

## Improved methods for calculating WUE and Transpiration in PnET. Mark E. Kubiske, USFS, NRS, Rhinelander, WI

PnET is ultimately a hydrologic model so the plant-soil hydrologic relationship is critical. However, in the present model, the plant side of that relationship depends almost entirely upon an user-supplied, variable (spec.WUEconst) that is, essentially, an arbitrary fudge-factor to make the transpiration values seem reasonable. Blegh!!!

The method presented here is rooted in the physics governing CO<sub>2</sub> and H<sub>2</sub>O vapor diffusion between plant and atmosphere, and ultimately the physics translating H<sub>2</sub>O vapor lost to volume of ground water extracted. It involves no input variables other than those already used by PnET that are directly related to the physiological mechanisms of photosynthesis and transpiration.

This new expression for WUE (we'll call it WUE<sub>MEK</sub> – I've always wanted to have a variable named after me) is a pure mass-flux ratio. It is determined from temperature and the diffusion gradients of CO<sub>2</sub> and H<sub>2</sub>O vapor that PnET already uses. It is not constrained by conductance; however, when transpiration is calculated as NetPsn / WUE<sub>MEK</sub>, the transpiration rate will be constrained by conductance because NetPsn is so constrained.

All equations and constants are from the *Handbook of Chemistry and Physics*.

### Theory

According to Fick's Law, the flux of any substance ( $J$ , in mole cm<sup>-2</sup> s<sup>-1</sup>) is equal to the concentration gradient ( $\partial c / \partial x$ ), where  $c$  is the concentration in mol cm<sup>-3</sup> and  $x$  is the diffusion path in cm, times the diffusivity ( $D$ , in cm<sup>2</sup> s<sup>-1</sup>) of the gas in air:

$$J = D \left( \partial c / \partial x \right)$$

Translated into finite form:

$$J = D \left( \Delta c / x \right) \quad \text{Equation 1}$$

Mechanistically, the diffusion gradient for CO<sub>2</sub> into leaves is the concentration difference (Ca-Ci) in  $\mu\text{mol mol}^{-1}$ . The diffusivity of CO<sub>2</sub> in air is  $D = 0.139 \text{ cm}^2 \text{ s}^{-1}$

The diffusion gradient for H<sub>2</sub>O vapor is the pressure difference VPD in kPa. The diffusivity of H<sub>2</sub>O vapor in air is  $D = 0.239 \text{ cm}^2 \text{ s}^{-1}$

Given the units for  $J$  (mole cm<sup>-2</sup> s<sup>-1</sup>) we need to convert the CO<sub>2</sub> concentration difference and H<sub>2</sub>O VPD into units of *mole CO<sub>2</sub> per cm<sup>3</sup> of air*, and *mole H<sub>2</sub>O per cm<sup>3</sup> of air*, respectively. To make these conversions, we're going to apply the Universal Gas Law:

$$PV = nRT \quad \text{Equation 2}$$

Where  $P$  is pressure (kPa),  $V$  is volume (cm<sup>3</sup>),  $n$  is number of moles,  $R$  is the universal gas constant, and  $T$  is temperature (K). In the appropriate units, the value of  $R$  is:

$$R = 8314.47 \frac{\text{kPa cm}^3}{\text{mol K}}$$

**Mass flux density of CO<sub>2</sub>:** Based on the units described above, we need to convert (Ca-Ci) from  $\mu\text{mol CO}_2 \text{ per mol air}$  to  $\text{mol CO}_2 \text{ per cm}^3 \text{ air}$ .

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Apply the universal gas law to convert 1 mol of air into  $\text{cm}^3$  of air. Assume 1 atm of pressure (101.3 kPa) -- this assumption is necessary because PnET does not otherwise make use of atmospheric pressure. *(To improve the accuracy of the modeled transpiration, a user input variable for elevation could be employed)*. The temperature used in the calculations will be the minimum temperature that was used to calculate VPD; as used by PnET this variable is  $t_{min}$ . Thus:

$$V_{air} = \frac{nRT}{P} = \frac{1 \text{ mol air} \cdot 8314.47 \frac{\text{kPa cm}^3}{\text{mol K}} \cdot (t_{min} + 273 \text{ K})}{101.3 \text{ kPa}}$$

The concentration difference for  $\text{CO}_2$  from Equation 1, and with the conversion of  $\mu\text{mol CO}_2$  to mol:

$$\Delta c \frac{\text{mol CO}_2}{\text{cm}^3 \text{ air}} = \left( C_a - C_i \frac{\mu\text{mol CO}_2}{V_{air} \text{ cm}^3} \right) \cdot 10^{-6} \frac{\text{mol}}{\mu\text{mol}}$$

And mass flux of  $\text{CO}_2$  is:

$$J_{CO_2} \text{ mol/cm}^2/\text{s} = D \cdot \left( \frac{\Delta c}{x} \right) = 0.139 \frac{\text{cm}^2}{\text{s}} \cdot \left[ \left( \frac{C_a - C_i \mu\text{mol CO}_2}{V_{air} \text{ cm}^3} \right) \cdot 10^{-6} \frac{\text{mol}}{\mu\text{mol}} \right] / x \text{ cm}$$

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**Mass flux density of H<sub>2</sub>O vapor:** Again, based on the units described above, the pressure gradient VPD needs to be converted into mol H<sub>2</sub>O vapor per cm<sup>3</sup> of air. So, in any volume of air, the partial pressure deficit of H<sub>2</sub>O is 1.3 kPa. Thus, the concentration difference, in moles of H<sub>2</sub>O per volume of air are:

$$\Delta c \frac{\text{mol H}_2\text{O}}{\text{cm}^3 \text{ air}} = \frac{n_{\text{H}_2\text{O}}}{V} = \frac{P}{RT} = \frac{\text{VPD kPa}}{8.314.47 \frac{\text{kPa cm}^3}{\text{mol K}} \cdot (t_{\text{min}} + 273 \text{ K})}$$

And mass flux of H<sub>2</sub>O is:

$$J_{\text{H}_2\text{O}} \text{ mol/cm}^2/\text{s} = D \cdot \left( \frac{\Delta c}{x} \right) = 0.239 \frac{\text{cm}^2}{\text{s}} \cdot \left[ \frac{\text{VPD kPa}}{8.314.47 \frac{\text{kPa cm}^3}{\text{mol K}} \cdot (t_{\text{min}} + 273 \text{ K})} \right] / x \text{ cm}$$

**WUE<sub>MEK</sub>:** Photosynthetic water use efficiency is defined as:

$$WUE_{\text{MEK}} = \frac{J_{\text{CO}_2}}{J_{\text{H}_2\text{O}}}$$

Note that from the equations above for mass flux density, length of the diffusion path,  $x$ , cancel.

### **Transpiration Rate:**

The usual method of calculating Transpiration from PnET is:

$$E_{\text{H}_2\text{O}} = \frac{\text{Photosynthesis rate}}{WUE}$$

In PnET,  $\text{NetPsn}$  is in g CO<sub>2</sub>/m<sup>2</sup> ground area/day.

WUE<sub>MEK</sub> is expressed as mol CO<sub>2</sub> per mol H<sub>2</sub>O, which is easily converted to grams using the gram-molecular weights:

$$WUE_{\text{MEK}} = \left( \frac{J_{\text{CO}_2}}{J_{\text{H}_2\text{O}}} \right) \left( \frac{44}{18} \right)$$

So Transpiration rate is:

$$E_{\text{H}_2\text{O}} \text{ g H}_2\text{O/m}^2/\text{day} = \frac{\text{NetPsn g CO}_2/\text{m}^2/\text{day}}{WUE_{\text{MEK}} \text{ g CO}_2/\text{g H}_2\text{O}}$$

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The transpiration rate expressed by PnET is (I'll just refer to the variable as  $TR$ ) mm H<sub>2</sub>O/month.

The units for  $E_{H_2O}$  above are g H<sub>2</sub>O/m<sup>2</sup>/day and are easily converted to mm/month. Convert g of H<sub>2</sub>O vapor into mm<sup>3</sup> of liquid water: because mass is conserved, 1 g of H<sub>2</sub>O vapor = 1 g of liquid water, and 1 g liquid H<sub>2</sub>O occupies 1 cm<sup>3</sup>.

The other needed conversions are: cm<sup>3</sup> H<sub>2</sub>O to mm<sup>3</sup>  
m<sup>2</sup> ground area to mm<sup>2</sup>  
day to month

$$TR \frac{\text{mm}}{\text{mo}} = E_{H_2O} \frac{\text{cm}^3 \text{ H}_2\text{O}}{\text{m}^2 \text{ day}} \cdot \frac{1000 \text{ mm}^3}{\text{cm}^3} \cdot \frac{\text{m}^2}{1,000,000 \text{ mm}^2} \cdot \frac{30 \text{ day}}{\text{mo}}$$

Combining all the conversion factors, including that for mol into g, into a single constant, a final expression for transpiration rate can be:

$$TR = 0.01227 \cdot \left( \frac{NetPsn}{J_{CO_2}/J_{H_2O}} \right)$$

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