Supplemental Information:

In this session, we describe the major equations used in WIMOVAC.

1. Macroclimate

Actual macroclimate data may be input in runs of WIMOVAC, or WIMOVAC simulates a generalized macroclimate based on latitude and any climatic averages that can be provided. The macroclimate conditions (i.e. light, relative humidity, rainfall, and wind speed) for a given Julian date (D_j) and location are simulated separately. Date, time, and latitude (Ω) determine the solar declination (δ) and solar zenith (Θ) angles. For site dependent variables such as atmospheric transmittance (α) WIMOVAC provides an average value from the literature. The user may view this value and its source in the parameter file, and may input a more appropriate value as necessary. Direct (I_{dir}) and diffuse solar radiation (I_{diff}) above canopy may then be predicted (Norman, 1980) (Eqn.1)–(Eqn.5). Where air temperature is not available it follows the typical daily and seasonal cycles, slightly offset from the daily and seasonal peaks of radiation input (Spain & Keen, 1992b). In many biological situations, extremes of temperatures are more important than the mean of temperature (Wang, Vinocur & Altman, 2003). In WIMOVAC, temperature is simulated using three elements (Eqn.9), i.e. the daily mean temperature (Eqn.6), range (Eqn.7) and excursion (Eqn.8). The calculation of excursion allows an offset between the maximum incident solar radiation and the maximum temperature of simulated days, which reflects the local heat capacity of the surroundings (Eqn. 8).

$$\delta = -23.5 \cdot cos\left(\frac{360 \cdot (D_j + 10)}{365}\right) \qquad \text{Eqn 1.}$$

$$\cos(\theta) = \sin(\Omega) \cdot \sin(\delta) + \cos(\Omega) \cdot \cos(\delta) \cdot \cos(15 \cdot (t - t_{sn})) \qquad \text{Eqn 2.}$$

$$I_{dir} = I_s \cdot \alpha^{((P/P_o)/\cos(\theta))} \cos(\theta) \qquad \text{Eqn 3.}$$

$$I_{diff} = 0.5 \cdot I_s \cdot (1 - \alpha^{(P/P_o)/\cos(\theta)}) \cdot \cos(\theta) \qquad \text{Eqn 4.}$$

$$\cos\left(\frac{15 \cdot t_{len}}{2}\right) = -\tan(\Omega) * \tan(\delta) \qquad \text{Eqn 5.}$$

$$Mean = T_1 + T_2 \cdot \sin\left(2 \cdot \pi \cdot \frac{D_j - D_{start}}{365}\right) \qquad \text{Eqn 6.}$$

$$Range = T_3 + (T_4 - T_3) \cdot \sin\left(2 \cdot \pi \cdot \frac{D_j - D_{start}}{365}\right)$$

Eqn 7.

$$Excursion = \sin\left(2 \cdot \pi \cdot \frac{h_r - (h_{peak} - 6)}{24}\right)$$

Eqn 8.

$$T_{air} = Mean + Range \cdot Excursion$$

Eqn 9.

2. Leaf level photosynthesis and stomata conductance

The steady state biochemical model of C3 photosynthesis (Farquhar, von Caemmerer & Berry, 1980) is used in WIMOVAC to simulate the response of C3 leaf photosynthesis to changes in CO_2, light, temperature, relative humidity etc. In this model, the leaf level photosynthesis is limited by one of three biochemical processes, *i.e.* RuBISCO limited photosynthesis (Eqn 13), RuBP-regeneration limited photosynthesis (Eqn 14), and triose phosphate limited photosynthesis(Sharkey 1985) (Eqn 15). Under any particular atmospheric CO_2, O_2, light, humidity, and temperature conditions, the slowest of these three processes limits the rate of leaf photosynthesis (Eqn 12). The value of intercellular $[CO_2]$ (C_i) is governed by the interaction of A as given by eqn. 12 and A as limited by stomatal conductance (g_s). Stomatal conductance for C3 plant is predicted from A, relative humidity and surface CO_2 concentration in a modified version (Eqn. 18-21) of the Ball, Woodrow & Berry (1987). C_i is solved by iteratively seeking a matching A from the leaf photosynthesis (Eqn. 12) and stomatal conductance equations (Eqn. 24) using the Newton-Raphson procedure (Press, Flannery, Teukolsly & Vetterling, 1986) as implemented by Humphries and Long (Humphries & Long, 1995). Eqns 10-11 were used to predict the potential rate of electron transport governing the RuBP-limited rate of photosynthesis (Evans & Farquhar, 1991). For C4 photosynthesis, the CO_2 concentration in mesophyll cell (C_m) was calculated through multiplying air CO_2 concentration (C_a) by the ratio of C_m to C_a and the ratio of C_m to C_a can be input from the parameter file. The equations in Von Caemmerer et al. (2000) (Eqn. 24– Eqn. 31) are used to calculate C4 photosynthesis rate under a certain C_m and light environment.

$$J = \frac{I_2 + J_{max} - \sqrt{(I_2 + J_{max})^2 - 4\Theta I_2 J_{max}}}{2\Theta}$$

Eqn 10

$$I_2 = \frac{I_0 \times (1 - S_p)(1 - r)}{2}$$

Eqn 11

$$A = (1 - \frac{\Gamma^*}{C_i}) \min(W_c, W_j, W_p) - R_d$$

Eqn 12

$$W_c = \frac{V_{c\max} \cdot C_i}{C_i + K_c [1 + O_i / K_o]}$$

Eqn 13

$$W_j = \frac{J\, C_i}{4C_i + 8\Gamma^*}$$

Eqn 14

$$W_p = \frac{3 \cdot T_u}{1 - \Gamma^* / C_i}$$

Eqn 15

$$C_i = 0.7C_a \cdot [(1.6740 - 6.1294 \cdot 10^{-2}T + 1.1688 \cdot 10^{-3}T^2 - 8.8741 \cdot 10^{-6}T^3)/0.73547]$$
$$At\, 25^o C, C_i = 0.7C_a$$

Eqn. 16

$$O_i = 210[(4.7000 \cdot 10^{-2} - 1.3087 \cdot 10^{-3}T + 2.5603 \cdot 10^{-5}T^2 - 2.1441 \cdot 10^{-7}T^3)/2.6934 \cdot 10^{-2}]$$
$$At\, 25^o C, O_i = O_a$$

Eqn. 17

$$g_s = \frac{-b + \sqrt{b^2 + 4ac}}{2a}$$

Eqn. 18

$$a = C_s$$

Eqn. 19

$$b = -(g_0 \cdot C_s + 100g_1 \cdot A - C_s \cdot g_b)$$

Eqn. 20

$$c = -(100g_1 \cdot A \cdot RH \cdot \frac{e_{air}}{e_{leaf}} \cdot g_b + g_0 \cdot C_s \cdot g_b)$$

Eqn. 21

$$C_s = C_a - \frac{A}{g_b}$$

Eqn. 22

$$C_i = C_s - \frac{A}{g_s}$$

Eqn. 23

$$V_p = \frac{C_m \cdot V_{p\max}}{C_m + K_p}$$

Eqn 24

$$A_{c1} = V_p - R_m + g_L \cdot C_m \qquad\qquad \text{Eqn 25}$$

$$A_{c2} = V_{c\max} - R_d \qquad\qquad \text{Eqn 26}$$

$$A_{j1} = \frac{(1-x) \cdot J}{3} - R_d \qquad\qquad \text{Eqn.27}$$

$$A_{j2} = \frac{x \cdot J}{2} - R_m + g_L \cdot C_m \qquad\qquad \text{Eqn. 28}$$

$$A_j = \min\left(A_{j1}, A_{j2}\right) \qquad\qquad \text{Eqn29}$$

$$A_c = \min(A_{c1}, A_{c2}) \qquad\qquad \text{Eqn. 30}$$

$$A = \min(A_c, A_j) \qquad\qquad \text{Eqn. 31}$$

Canopy level photosynthesis

WIMOVAC differentiates sunlit and shaded leaf area following Norman (1980) and Forseth and Norman (1991). The leaf area of sunlit and shaded leaves and the mean irradiances of these two populations are calculated dynamically (Eqn.32)–(Eqn.35). Sunlit leaves are assumed to receive direct (I_{dir}) and diffuse (I_{diff}) solar radiation (Eqn.36-38) while shaded leaves receive diffuse and scattered light (I_{scat}) from other leaves in the canopy (Eqn.36-38). The total canopy photosynthesis is the sum of the photosynthesis at both the sunlit and shaded leaves (Eqn.40). In most natural canopies, leaves assume a range of orientations in which they may be predominantly horizontal (planophile), vertical (erectophile) or an intermediate mixture. A single parameter, χ (the ratio of the horizontal projection of the ellipsoid to the vertical) is used in WIMOVAC to describe the distribution and calculate the expected canopy extinction coefficient (k, Eqn.32). Total canopy assimilation, transpiration and conductance are obtained by integrating over individual leaf classes (Eqn.36)–(Eqn.40).

$$k = \frac{\sqrt{\chi^2 + \tan^2(\theta)} \cdot \cos(\theta)}{\chi + 1.744 \cdot [\chi + 1.183]^{-0.733}} \qquad\qquad \text{Eqn 32}$$

$$F_{sun} = \frac{[1 - e^{(-k \cdot F_{canopy}/\cos(\theta))}] \cdot \cos(\theta)}{k} \qquad\qquad \text{Eqn 33}$$

$$F_{shade} = F_{canopy} - F_{sun} \qquad\qquad \text{Eqn 34}$$

$$F_{canopy} = F_{sun} + F_{shade} \qquad \text{Eqn 35}$$

$$I_{sun} = I_{dir} \cdot k / \cos(\theta)) + I_{shade} \qquad \text{Eqn 36}$$

$$I_{shade} = I_{diff} \cdot e^{(-0.5 \cdot F_{canopy}^{0.7})} + I_{scat} \qquad \text{Eqn 37}$$

$$I_{scat} = 0.07 \cdot I_{dir} \cdot (1.1 - 0.1 \cdot F_{canopy}) \cdot e^{-(cos(\theta))} \qquad \text{Eqn 38}$$

$$I_{total} = I_{dir} + I_{dif} \qquad \text{Eqn 39}$$

$$A_c = (A_{c,sun} \cdot F_{sun}) + (A_{c,shade} \cdot F_{shade}) \qquad \text{Eqn 40}$$

Growth, partitioning and allocation

Partitioning fundamentally determines the efficiency with which both assimilated carbon (C) and nitrogen (N) are used (Farrar & Williams, 1991). Consequently, photosynthetic rates are often not directly correlated with growth rates (Mooney, Drake, Luxmoore, Oechel & Pitelka, 1991). For example, subtle differences in resource use such as maintenance respiration can lead to significant differences in productivity if averaged over an entire growing season, even if photosynthesis and water use are the same (Farrar & Williams, 1991). Resource allocation patterns are therefore critical in determining the relative growth rate, ultimate plant size and reproductive yields of plants. Changing patterns of allocation may also be one of the most significant factors in determining how plants respond and acclimate to different environments. This is because plants respond to environments differently at different developmental stages.

Although there is little mechanistic basis for using a partitioning calendar approach, its simplicity and ability to relate measurable partitioning coefficients, based upon experimentally determined dry weights, to identifiable developmental stages has led to its wide spread adoption (Hodges & French, (1985). , Jones, Hoogenboom, Porter, Boote, Batchelor, Hunt, Wilkens, Singh, Gijsman & Ritchie, 2003, Reynolds, Acock, Dougherty & Tenhunen, 1989). In WIMOVAC, the partitioning calendar is determined using thermal time, which is obtained by multiplying the average temperature over a threshold with the duration over which this temperature applies. A table of partitioning coefficients is associated with each stage. For each developmental stage, the table describes the fraction of available carbon allocated to each of the plant structural pools, *i.e.* leaf, stem, structural root, fine root, storage, pod, and seed at that stage. The partitioning coefficients in each table were determined experimentally. By varying this coefficient (-1

to 1), WIMVOAC simulates the dynamic source/sink demands during plant development. The total C available for growth during a given developmental stage is the sum of net photosynthetic assimilation and the remobilized carbohydrate from storage root/shoot (Eqn.41, 42). The new leaf area, stem or root length is predicted based on allocated carbon resources for each tissue (Eqn.43)–(Eqn.47) and the specific leaf area, specific stem length, and specific root length respectively (Eqn.48)–(Eqn.51). New leaf growth is assumed to occur uniformly at different height of the canopy. New stem growth is associated with an increase in canopy height.

$$A_{stroot} = abs\left(\omega_{stroot} \cdot k_{stroot}\right) ; \quad k_{stroot} < 0 \qquad \text{Eqn 41}$$

$$A_{total} = A_c + A_{seed} + A_{stroot} \qquad \text{Eqn 41}$$

$$\omega_{leaf} = \omega_{leaf} + \left(A_{total} \cdot k_{leaf}\right) \qquad \text{Eqn 43}$$

$$\omega_{stem} = \omega_{stem} + \left(A_{total} \cdot k_{stem}\right) \qquad \text{Eqn 44}$$

$$\omega_{sroot} = \omega_{sroot} + \left(A_{total} \cdot k_{sroot}\right) \qquad \text{Eqn 45}$$

$$\omega_{stroot} = \omega_{stroot} + \left(A_{total} \cdot k_{stroot}\right) \qquad \text{Eqn 46}$$

$$\omega_{froot} = \omega_{leaf} + \left(A_{total} \cdot k_{froot}\right) \qquad \text{Eqn 47}$$

$$\Delta F_{canopy} = \frac{\omega_{leaf}}{Sp_{leaf}} \qquad \text{Eqn 48}$$

$$\Delta L_{stem} = \frac{\omega_{stem}}{Sp_{stem}} \qquad \text{Eqn 49}$$

$$\Delta L_{sroot} = \frac{\omega_{root}}{Sp_{sroot}} \qquad \text{Eqn 50}$$

$$\Delta L_{froot} = \frac{\omega_{froot}}{Sp_{froot}} \qquad \text{Eqn 51}$$

Respiration

WIMOVAC simulates respiration (R_{total}) following Penning de Vries (1972). In this approach, the fraction of gross photosynthesis associated with growth respiration is assumed as constant but the respiratory cost of maintaining plant structures varies depending on the tissue type (Eqn 52). Temperature is assumed to influence maintenance respiration via a typical Q10 response following Spain and Keen (1992).

$$R_{total} = \left(a \cdot A_{gross}\right) + \left(b_{leaf} \cdot \omega_{leaf}\right) + \left(b_{stem} \cdot \omega_{stem}\right) + \left(b_{root} \cdot \omega_{root}\right)$$

Eqn 52

References:

Evans J.H. & Farquhar G.D. (1991) Modelling canopy photosynthesis from the biochemistry of C3 chloroplast. In Boote KJ and Loomis RS (eds), Modelling crop photosynthesis-from biochemistry to canopy, pp1-15. Crop science society of America, Madison.

Farquhar G.D., von Caemmerer S. & Berry J.A. (1980) A biochemical model of photosynthetic CO_2 assimilation in leaves of C_3 species. *Planta*, **149**, 78-90.

Farrar J.F. & Williams M.L. (1991) The effects of increased CO2 and temperature on carbon partitioning, source-sink relations and respiration. *Plant Cell and Environment* **14**, 819-830.

Forseth I. & Norman J. (1991) Photosynthesis and Productivity Research in a Changing Environment. In: *Modeling of solar irradiance, leaf energy budget, and canopy photosynthesis.*, pp. 207–219. Chapman & Hall, London.

Hodges H.W. & French V. ((1985).) SOYPHEN: Soybean growth stages modeled from temperature, day length and water availability. *Journal of Agronomy* **77**, 500-505.

Humphries S.W. & Long S.P. (1995) WIMOVAC: a software package for modelling the dynamics of plant leaf and canopy photosynthesis. *Computer Application in the Biosciences*, **11**, 361-371.

Jones J.W., Hoogenboom G., Porter C.H., Boote K.J., Batchelor W.D., Hunt L.A., Wilkens P.W., Singh U., Gijsman A.J. & Ritchie J.T. (2003) The DSSAT cropping system model. *European Journal of Agronomy*, **18**, 235-265.

Mooney H.A., Drake B.G., Luxmoore R.J., Oechel W.C. & Pitelka L.F. (1991) Predicting ecosystem responses to elevated CO_2 concentrations. . *Bioscience*, **41**, 96-104.

Norman J.M. (1980) Predicting Photosynthesis for Ecosystem Models. In: *Interfacing leaf and canopy light interception models* (ed J.D.J. Hesketh, J. W.), pp. 49-67. CRC Press, Boca Raton, Florida.

Penning de Vries F.W.T. (1972) Respiration and growth. In: *Crop processes in controlled environments.* (eds Rees AR & H.D. Cockshull KE, Hurd RJ, eds.), pp. 327-347. Academic Press, London.

Press W.H., Flannery B.P., Teukolsly S.A. & Vetterling W.T. (1986) Numerical recipes: The art of scientific computing. Cambridge University Press, Cambridge.

Reynolds J.F., Acock B., Dougherty R.S. & Tenhunen J.D. (1989) A modular structure for plant growth simulation models. In Biomass production by fast-growing trees (ed. J. J. Landsberg), pp. 123-134. Kluwer Academic Publishers, Boston.

Sharkey   T.D. (1985) O_2 insensitive photosynthesis in C_3 plants. *Plant Physiology*, **78**, 71-75.

Spain J.D. & Keen R.D. (1992a) Temperature and biological activity. In: *Computer simulation in biology.* Wiley-Liss, New York.

Spain J.D. & Keen R.E. (1992b) Temperature and biological activity. In Computer simulation in biology (ed. R. E. Keen and J. D. Spain), pp. 183-200. Wiley-Liss, New York.

Wang W.X., Vinocur B. & Altman A. (2003) Plant responses to drought, salinity and extreme temperatures: towards genetic engineering for stress tolerance. *Planta*, **218**, 1-14.