} \text{s}^{-1}$ ) are defined as the liquid water and water vapor fluxes, respectively. Additionally, the contribution of root water uptake due to plant transpiration is introduced through the source term  $s_r$  ( $\text{kg m}^{-3} \text{s}^{-1}$ ):

$$\frac{\partial w}{\partial t} = -\nabla \cdot (\mathbf{g}_l + \mathbf{g}_v) + s_r \quad (1.17)$$

The sink term due to root water uptake is explained in detail later in Section 1.3. In this thesis, the conservation of mass is solved using the  $p_c$ -form Richards equation, where Eq. (1.17) becomes:

$$\frac{\partial w}{\partial p_c} \frac{\partial p_c}{\partial t} = -\nabla \cdot (\mathbf{g}_l + \mathbf{g}_v) + s_r \quad (1.18)$$

with  $C_{mm} \equiv \partial w / \partial p_c$  ( $\text{kg m}^{-3} \text{Pa}^{-1}$ ) is defined as the moisture capacity. Thus, the change in water content in the porous material is simply due to the liquid and vapor fluxes, and root water uptake. The liquid water flux  $g_l$  in porous media is given by:

$$g_l = -K_{lp} \nabla (p_c + \rho_l g z) \quad (1.19)$$

and assumes the air pressure effects be negligible with respect to capillary and gravitational effects, where  $K_{lp}$  (s) the liquid water permeability. We assume that the liquid water permeability is only due to pressure gradient, and the influence of thermal gradient is neglected (Carmeliet 2005). The water vapor flux in the porous media is given by:

$$g_v = K_{vp} \nabla p_c + K_{vT} \nabla T \quad (1.20)$$

where

$$K_{vp} = -\delta_v \frac{p_v}{\rho_l R_v T} \quad (1.21)$$

is the water vapor permeability (s) due to pressure,

$$K_{vT} = -\delta_v \frac{p_v}{\rho_l R_v T^2} (\rho_l L_v - p_c) \quad (1.22)$$

is the water vapor permeability (s) due to temperature, and

$$\delta_v = \frac{D_{va,mat}}{R_v T} \quad (1.23)$$

is the water vapor diffusion coefficient (s) where  $D_{va,mat}$  ( $\text{m}^2 \text{s}^{-1}$ ) is the binary apparent diffusion coefficient between dry air and water vapor (Carmeliet 2005; Defraeye 2011; Saneinejad 2013; Kubilay 2014). Thus, substituting the fluxes Eqs. (1.19) and (1.20) into Eq. (1.18), the expanded form of conservation of mass is given as:

$$C_{mm} \frac{\partial p_c}{\partial t} = \nabla \cdot \left( K_{lp} \nabla (p_c + \rho_l g z) + K_{vp} \nabla p_c + K_{vT} \nabla T \right) + s_r \quad (1.24)$$

The conservation of energy is given as:

$$\frac{\partial h}{\partial t} + \nabla \cdot (hu) = -\nabla \cdot q \quad (1.25)$$

where  $h$  ( $\text{J kg}^{-1}$ ) is the enthalpy of total solid domain:

$$h = \sum_i w_i h_i = w_s h_s + w_a h_a + w_l h_l + w_v h_v \quad (1.26)$$

assuming that thermal contribution of soil and liquid water is much higher than dry air and water vapor. The heat conduction  $q$  ( $\text{W m}^{-2}$ ) is given by Fourier's law as:

$$q = -\lambda \nabla T \quad (1.27)$$

where  $T$  (K) is temperature,  $\lambda$  ( $\text{W m}^{-1} \text{K}^{-1}$ ) is thermal conductivity. Substituting Eq. (1.26) into Eq. (1.25) gives:

$$\frac{\partial}{\partial t} (w_s h_s + w_l h_l) = -\nabla \cdot \mathbf{q} - \nabla \cdot (w_l h_l \mathbf{u}_l + w_v h_v \mathbf{u}_v) \quad (1.28)$$

or equivalently written as:

$$\frac{\partial}{\partial t} (w_s h_s + w_l h_l) = -\nabla \cdot \mathbf{q} - \nabla \cdot (h_l \mathbf{g}_l + h_v \mathbf{g}_v) \quad (1.29)$$

where the enthalpy of liquid water  $h_l$  and water vapor  $h_v$  are defined as:

$$h_l = c_{p,l} (T - T_{ref}) \quad (1.30)$$

$$h_v = c_{p,v} (T - T_{ref}) + L_v \quad (1.31)$$

and  $L_v$  is the latent heat of vaporization of water. Substituting Eqs. (1.30) and (1.31) into Eq. (1.29), the conservation of energy is given as:

$$\begin{aligned} & (c_{ps} w_s + c_{pl} w) \frac{\partial T}{\partial t} + \left[ c_{pl} (T - T_{ref}) \frac{\partial w}{\partial p_c} \right] \frac{\partial p_c}{\partial t} = \\ & -\nabla \cdot \left\{ \mathbf{q} + \underbrace{c_{pl} (T - T_{ref}) \mathbf{g}_l}_{q_l} + \underbrace{[c_{pv} (T - T_{ref}) + L_v] \mathbf{g}_v}_{q_v} \right\} \end{aligned} \quad (1.32)$$

where the capacity terms are:

$$C_{TT} = c_{ps} w_s + c_{pl} w \quad (1.33)$$

$$C_{Tp} = c_{pl} (T - T_{ref}) \frac{\partial w}{\partial p_c} \quad (1.34)$$

Substituting liquid and vapour fluxes, Eqs. (1.19) and (1.20), respectively, thermal capacities Eqs. (1.33) and (1.34) and heat conduction Eq. (1.27) into conservation of energy expands Eq. (1.32) to:

$$\begin{aligned} C_{TT} \frac{\partial T}{\partial t} + C_{Tp} \frac{\partial p_c}{\partial t} = & \nabla \cdot \left( \lambda \nabla T + K_{lp} c_{pl} (T - T_{ref}) \nabla p_c \right. \\ & + K_{lp} c_{pl} (T - T_{ref}) \rho_l \mathbf{g}_z \\ & - K_{vp} [c_{pv} (T - T_{ref}) + L_v] \nabla p_c \\ & \left. - K_{vT} [c_{pv} (T - T_{ref}) + L_v] \nabla T \right) \end{aligned} \quad (1.35)$$

### 1.2.4 Linearized heat and mass transport equation

In the present study, the conservation of mass and energy is coupled together as a heat and mass model (HAM) according to (Janssen 2002; Carmeliet 2005; Defraeye 2011; Saneinejad 2013; Kubilay et al. 2018). Due to the shape of the water retention curve and the hydraulic conductivity curve, the Richards equation is highly non-linear. Therefore, the numerical solution of the equation is very sensitive to convergence tolerance and requires linearization techniques to maintain accuracy and computational efficiency. Therefore, methods such as fixed-point Picard iterations is used to solve the non-linear equations. More details on the discretization is provided in Janssen (2002), Liu (2012), and Kubilay et al. (2018).

The conservation of mass (i.e., the moisture transport equation), Eq. (1.24), in the linearized form is given as:

$$\begin{aligned} C_{mm}^{n+1,k} \frac{p_c^{n+1,k+1} - p_c^n}{\Delta t} = \nabla \cdot \left( K_{lp}^{n+1,k} \nabla \left( p_c^{n+1,k+1} + \rho_l g z \right) \right. \\ \left. + K_{vp}^{n+1,k} \nabla p_c^{n+1,k+1} \right. \\ \left. + K_{vT}^{n+1,k} \nabla T^{n+1,k} \right) \\ + s_r^{n+1,k+1} \end{aligned} \quad (1.36)$$

where the capacity, permeabilities and temperature are determined from the previous Picard iteration ( $k$ ). The subscript ( $n$ ) denotes the global (i.e., outer) time step of  $t$  and  $k$  denoting the internal Picard iteration step. When the Picard solution approaches converges,  $p_c^{n+1,k} \rightarrow p_c^{n+1,k+1}$  and the influence of  $\partial w / \partial p_c$  becomes negligible. This can results in larger mass conservation errors and can be minimized by using mixed-from:

$$\begin{aligned} C_{mm}^{n+1,k} \frac{p_c^{n+1,k+1} - p_c^n}{\Delta t} = \nabla \cdot \left( K_{lp}^{n+1,k} \nabla \left( p_c^{n+1,k+1} + \rho_l g z \right) \right. \\ \left. + K_{vp}^{n+1,k} \nabla p_c^{n+1,k+1} \right. \\ \left. + K_{vT}^{n+1,k} \nabla T^{n+1,k} \right) \\ + s_r^{n+1,k+1} - \frac{w^{n+1,k+1} - w^n}{\Delta t} \end{aligned} \quad (1.37)$$



Similarly, the linearized form of the heat equation is defined as:

$$\begin{aligned}
C_{TT}^{n+1,k} \frac{T^{n+1,k+1} - T^n}{\Delta t} = & \nabla \cdot \left( \lambda \nabla T^{n+1,k+1} \right. \\
& + K_{lp}^{n+1,k} c_{pl} \left( T^{n+1,k+1} - T_{ref} \right) \nabla p_c^{n+1,k+1} \\
& + K_{lp}^{n+1,k} c_{pl} \left( T^{n+1,k+1} - T_{ref} \right) \rho_l g z \\
& - K_{vp}^{n+1,k} \left[ c_{pv} \left( T^{n+1,k+1} - T_{ref} \right) + L_v \right] \nabla p_c^{n+1,k} \\
& \left. - K_{vT}^{n+1,k} \left[ c_{pv} \left( T^{n+1,k+1} - T_{ref} \right) + L_v \right] \nabla T^{n+1,k+1} \right)
\end{aligned} \tag{1.38}$$

where the capillary pressure time derivative term is ignored. The mixed-form the heat equation is given as:

$$\begin{aligned}
C_{TT}^{n+1,k} \frac{T^{n+1,k+1} - T^n}{\Delta t} = & \nabla \cdot \left( \lambda \nabla T^{n+1,k+1} \right. \\
& + K_{lp}^{n+1,k} c_{pl} \left( T^{n+1,k+1} - T_{ref} \right) \nabla p_c^{n+1,k+1} \\
& + K_{lp}^{n+1,k} c_{pl} \left( T^{n+1,k+1} - T_{ref} \right) \rho_l g z \\
& - K_{vp}^{n+1,k} \left[ c_{pv} \left( T^{n+1,k+1} - T_{ref} \right) + L_v \right] \nabla p_c^{n+1,k} \\
& \left. - K_{vT}^{n+1,k} \left[ c_{pv} \left( T^{n+1,k+1} - T_{ref} \right) + L_v \right] \nabla T^{n+1,k+1} \right) \\
& - \frac{C_{TT}^{n+1} T^{n+1} - C_{TT}^n T^n}{\Delta t}
\end{aligned} \tag{1.39}$$

The system of linear equations is solved by Krylov subspace iteration solver, i.e. preconditioned conjugate gradient (PCG) with diagonal-based incomplete Cholesky (DIG) preconditioning. The convergence criteria for the Picard iteration is user-defined:

$$|p_c^{n+1,k+1} - p_c^{n+1,k}| \leq \delta p_c \tag{1.40}$$

$$|T^{n+1,k+1} - T^{n+1,k}| \leq \delta T \tag{1.41}$$

where  $\delta p_c = \delta T = 10^{-2}$ .

### 1.3 SOIL-PLANT-ATMOSPHERIC CONTINUUM

In the present study, the components of the water potential inside the plants are not directly determined. The soil-plant-atmosphere continuum model that is integrated into the vegetation model is described in this section, implemented according the state-of-art techniques: (Idso 1977; Farquhar et al. 1980; Manzoni et al. 2011; Volpe et al. 2013;

Manoli et al. 2014; Launiainen et al. 2015). The root-system of the plants are represented as a network-like structure assuming cooperative strategy among the individual roots and a bulk plant transpiration through a single xylem is assumed.

### 1.3.1 Water transport in soil-root system

The hydraulic conductivity in soil  $K$  ( $\text{m s}^{-1}$ ) is given as:

$$K(\mathbf{x}) = K_{lp}(\mathbf{x}) |g| \quad (1.42)$$

where  $K_l$  (s) is the liquid permeability defined in the previous section and function on the moisture content. The soil conductance in the root region  $k_s$  ( $\text{s}^{-1}$ ) is:

$$k_s(\mathbf{x}) = \alpha K(\mathbf{x}) r(\mathbf{x}) \quad (1.43)$$

where  $\alpha$  is

$$\alpha = \sqrt{\left(\frac{L}{RAI}\right) \frac{1}{d}} \quad (1.44)$$

and  $d$  is the root diameter and  $RAI = \int r \, dz$  is the root area index ( $\text{m}^2 \text{m}^{-2}$ ) and is the vertical integral of the root area density  $r$  ( $\text{m}^2 \text{m}^{-3}$ ). The conductance of the root system  $k_r$  ( $\text{s}^{-1}$ ) is given as:

$$k_r(\mathbf{x}) = r(\mathbf{x}) \frac{\Delta z}{\beta} \quad (1.45)$$

where  $\Delta z$  is the vertical height of the root layer mesh and  $\beta = 3 \times 10^8$  s. The effective conductance of the soil-root system (or rhizosphere)  $k_{sr}^*$  ( $\text{s m}^{-1}$ ) is given as:

$$k_{sr}^*(\mathbf{x}) = \frac{1}{|g|} \frac{k_s(\mathbf{x}) k_r(\mathbf{x})}{k_s(\mathbf{x}) + k_r(\mathbf{x})} \quad (1.46)$$

The sink in soil moisture  $s_r$  ( $\text{kg m}^{-3} \text{s}^{-1}$ ) is given as:

$$s_r(\mathbf{x}) = r(\mathbf{x}) g_{v,root}(\mathbf{x}) \quad (1.47)$$

where  $g_{v,root}$  is the root water uptake ( $\text{kg m}^{-2} \text{s}^{-1}$ )

$$g_{v,root}(\mathbf{x}) = k_{sr}^*(\mathbf{x}) (\psi_s(\mathbf{x}) - \psi_R) \quad (1.48)$$

and simply dependent on the soil-root system conductance, soil water potential  $\psi_s$  and the (bulk) root water potential  $\psi_R$ . The resulting net sink is soil moisture  $G_{v,root}$  ( $\text{kg s}^{-1}$ ) due to transpiration is thus:

$$G_{v,root} = \int_{\Omega_s} r(\mathbf{x}) g_{v,root}(\mathbf{x}) \, dV \quad (1.49)$$

where  $\Omega_s$  is the soil domain. The water uptake from the root is equal to the water transport in the xylem as so:

$$G_{v,root} = G_{v,xylem} \quad (1.50)$$

### 1.3.2 Water transport in xylem-leaf system

The plant xylem conductance is modeled using a “*vulnerability curve*” approach, where xylem conductance becomes exponentially smaller with increasing leaf water potential (Volpe et al. 2013). This empirical model is based on plant response to the vulnerability to xylem cavitation and embolism that could occur at high water potential gradients. The xylem conductance  $k_x$  ( $\text{m Pa}^{-1} \text{s}^{-1}$ ) is given by:

$$k_x(\psi_L) = k_{x,max} \exp \left\{ - \left( -\frac{\psi_L}{d} \right)^c \right\} \quad (1.51)$$

where  $k_{x,max}$  ( $\text{m Pa}^{-1} \text{s}^{-1}$ ) is the maximum xylem conductance,  $c$  and  $d$  are fit coefficients (Volpe et al. 2013), and  $\psi_L$  (Pa) is the (bulk) leaf water potential. The effective xylem conductance  $k_x^*$  ( $\text{s m}^{-1}$ ) of water is:

$$k_x^*(\psi_L) = k_x(\psi_L) \rho_l \quad (1.52)$$

Thus, the water flux through the plant in xylem  $g_{v,xylem}$  ( $\text{kg m}^{-2} \text{s}^{-1}$ ) is given as:

$$g_{v,xylem}(\psi_L) = k_x^*(\psi_L) (\psi_R - \psi_L) \quad (1.53)$$

where is governed by the water potential gradient. The net water flux  $G_{v,xylem}$  ( $\text{kg s}^{-1}$ ) is given as:

$$G_{v,xylem}(\psi_L) = \int_{\partial\Omega_x|s} g_{v,xylem}(\psi_L) dA = g_{v,xylem} A_x \quad (1.54)$$

where  $A_x$  ( $\text{m}^2$ ) is the xylem cross-sectional area, assuming that the net water flux through the xylem is equal (i.e. no water storage).

Similarly, the net flux of water in xylem should be equal to the net transpiration rate, as storage is negligible. Therefore,

$$G_{v,xylem} = G_{v,leaf} \quad (1.55)$$

and moreover,

$$G_{v,root} = G_{v,xylem} = G_{v,leaf} \quad (1.56)$$

### 1.3.3 Water transport from leaf to air

The leaf transpiration rate  $g_{v,leaf}$  ( $\text{kg m}^{-2} \text{s}^{-1}$ ) is defined in ??, and is simply defined as:

$$g_{v,leaf} = k_{st,v}^* (p_{v,leaf} - p_v) \quad (1.57)$$

where  $k_{st,v}^*$  ( $\text{s m}^{-1}$ ) is the effective stomatal conductance to water vapor,  $p_{v,leaf}$  (Pa) is the leaf surface vapor pressure and  $p_v$  (Pa) is the atmospheric vapor pressure. The net plant transpiration rate is given as:

$$G_{v,leaf} = \int_{\Omega_a} a g_{v,leaf} dV \quad (1.58)$$

where  $a$  ( $\text{m}^2 \text{m}^{-3}$ ) is the leaf area density. The water mass flux to the atmosphere is assumed to be in equilibrium with the water vapor flux through xylem:

$$G_{v,xylem} = G_{v,leaf} \quad (1.59)$$

and so:

$$k_x^* (\psi_R - \psi_L) A_x = \int_{\Omega_a} a g_{v,leaf} dV \quad (1.60)$$

Therefore, the root water potential  $\psi_R$  can be determined once leaf water potential  $\psi_L$  (Pa), net plant transpiration rate  $G_{v,leaf}$  ( $\text{kg s}^{-1}$ ), effective xylem conductance  $k_x^*$  ( $\text{s m}^{-1}$ ) and xylem cross-section area  $A_x$  ( $\text{m}^2$ ):

$$\psi_R (\psi_L) = \psi_L + \frac{G_{v,leaf}}{A_x k_x^*} \quad (1.61)$$

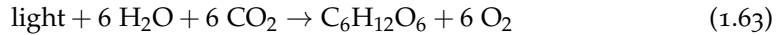
The assumption is that water extract by roots only feed the transpiration and storage inside the plant is neglected. Furthermore, one can also take in account of the gravitation potential change due to tree height:

$$\psi_R (\psi_L) = \psi_L + \frac{G_{v,leaf}}{A_x k_x^*} + \rho_l g H \quad (1.62)$$

however, with a tree height of  $H = 10$  m, the additional potential is only  $\psi_g = 0.1$  MPa.

### 1.3.4 Improved stomatal model

The photosynthetic reaction takes light, water and  $\text{CO}_2$  and creates carbohydrate and oxygen:



and additional moisture is lost by evaporation when stomatal cavity is exposed to atmosphere. Therefore, the photosynthetic process is directly related to atmospheric condition such as  $\text{CO}_2$  concentration, availability of light and temperature. Furthermore, the transpiration rate is also dependent on the atmospheric humidity and the availability of water for transpiration (Ball 1987; Leuning et al. 1995). Based on these conditions, a generally accepted theory is the plant regulates the stomatal aperture to optimize the photosynthetic rate for a given transpiration rate. Moreover, the function of vegetation can be simplified as just maximizing the photosynthesis (or  $\text{CO}_2$  assimilation) for a given transpiration rate (water use) (Medlyn et al. 2011). The water use

efficiency or WUE quantifies the efficiency of the plant of reaching this target. The WUE is defined as:

$$WUE = \frac{f_c}{f_v} \quad (1.64)$$

where  $f_c$  ( $\text{mol m}^{-2} \text{s}^{-1}$ ) is the  $\text{CO}_2$  assimilation rate (i.e., denoted also as  $A_n$  (in plant-science) or  $G_{c,leaf}$  (in building physics), also known as photosynthesis rate) and  $f_v$  ( $\text{mol m}^{-2} \text{s}^{-1}$ ) is the transpiration rate (i.e. denoted also as  $f_e$  (in plant-science) or  $G_{v,leaf}$  (in building physics), also known as water use).

The stomatal optimality model reflects the theory of the stomatal behavior (Cowan 1978). The optimal stomatal control is derived from the minimization problem described by the Lagrangian:

$$\mathcal{L}(k_{st}) = f_c - \lambda f_v \quad (1.65)$$

where  $\lambda$  ( $\text{mol mol}^{-1}$ ) is a Lagrange multiplier and represents the marginal water cost of plant carbon gain (Katul et al. 2010; Medlyn et al. 2011; Manoli et al. 2014) and  $f_c = f_c(k_{st})$  and  $f_v = f_v(k_{st})$  where both assimilation rate and transpiration rate are both dependent on the stomatal conductance  $k_{st}$  ( $\text{mol m}^{-2} \text{s}^{-1}$ ) (i.e.  $g_s$  (in plant-science) or  $h_{c,m}$  (in building-physics) or  $1/r_s$  where  $r_s$  is stomatal resistance). Cowan (1978) shows that optimal stomatal behaviour is at the minima of the Lagrangian:

$$\frac{\partial \mathcal{L}}{\partial k_{st}} = 0 \quad (1.66)$$

leading to the following constraint:

$$\lambda = \frac{\partial f_v}{\partial k_{st}} \frac{\partial k_{st}}{\partial f_c} \quad (1.67)$$

or simply:

$$\lambda = \frac{\partial f_v}{\partial f_c} \quad (1.68)$$

Following, these constraints, the stomatal conductance is can be determined with additional closure model for assimilation rate and transpiration rate. The assimilation rate  $f_c$  can be described from the perspective of photochemical reaction model and the Fickian diffusion model from the stomatal cavity.

The Farquhar model of photosynthesis describing the biochemical demand function is given as:

$$f_c = \frac{a_1 c_i}{a_2 + s c_a} \quad (1.69)$$

where  $c_i$  ( $\text{mol mol}^{-1}$ ) is the intercellular  $\text{CO}_2$  concentration,  $c_a$  ( $\text{mol mol}^{-1}$ ) is the ambient  $\text{CO}_2$  concentration, and  $a_1$  and  $a_2$  are parameters dependent on whether photosynthetic reaction rate is limited by light or Rubisco (Rubilose biphosphate (RuBP) carboxylase-oxygenase) (Farquhar et al. 1980; Katul et al. 2010) and  $s = 0.7$  is the constant representing long-term intercellular to ambient  $\text{CO}_2$  concentration ratio (Volpe et al. 2013). Note that we use a linearized model assuming  $c_p \ll c_i$  where  $c_p$  is the

CO<sub>2</sub> compensation point. As the photosynthesis can either be light-limited or Rubisco limited, the true assimilation rate  $f_c$  is given as:

$$f_c = \min(f_c^l, f_c^r) \quad (1.70)$$

where  $f_c^l$  is the light-limited assimilation rate and  $f_c^r$  is the Rubisco limited assimilation rate. Note that it is also possible to incorporate the dark (or night) respiration and in that case  $f_c = \min(f_c^l, f_c^r) - r_d$ , but is simplified in our study.

#### *Light-limited*

When the assimilation (or photosynthesis) rate is *light-limited*:

$$a_1(\mathbf{x}) = \alpha_p e_m Q_p = \gamma Q_p(\mathbf{x}) \quad (1.71)$$

and

$$a_2(\mathbf{x}) = 2c_p(\mathbf{x}) \quad (1.72)$$

where  $\alpha_p$  is the leaf absorptivity of photosynthetically active radiation (PAR),  $e_m$  is the maximum quantum efficiency of the leaf,  $\gamma = 0.015$  is the apparent quantum yield,  $Q_p$  (mol m<sup>-2</sup> s<sup>-1</sup>) is the flux of incoming PAR and  $c_p$  (mol mol<sup>-1</sup>) is the the CO<sub>2</sub> compensation point with:

$$c_p(\mathbf{x}) = \frac{K_c(\mathbf{x})}{2K_o(\mathbf{x})} C_{o,a} \frac{k_o}{k_c} \quad (1.73)$$

where  $k_c = 2.5$  s<sup>-1</sup> and  $k_o = 0.18k_c$  (Farquhar et al. 1980). Therefore, the light-limited assimilation rate is:

$$f_c^l(\mathbf{x}) = \frac{\gamma Q_p(\mathbf{x}) c_i(\mathbf{x})}{2c_p(\mathbf{x}) + s_{c_a}(\mathbf{x})} \quad (1.74)$$

#### *Rubisco-limited*

If the assimilation rate is *Rubisco-limited*:

$$a_1(\mathbf{x}) = V_{cmax}(\mathbf{x}) \quad (1.75)$$

and

$$a_2(\mathbf{x}) = K_c(\mathbf{x}) \left( 1 + \frac{C_{o,a}}{K_o(\mathbf{x})} \right) \quad (1.76)$$

where  $V_{cmax}$  is the maximum carboxylation capacity (referenced at 25 °C),  $K_c$  and  $K_o$  are Michaelis constant for CO<sub>2</sub> and O<sub>2</sub> inhibition (referenced at 25 °C), and  $C_{o,a} = 0.21$  mol mol<sup>-1</sup> is the oxygen concentration in the atmosphere. The maximum carboxylation capacity is given as:

$$V_{cmax}(\mathbf{x}) = V_{cmax,25} \frac{\exp\{0.088(T_l(\mathbf{x}) - 298.15)\}}{1 + \exp\{0.29(T_l(\mathbf{x}) - 314.15)\}} \quad (1.77)$$

and  $K_c$  and  $K_o$  are

$$K_c(\mathbf{x}) = K_{c,25} \exp \{ \gamma_c (T_l(\mathbf{x}) - 298.15) \} \quad (1.78)$$

$$K_o(\mathbf{x}) = K_{o,25} \exp \{ \gamma_o (T_l(\mathbf{x}) - 298.15) \} \quad (1.79)$$

where  $T_l$  (K) is the leaf temperature,  $V_{cmax,25} = 5.9 \times 10^{-5} \text{ mol m}^{-2} \text{ s}^{-1}$ ,  $\gamma_c = 0.074$ ,  $\gamma_o = 0.015$ ,  $K_{c,25} = 3 \times 10^{-3} \text{ mol mol}^{-1}$  and  $K_{o,25} = 0.3 \text{ mol mol}^{-1}$ . Therefore, the Rubisco-limited assimilation rate is:

$$f_c^r(\mathbf{x}) = \frac{V_{cmax}(\mathbf{x})c_i}{K_c(\mathbf{x}) \left( 1 + \frac{C_{o,a}}{K_o(\mathbf{x})} \right) + sc_a(\mathbf{x})} \quad (1.80)$$

The Fickian diffusion through stomata is given as:

$$f_c = k_{st} (c_a - c_i) \quad (1.81)$$

$$f_v = k_{st,v} \left( \frac{p_{v,i} - p_v}{p} \right) \quad (1.82)$$

where  $k_{st,v}$  ( $\text{mol m}^{-2} \text{ s}^{-1}$ ) is the stomatal conductance to water vapor:

$$k_{st,v} = a_c k_{st} \quad (1.83)$$

where  $a_c = 1.6$  is the relative diffusion of water vapor to  $\text{CO}_2$ . Furthermore,  $p_{v,i} = p_{v,sat}(T_l)$  (Pa) is the intercellular vapor pressure inside the stomatal cavity assumed to be at saturation at the leaf temperature  $T_l$ . Thus, equating Fickian  $\text{CO}_2$  flux to the Farquhar biochemical demand, we have:

$$f_c = \frac{a_1 c_i}{a_2 + sc_a} = k_{st} (c_a - c_i) \quad (1.84)$$

where  $c_i$  is the unknown. Rewriting, we get:

$$c_i = c_a \frac{a_2 + sc_a}{a_1/k_{st} + a_2 + sc_a} \quad (1.85)$$

and substituting  $c_i$  into the biochemical demand function, the assimilation rate is a closed-problem as:

$$f_c = \frac{k_{st} a_1 c_a}{a_1 + k_{st} (a_2 + sc_a)} \quad (1.86)$$

Thus, the stomatal conductance can be finally obtained from the minimizing the problem:

$$\frac{\partial \mathcal{L}}{\partial k_{st}} = \frac{\partial f_c}{\partial k_{st}} - \lambda \frac{\partial f_v}{\partial k_{st}} = 0 \quad (1.87)$$

which becomes:

$$\frac{\partial}{\partial k_{st}} \left[ \left( \frac{k_{st} a_1 c_a}{a_1 + k_{st} (a_2 + s c_a)} \right) - \lambda a_c k_{st} VPD \right] = 0 \quad (1.88)$$

where  $VPD = (p_{v,i} - p_v) / p$  (mol mol<sup>-1</sup>). The derivative becomes:

$$\frac{a_1^2 c_a}{[a_1 + k_{st} (a_2 + s c_a)]^2} - \lambda a_c VPD = 0 \quad (1.89)$$

Therefore, solving for  $k_{st}$  we obtain:

$$k_{st}(x) = \frac{a_1(x)}{a_2(x) + s c_a(x)} \left( -1 + \sqrt{\frac{c_a(x)}{a_c \lambda(\psi_l) VPD(x)}} \right) \quad (1.90)$$

where the marginal water use is empirically related to the leaf water potential  $\lambda = \lambda(\psi_l)$  (Katul et al. 2010; Manoli et al. 2014). Therefore, the stomatal response change to water availability is reflected through the change in leaf water potential  $\psi_l$ . Additionally, in literature it is known that stomata does not completely close during night allowing for respiration. Therefore, taking this into account:

$$k_{st}(x) = \frac{a_1(x)}{a_2(x) + s c_a(x)} \left( -1 + \sqrt{\frac{c_a(x)}{a_c \lambda(\psi_l) VPD(x)}} \right) + k_{st,n} \quad (1.91)$$

where  $k_{st,n}$  (mol m<sup>-2</sup> s<sup>-1</sup>) is the nocturnal stomatal conductance ( $k_{st,n} = 0.018$  mol m<sup>-2</sup> s<sup>-1</sup> (Manoli et al. 2014)). The intercellular CO<sub>2</sub> concentration simplifies to:

$$c_i = c_a \left( 1 - \sqrt{\frac{a \lambda VPD}{c_a}} \right) \quad (1.92)$$

and thus closing the (with the exception of  $\lambda$ ) the photosynthetic rate. So far, the stomatal conductance model is derived by neglecting the contribution of boundary layer conductance  $k_b$  (i.e.  $g_b$  (in plant-science), or inverse of boundary layer resistance  $r_b$ , assumed to be equivalent to aerodynamic resistance  $r_a$ ). Therefore, the effective stomatal conductance  $k_{st}^*$  is defined as:

$$k_{st}^* = \frac{k_{st} k_b}{k_{st} + k_b} \quad (1.93)$$

assuming the resistance are in series. Therefore, the plant fluxes into atmosphere become:

$$f_c = k_{st}^* f_c \quad (1.94)$$

$$f_v = k_{st,v}^* f_v \quad (1.95)$$



Furthermore, the fluxes in units  $\text{kg m}^{-2} \text{s}^{-1}$  can be simply determined as:

$$g_{c,leaf} = M_c f_c \quad (1.96)$$

$$g_{v,leaf} = M_v f_v \quad (1.97)$$

where  $M_c = 4.401 \times 10^{-2} \text{ kg mol}^{-1}$  and  $M_v = 1.8015 \times 10^{-2} \text{ kg mol}^{-1}$  are the molar mass of  $\text{CO}_2$  and water vapor, respectively.

### 1.3.5 Marginal water use

The marginal water use efficiency (WUE)  $\lambda$  or the cost-parameter for the cost of water lost from leaves. The marginal WUE should change over time depending on the water availability Manzoni et al. (2011). The marginal WUE is estimated from photosynthesis, transpiration and stomatal conductance measurement, obtained simply from the gradient of WUE:

$$WUE = \frac{f_c}{f_v} \quad (1.98)$$

The observations derive a marginal WUE as a function of leaf water potential  $\psi_L$ :

$$\lambda(\psi_L) = \lambda_{max}^* \frac{c_a}{c_a^*} \exp \left\{ -\beta \left( \langle \psi_L \rangle_{24h} - \psi_{L,max} \right)^2 \right\} \quad (1.99)$$

where  $\psi_L$  is assumed to vary slowly such that  $\langle \psi_L \rangle_{24h}$  is fixed within the secant iteration,  $\lambda_{max}^*$  is the marginal WUE under well-watered soil condition at reference  $\text{CO}_2$  concentration  $c_a^* = 400 \mu\text{mol mol}^{-1}$  or parts-per-million (ppm),  $\beta$  is the plant-specific sensitivity parameter (Huang et al. 2017).

### 1.3.6 Numerical method for determining leaf water potential

The water transport through the plant from soil to root, from root to xylem, through the xylem, and finally, from leaf stomata to air is a closed-problem once the leaf water potential is known. The leaf water potential is determined from the following constraint:

$$G_{v,leaf}(\psi_L) = G_{v,root}(\psi_L) \quad (1.100)$$

or as an optimization problem, it is defined as:

$$\arg \min_{\psi_L} \mathcal{G}(\psi_L) = \left| G_{v,leaf} - G_{v,root} \right| \quad (1.101)$$

As this is a non-linear closure problem (Manoli et al. 2014), a secant method is employed to iteratively converge to the leaf water potential. The  $j + 1^{\text{th}}$  leaf water potential estimate is determined as:

$$\psi_L^{j+1} = \psi_L^j - G(\psi_L^j) \frac{\psi_L^j - \psi_L^{j-1}}{G(\psi_L^j) - G(\psi_L^{j-1})} \quad (1.102)$$

where the initial estimate of  $\psi_L^{j=0} = 0$  MPa and  $\psi_L^{j=1} = -10$  MPa and with the additional constraint that  $-10 \leq \psi_L \leq 0$  MPa, enforcing that leaf water potential is negative and not larger than  $-10$  MPa (typically known to lower). The detailed solution strategy for determining for coupling all the models is detailed in next section.

### 1.3.7 Solution strategy for coupling

The numerical model for air domain, solid domains (soil, ground, building), the radiation model and the vegetation model is implemented into OpenFOAM. The solid and air domains are coupled at regular intervals  $t^m$  defined as exchange timesteps or air time steps (Saneinejad et al. 2014; Kubilay et al. 2018). The fluxes between air and solid domain consisting for thermal, moisture and radiative transfers are coupled at this step, chosen to be 10 min. At each  $t^m$ , the air domain is assumed to the quasi-steady and solving using steady-state RANS approach converged when residuals of  $\rho$ ,  $u$ ,  $h$ ,  $k$ ,  $\varepsilon$  are below threshold. During the steady-state computation, the leaf energy balance is evaluated periodically to correct the heat and mass fluxes,  $q_{sen,leaf}$  and  $g_{v,leaf}$ , respectively.

The algorithm of the air domain  $t^m \rightarrow t^{m+1}$  with  $\Delta t^m$  the air domain pseudo-timesteps of 10 min, is as follows:

1. Update the radiation fields in the air domain using  $q_{rad}$  from building surfaces and determined  $q_{r,lw}$  and  $q_{r,sw}$ .
2. Solve the energy balance at the leaf surface:
  - a) Determine the radiative flux  $q_{rad,leaf}$  using ??.
  - b) Calculate the stomatal and aerodynamic resistances  $r_a$  and  $r_s$  using ?? and ??, respectively. Note that  $r_s = (k_{st,v})^{-1}$  and  $\lambda(\psi_L)$  is constant. Therefore,  $r_s$  is only dependent on assimilation rate  $f_c$ , and the VPD.
  - c) Perform an initial estimate of leaf temperature  $T_{leaf} = T$ .
  - d) Calculate the saturated vapor pressure at the leaf surface  $p_{vsat,leaf} = f(T_{leaf})$ .
  - e) Calculate the latent heat flux  $q_{lat,leaf}$  using ??.
  - f) Correct the leaf temperature  $T_{leaf}$  using ??.
  - g) Repeat steps (d) to (f) until the leaf temperature has converged with a convergence criterion of  $10^{-8}$ .
3. Calculate all vegetation source terms  $s_\rho$ ,  $s_u$ ,  $s_T$ ,  $s_w$ ,  $s_k$  and  $s_\varepsilon$  using Eqs. ????????????

4. Solve for the steady-state flow field for  $t^{m+1}$ , ??-??.
5. Repeat steps (2) to (4) until residuals of ??-?? have reached the convergence limit of  $10^{-8}$ ,  $\delta f^{m+1} \leq \epsilon$

For every  $m$  exchange timesteps, the solid domains are solved using a transient approach with  $n$  adaptive solid timesteps (Janssen 2002; Kubilay et al. 2018). The solution from the air domain consisting of thermal and moisture fluxes are taken as boundary conditions for the solid domain equations. For each internal  $n$  iterations, the thermal and radiative fluxes from solid domain are corrected until converges. For each of  $n$  solid timesteps, the linearized heat and mass transport equation are solved using  $k$  Picard iterations. Finally, for each  $k$  Picard iteration, the root water uptake is determined through  $j$  secant iterations minimizing the cost function  $\mathcal{G}$ .

The algorithm of the solid domain  $t^m \leq t^n \leq t^{m+1}$ , for  $n \in 0, \dots, N$  with  $t^{n=0} = t^m$  and  $t^N = t^{m+1}$  such that  $\Delta t^n < \Delta t^m$ , is as follows:

1. Solve the linearized heat and mass transport transport equation using  $k$  Picard iteration such that  $t^n \leq t^{n,k} \leq t^{n+1}$  with  $k \in \{0, \dots, K\}$  where  $t^{n,k=0} = t^n$  and  $t^{n,k=K} = t^{n+1}$ .
  - (a) Determine marginal WUE  $\lambda (\langle \psi_L \rangle_{24h})$ . As  $\psi_L$  is assumed to be slowly varying,  $\lambda$  is constant in secant iteration.
  - (b) Determine the stomatal conductance  $k_{st}$ , constant in the secant iteration.
  - (c) Determine the assimilation rate  $f_c$  and transpiration rate  $f_v$ , constant in the secant iteration.
  - (d) Determine the net transpiration rate  $G_{v,leaf}$ .
  - (e) Determine the effective soil-root conductance  $k_{sr}^*$ , constant in the secant iteration.
  - (f) Solve for leaf water potential  $\psi_L^{n,k}$  of the  $k^{\text{th}}$  Picard iteration using  $j \in \{0, \dots, J\}$  secant iterations.
    - (a) Initial guess of leaf water potential,  $\psi_L^{j=0} = 0$  MPa,  $\psi_L^{j=1} = -10$  MPa.
    - (b) Calculate the effective xylem conductance  $k_x^*$ .
    - (c) Calculate root water potential  $\psi_R^j$ .
    - (d) Calculate the root uptake  $g_{v,root}$  and the net root uptake  $G_{v,root}$ .
    - (e) Determine the cost function  $\mathcal{G}$ .
    - (f) Correct the leaf water potential using secant method  $\psi_L^j \rightarrow \psi_L^{j+1}$ .
    - (g) Repeat till leaf water potential converged,  $\delta \psi_L \leq \epsilon$ .
  - (g) Calculate the sink in soil moisture due to root water uptake  $s_r$ .
  - (h) Solve linearized form of heat and mass equation using PCG until  $\delta p_c = \delta T = 10^{-2}$ , repeating steps before.

2. Use the final surface temperature  $T_s^N$  to update the radiation model updating  $q_{r,lw}$  fluxes from all surfaces.
3. Final surface temperature  $T_s^N$  and moisture fluxes  $g_v^N$  are boundary condition for the air domain for  $t^m \rightarrow t^{m+1}$ .

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