

(From correspondence with co-author Junming Wang, deriving a semi-mechanistic model of pecan water-use efficiency that was incorporated into a manuscript accepted recently:

A. Andales, J. Wang, T. W. Sammis, J. G. Mexal, L. J. Simmons, D. R. Miller, and V. P. Gutschick. 2006. A model of pecan tree growth for the management of pruning and irrigation. *Agricultural Water Management* 84: 77-88.)

Hi, Junming,

This problem, explaining WUE in terms of gross meteorological observables, but using a mechanistic basis for the form of the regression relation, is tricky!

To get a mechanistic basis, I have to turn to the leaf-level expression,

$$WUE = \frac{A}{E} = \frac{g_s'(C_a - C_i)}{g_s(e_i - e_a)} = \frac{0.62C_a(1 - C_i/C_a)}{D_{La}}$$

The ready observables include the air-to-air VPD,  $D_{aa}$ , but not the leaf-to-air VPD,  $D_{La}$ , nor the  $C_i/C_a$  ratio.

You tested one idea I had, that VPD (that is,  $D_{aa}$ ) also affects  $C_i/C_a$ , which makes WUE a power function like  $1/D_{aa}^{1.5}$  or the more complex function I derived by using the Leuning model of stomatal control combined with a simple resistance model. That added only a little explanatory power;  $r^2$  went from 0.715 to 0.74.

The high correlation ( $r^2 = 0.84$ ) with  $1/(D_{aa} * Solar^2)$  implied that Solar is related to something like leaf temperature, which affects  $D_{La}$ . I theorized that high Solar means higher leaf temperatures (all else constant), because leaf conductance does not change much with higher PPFD (photosynthetic photon flux density, proportional to Solar, one may think), while the heat load increases. Today I realized that this is a poor explanation. From month to month, Solar varies because the solar elevation varies, not the intensity of the direct solar beam. In a simple but reasonably accurate model of light interception, a change in canopy light interception (a change in Solar, that is) comes from a change in the fraction of leaves illuminated, but the average light intensity (PPFD) on illuminated leaves does NOT change.

There is a more subtle effect of leaf temperature: because saturated vapor pressure rises with temperature at a different rate than photosynthetic rate (A) rises, the stomatal conductance, which is linked tightly to A, changes with leaf temperature, even at constant VPD. First, to see if this is a reasonable lead, I had to show that, in the field data, there is a correlation of  $1/Solar^2$  with a plausible function of air temperature related to WUE. I chose a form  $\exp(-0.03 * T_{air})$ , based on my intuition about the difference in scaling of A and  $e_{sat}$  with temperature. Yes, there is a strong correlation, with  $r^2 = 0.72$ . Next, I ran simulations at the leaf level with constant  $D_{aa}$  but varied leaf T. There is a major drop of WUE with increasing leaf T,  $T_L$ . There is a chain of causality, but the final effect is that  $C_i/C_a$  rises at high  $T_L$  and WUE drops.

I now propose that the correlation of WUE should be with  $D_{aa}$  and air T, and possibly windspeed, u (which affects boundary-layer conductance, thereby affecting surface humidity and stomatal conductance). That is, I would replace Solar with a function of  $T_{air}$  such as I proposed. The challenge now is to generate a mechanistic form for WUE as a function of  $D_{aa}$ ,  $T_{air}$ , and possibly u. I don't have an answer yet, but we must start by factoring WUE:

$$WUE = \frac{0.62C_a(1 - C_i/C_a)}{D_{La}} = \frac{0.62C_a}{D_{aa}} \left( \frac{D_{aa}}{D_{La}} \right) \left( 1 - \frac{C_i}{C_a} \right)$$

We need to formulate the behavior of the last two terms in large parentheses as functions of  $D_{aa}$ ,  $T_{air}$ , and  $u$ ...without using a gigantic model. This is where I am stuck right now, but I will keep thinking. There are some clues. The term  $(D_{aa}/D_{La})$  should increase somewhat with temperature, in a form I will try to work out, because hotter leaves have higher  $A$  --> higher  $g_s$  --> lower  $T_L - T_a$  (leaf cooling). The last term, in my simulations, decreases strongly with  $T_L$  (hence, with  $T_{air}$ ) at constant  $D_{aa}$ , because higher  $T_L$  --> higher  $g_s$  --> higher surface humidity and there is a positive feedback loop to higher  $g_s$ . At constant photosynthetic capacity (constant mesophyll conductance,  $g_m$ , in my simple resistance model), higher  $g_s$  --> higher  $C_i/C_a$ . The effect is moderated, because  $g_m$  also increases with  $T_L$ , but not as fast as does  $g_s$ . There are many other links, but we can't make the model too complicated.

In the end, we have to decide two things about the more mechanistically-based empirical form for WUE: 1) what functional form should the expression for WUE take? 2) are we willing to specify the numerical values of any coefficients in this expression, claiming that they are set by physiology or physics? If we just add adjustable coefficients, the gain in  $r^2$  must be very large to justify the giving up of a part of the mechanistic view.

It might be useful if I give you my combined model of photosynthesis, stomatal control, and energy balance so that you can play with the simulations. I will need to explain the meaning of some inputs, as well as some correlations among inputs (e.g., sky radiative temperature is linked to air temperature and, less so, to humidity).

Cheers,  
Vince

Some late-breaking news:

I just fit WUE in your spreadsheet to the form

$$WUE = \text{constant} * (1/D_{aa}) * \exp(-0.03 * T_{air})$$

I obtained an  $r^2$  of 0.944! This is so good that we might try simulations with the leaf model to see if the exponent 0.03 is stable, for different kinds of leaves, etc. (different photosynthetic capacities, etc.). To keep a mechanistic 'edge', we might want to show that  $C_i/C_a$  follows this last functional form.

What it looks like is that there is an intrinsic effect of temperature on WUE, over and above the correlation with  $D_{aa}$ , and that it has to do with the different pacing of the temperature dependences of water-vapor pressure and photosynthetic rate.

