Integrating Information on ‘Biosphere Breathing’ from Chloroplast to the Globe

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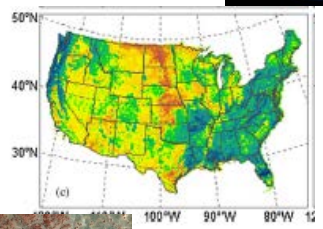
Outline

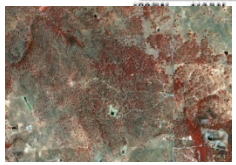
- Overview on Principles of Leaf-Canopy Scaling and Integration Concepts
- Show Tests of Such Models over Multiple Time Scales
- Use the CANVEG Model to Ask Ecophysiological and Micrometeorological Questions Relating to Trace Gas Fluxes

Spatial Scales of Inquiry:
Span 13-14 orders of Magnitude

Globe: 10,000 km (10^7 m)

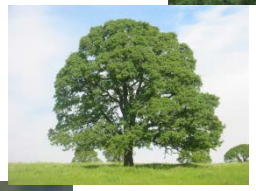


Continent: 1000 km (10^6 m)



Landscape: 1-100 km

Canopy: 100-1000 m



Plant: 1-10 m

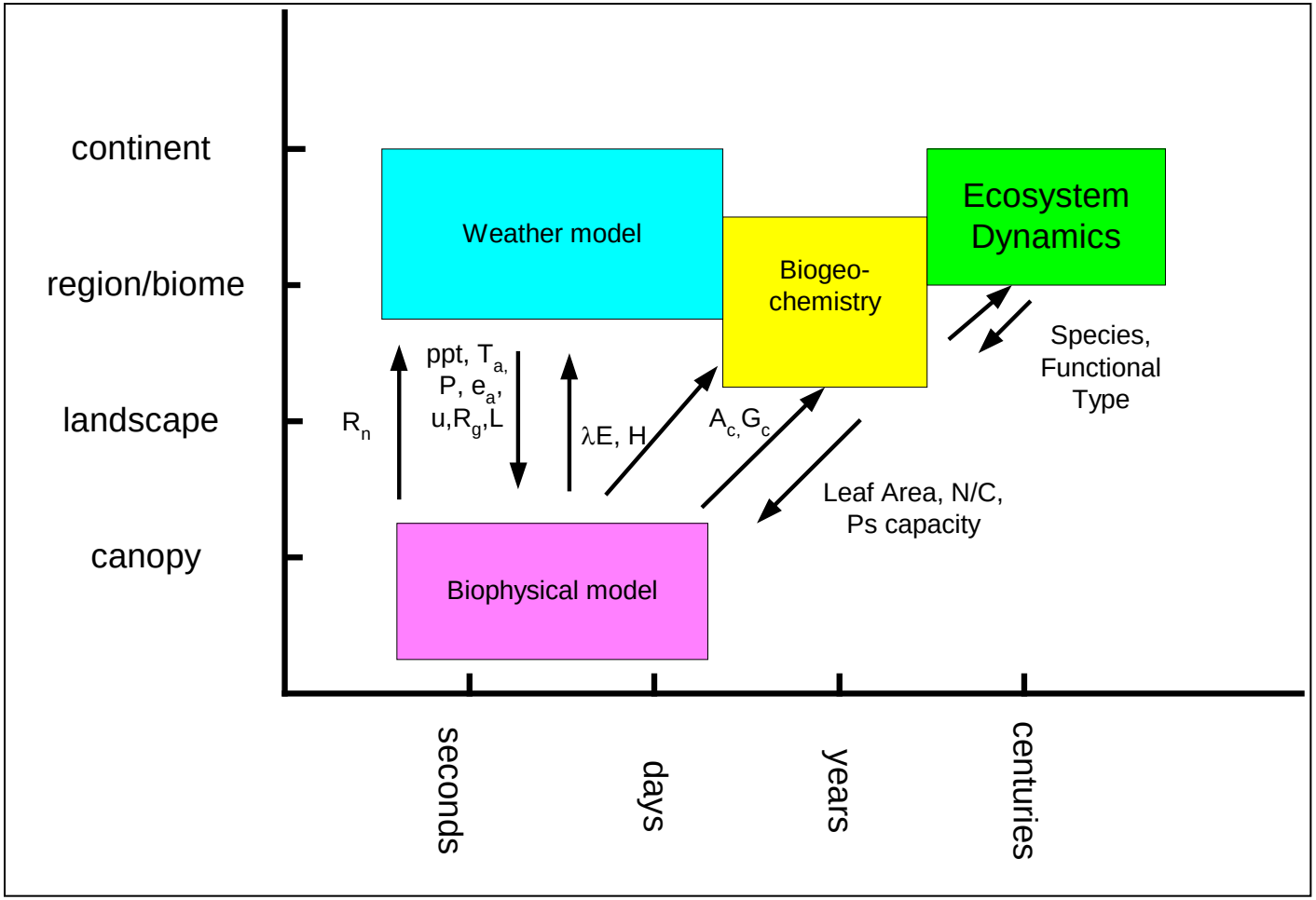
Leaf: 0.01-0.1 m

Stomata: 10^{-5} m

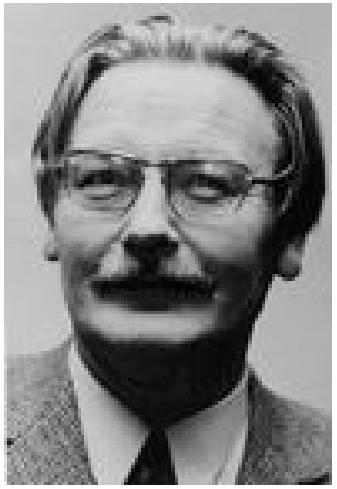
Bacteria/Chloroplast: 10^{-6} m

The Breathing of an Ecosystem is Defined by the Sum of an Array of Coupled, Non-Linear, Biophysical Processes that Operate across a Hierarchy/Spectrum of Time and Space Scales

Processes and Linkages: Roles of Time and Space Scales



Biophysical Modeling, Circa 1969



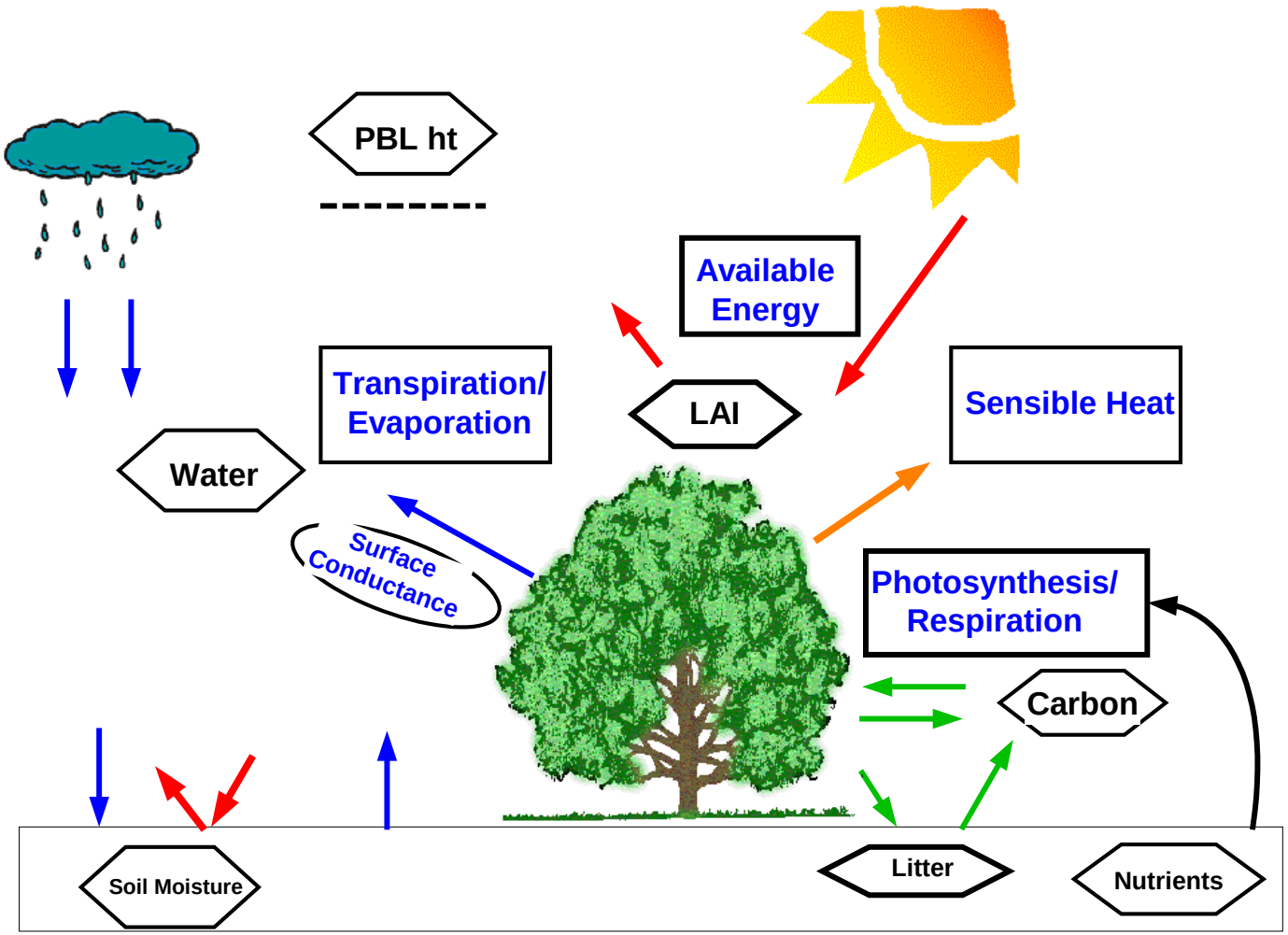
Cornelius T. deWit

‘Seven-stage simulation models by means of which ecosystems may be explained on basis of the molecular sciences are impossible large and detailed and it is naïve to pursue their construction’

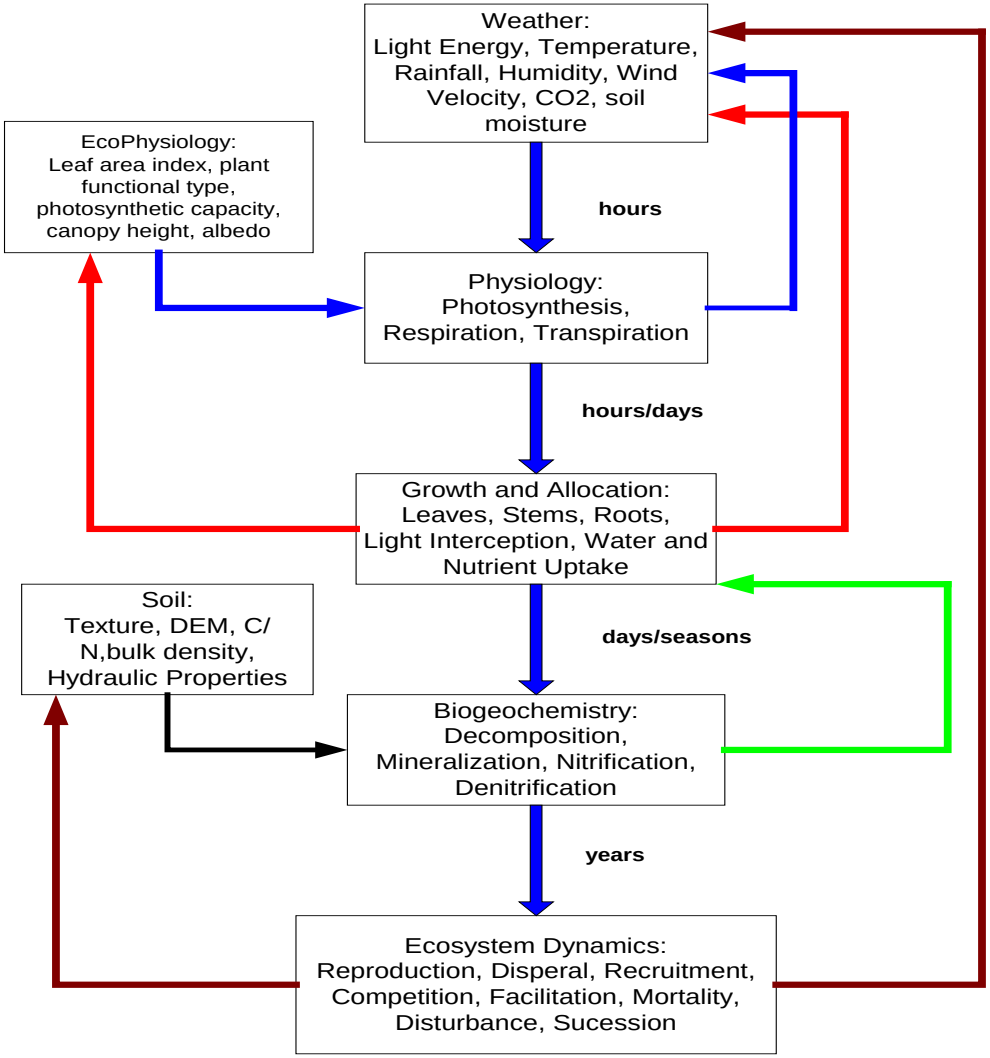
All models are wrong; some models are useful

Attributed to George Box, statistician

System Complexity:
Interconnection of Key Ecosystem Processes



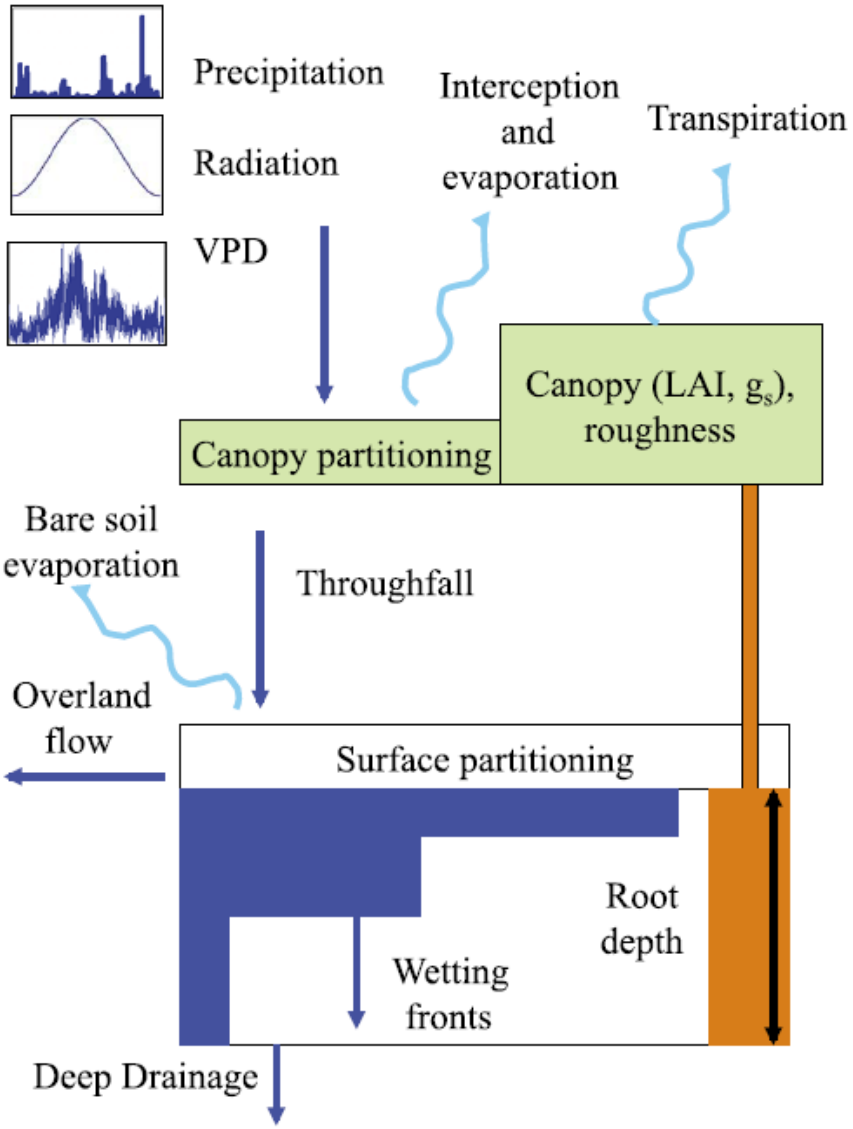
Biometeorology/Ecosystem Ecology, v2, the Processes



- Numerous and Coupled
- Biophysical Processes,
- Fast and Slow

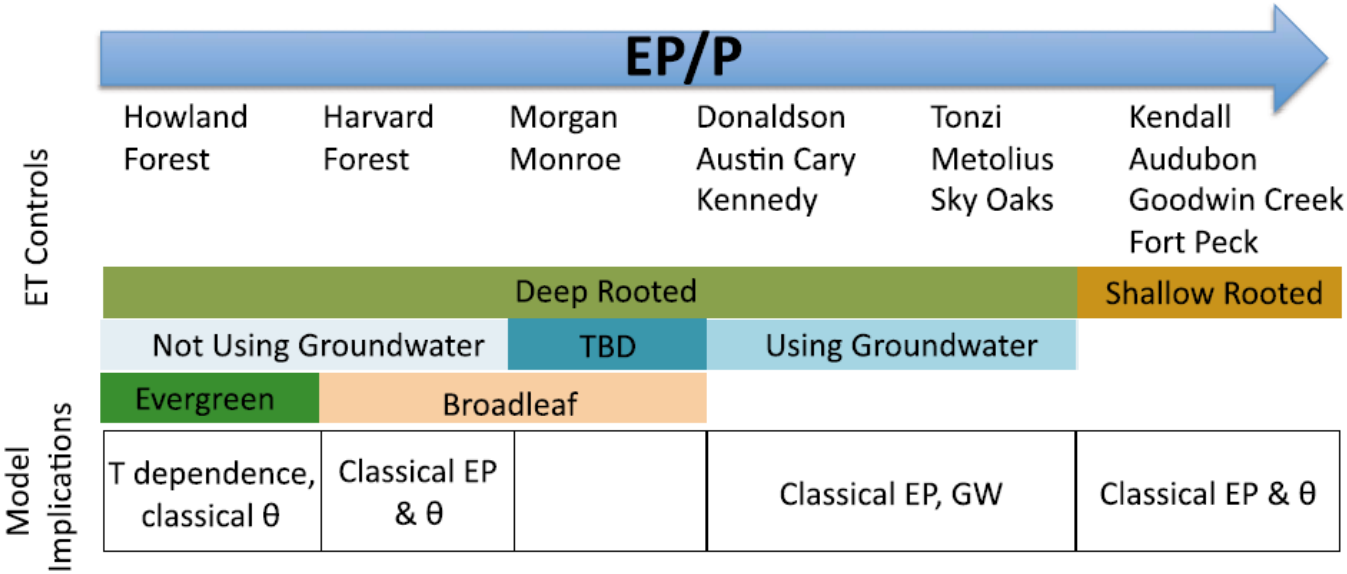
- Numerous Feedbacks,
- Positive and Negative

EcoHydrology Has Other Demands



Thompson et al 2011, WRR

Model Detail =f(ecosystem, climate)

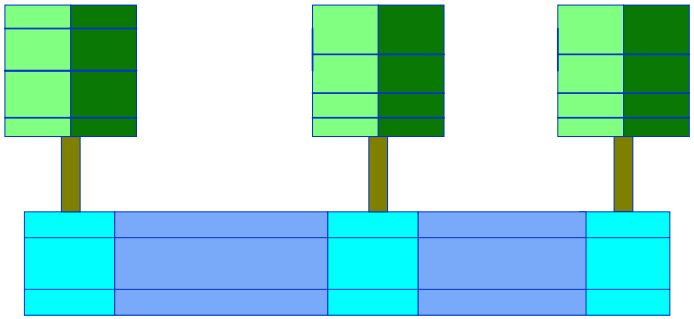


EP: Evaporation potential; GW: Groundwater

Thompson et al 2011, WRR

Big-Leaf Vegetation/Bucket Soil

Multi-layer Vegetation/Soil & Sun/Shade



Hierarchy of Models:

Space:

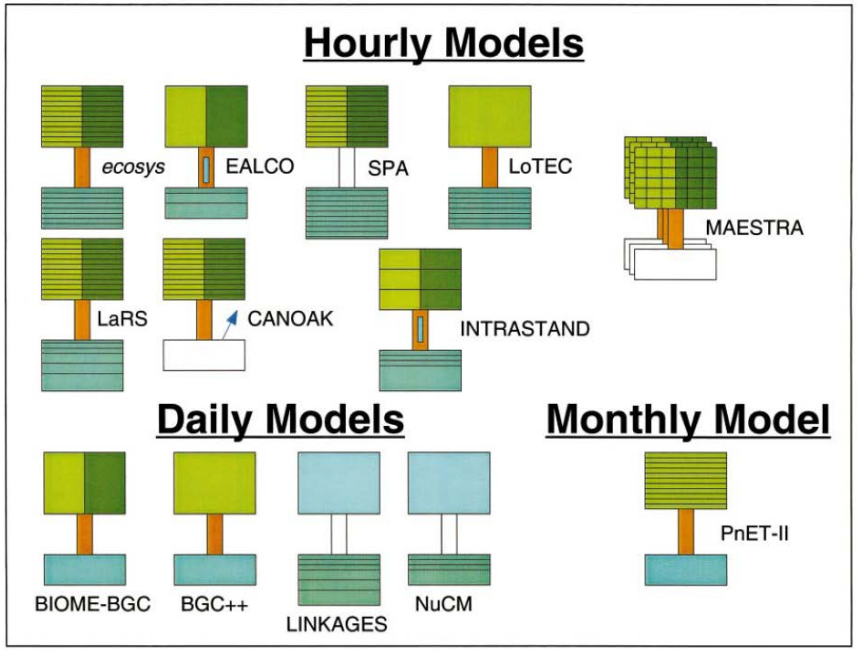
- Big-Leaf Vegetation/Bucket Soil
- Sun/Shade Vegetation
- 2-Layer, Vegetation and Soil
- Multi-Layer 1-D
- 3-D Model

Time:

- Hour
- Day
- Month

Geometrical Abstraction of the Canopy

- One-Dimensional
  - Big-Leaf
  - Dual Source, Sun-Shade
  - 2-Layer
    - Vegetation and soil
  - Multi-Layered
- Two-Dimensional
  - Dual source
    - sunlit and shaded
    - Vegetated vs Bare Soil
- Three-Dimensional
  - Individual Plants and Trees



After Hanson et al Ecol Appl 2004

Sources of Model Complexity and Uncertainty

- Representation of System Complexity
  - Geometrical
  - Processes and Feedbacks
  - Non-Linearities
- Model Parameters, f(x,z,t)
- Driving, or Input, Variables and their Transformation
- Spatial and Temporal Resolution
- Accuracy/Representativeness of Test-Bed Flux Data

Model Pitfalls

- Garbage In = Garbage Out

- Watch out for Non-Linearities
  - Apply at Proper Time-Step and Space-Scale

- Validate, Validate, Validate
- Don’t Parameterize Model Algorithms with the Same data used to Validate
- Equifinality, a combination of parameters yield the same answer
  - An appeal to Multiple Constraints
- Avoid Auto-Correlation, y =f(y)
- Avoid Extrapolating Empirical Regression models beyond the range of the dataset
  - Data Assimilation Best for Gap Filling in Time/Space and Diagnosis
- Use Mechanistic and Prognostic Models to predict the Future and to Upscale information
- Closure: Equal number of Equations and Unknowns is needed

A Challenge for Leaf to Landscape Upscaling:

Transform Weather Conditions from
a Weather Station to that of the **Leaves** in a Canopy with
Their Assortment of Angles and Layers Relative to the Sun
and Sky

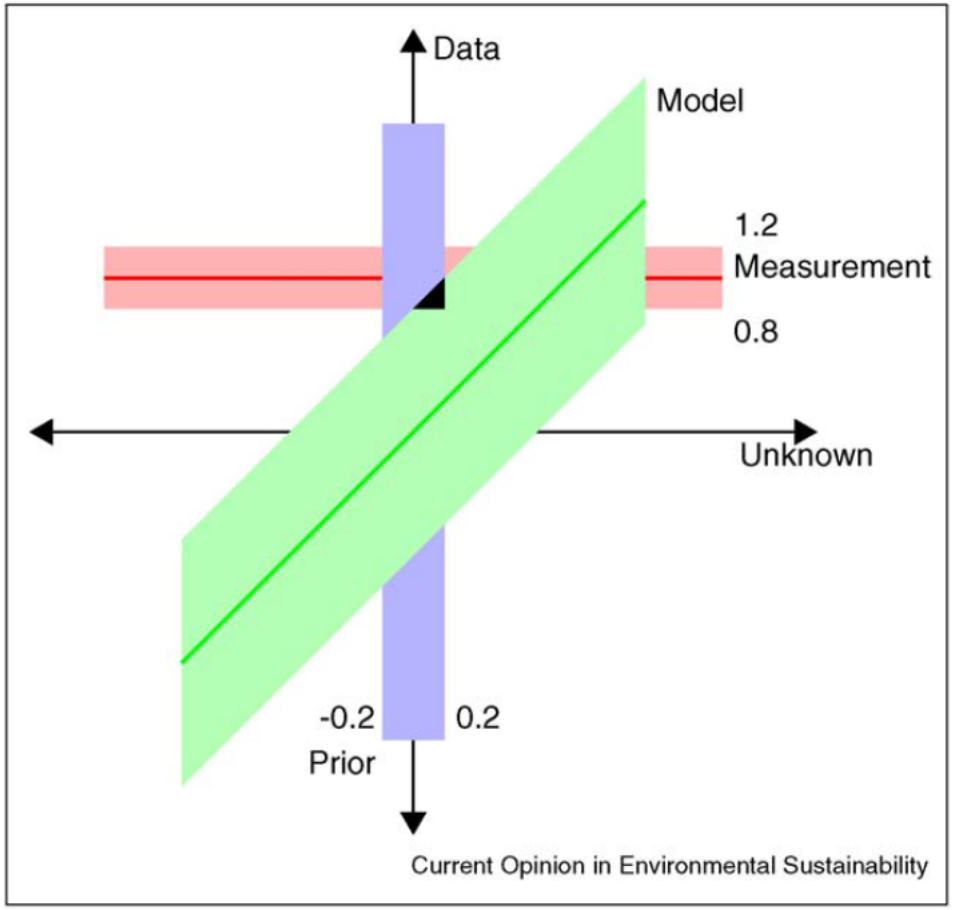
Challenge for Landscape to Global Upscaling

Converting Virtual ‘Cubism’ into Virtual ‘Reality’

Realistic Spatialization of Flux Data
Requires the Merging Numerous Data Layers with varying Time Stamps (hourly, daily, weekly), Spatial Resolution (1 km to 0.5 degree) and Data Sources (Satellites, Flux Networks, Climate Stations)

Model-Data Fusion

Figure 1



Rayner 2010 Current Opinions in Environment Sustainability

Mathematical Representation: Model Algorithms

1. Empirical, Regression Based
   1. Multiplicative
   2. Additive
2. Mechanistic/Diagnostic
3. Prognostic

$$f(t,x,y) = af(t) \cdot bf(x) \cdot cf(y)$$

$$f(t,x,y) = af(t) + bf(x) + cf(y)$$

$$Rn = H + \lambda E + G$$

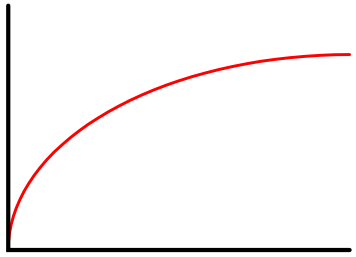
$$\frac{dc}{dt} = f(c,t)$$

Examples: Non-Linear Biophysical Processes

Photosynthesis

$$A \sim \frac{aI}{b+cI}; \frac{dC}{e+fC}$$

$$aA^3 + bA^2 + cA + d = 0$$



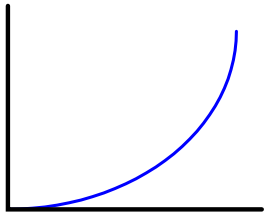
Transpiration

$$e_s(T) \sim \exp(T)$$

$$aLE^2 + bLE + c = 0$$

Respiration

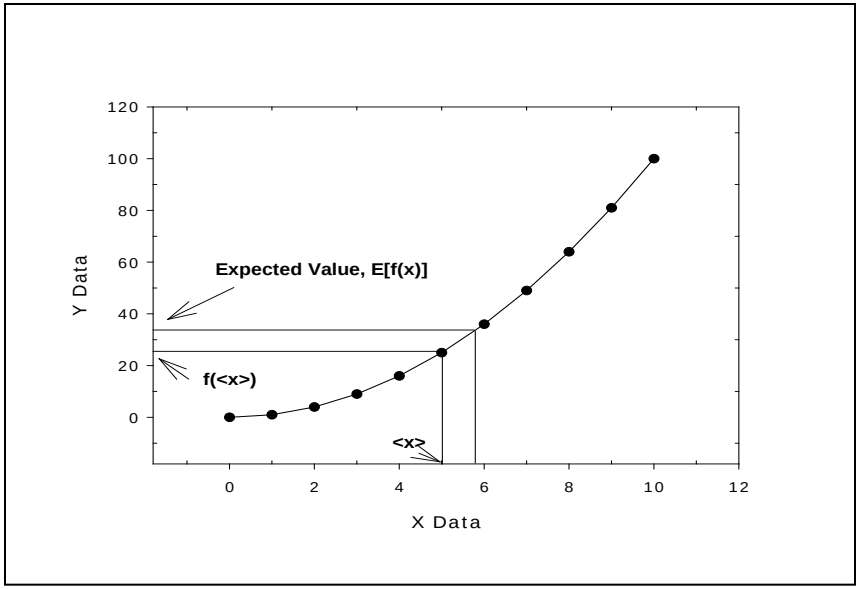
$$R_d \sim \exp(T)$$



Leaf Temperature

$$L\uparrow \sim T_s^4$$

Why Non-linearity is Important?



Jensen's Inequality

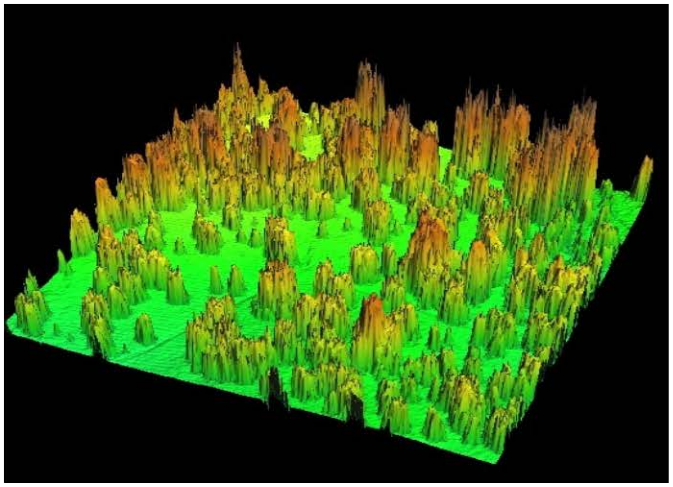
$$f([x]) \neq [f(x)]$$

$$E[f(x)] = f(\bar{x}) + \frac{1}{2}\frac{\partial^2 f(\bar{x})}{\partial x^2}\sigma(\bar{x})^2$$

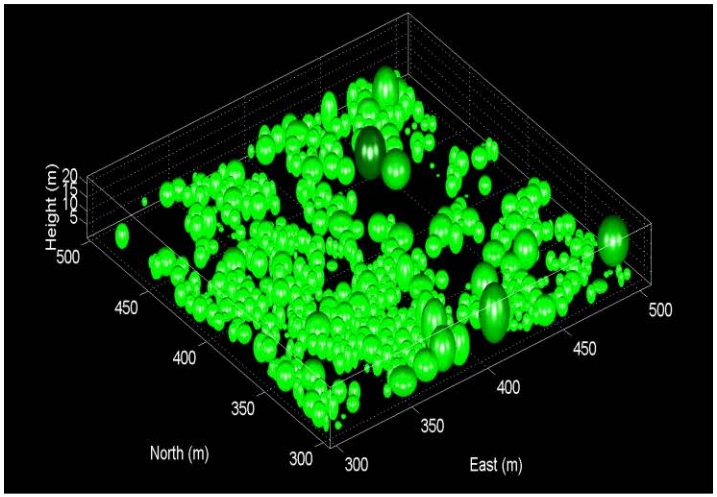
Taylor's Series Expansion

Hierarchy of Canopy Radiative Transfer Models

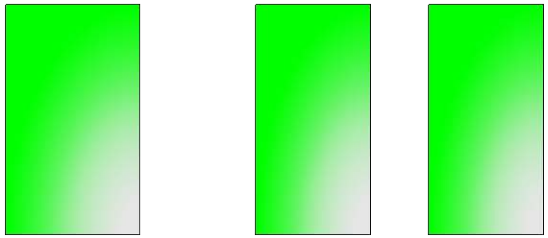
Reality



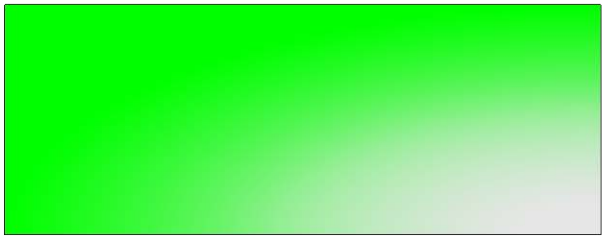
3-D Representation



2-D Representation



1-D Representation



Inverting LAI from Radiation Transfer Measurements

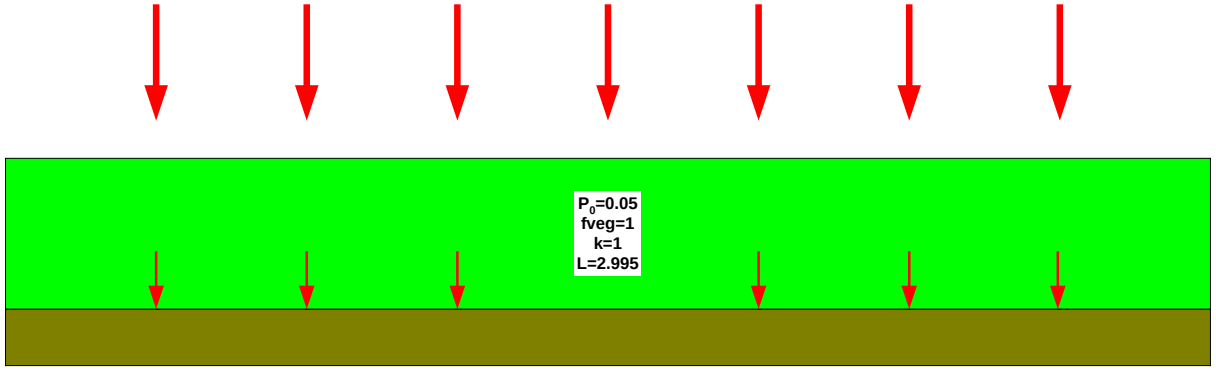
$$P_0 = \exp(-kL)$$

$$\overline{\ln(P_0)} \neq \ln(\overline{P_0})$$

$$L = -\frac{\overline{\ln(P_0)}}{k} = -\frac{\ln(\overline{P_0})}{k}$$

L = 2.996
[P_0]=0.05
[ln(P_0)]=-2.996

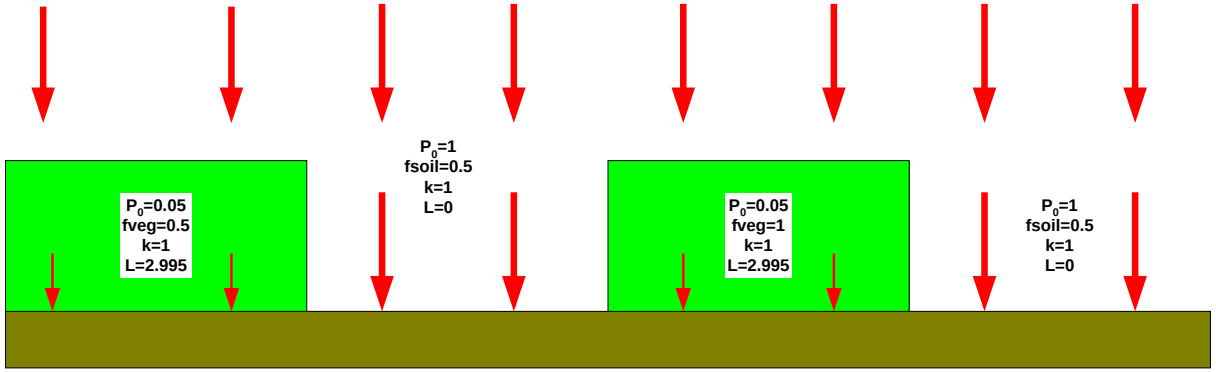
Ln[P_0]=-2.996
L*=2.996



$$L = -\frac{\overline{\ln(P_0)}}{k} \neq -\frac{\ln(\overline{P_0})}{k}$$

L = 1.497
[P_0]=0.525
[ln(P_0)]=-1.497

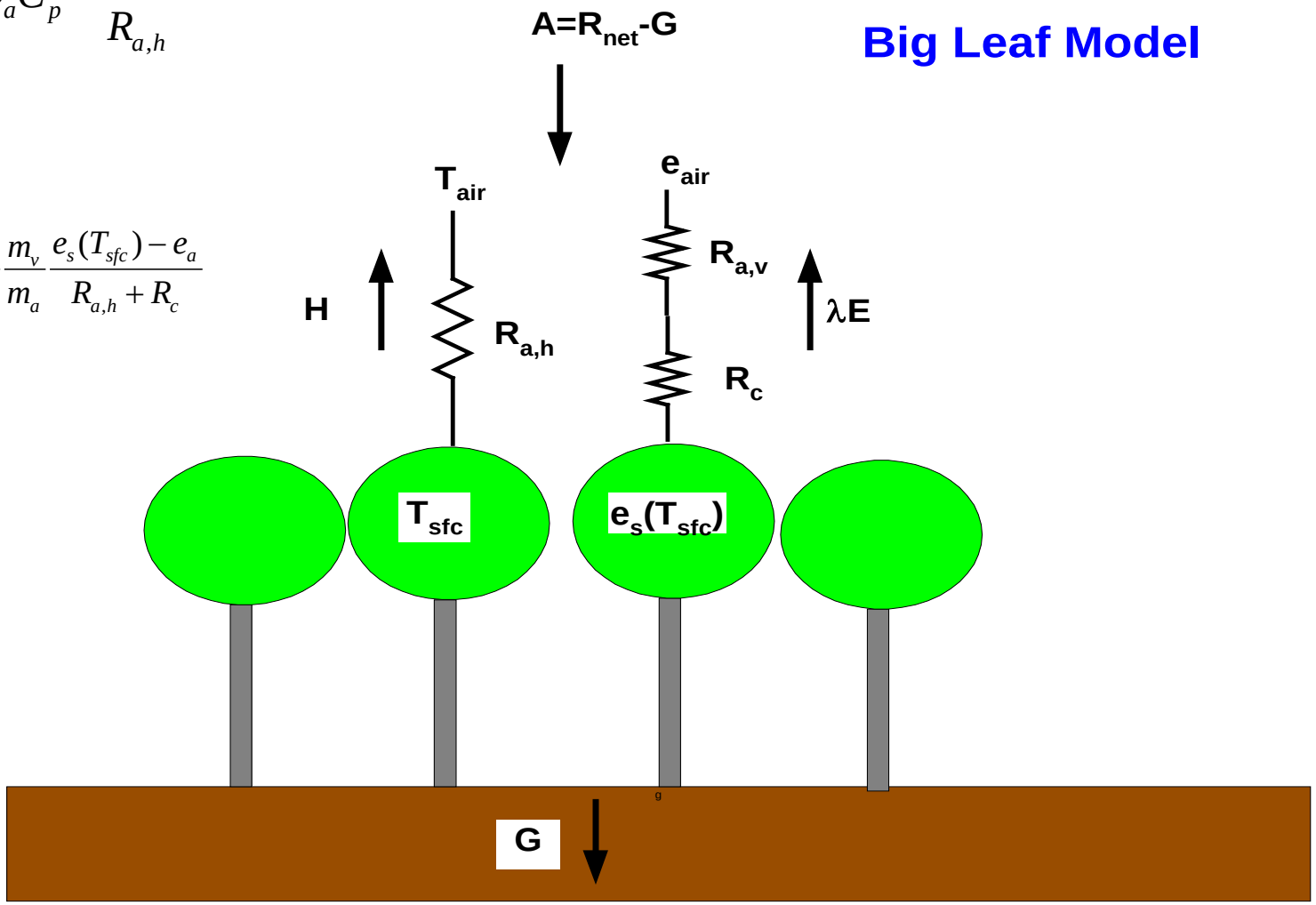
Ln[P_0]=-0.644
L*=0.644



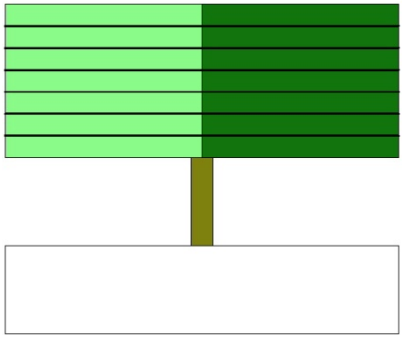
$$H = \rho_a C_p \frac{T_a - T_{sfc}}{R_{a,h}}$$

$$\lambda E = \frac{\rho_a \lambda}{P} \frac{m_v}{m_a} \frac{e_s(T_{sfc}) - e_a}{R_{a,h} + R_c}$$

Big Leaf Model



CANOAK



Role of Proper Model Abstraction

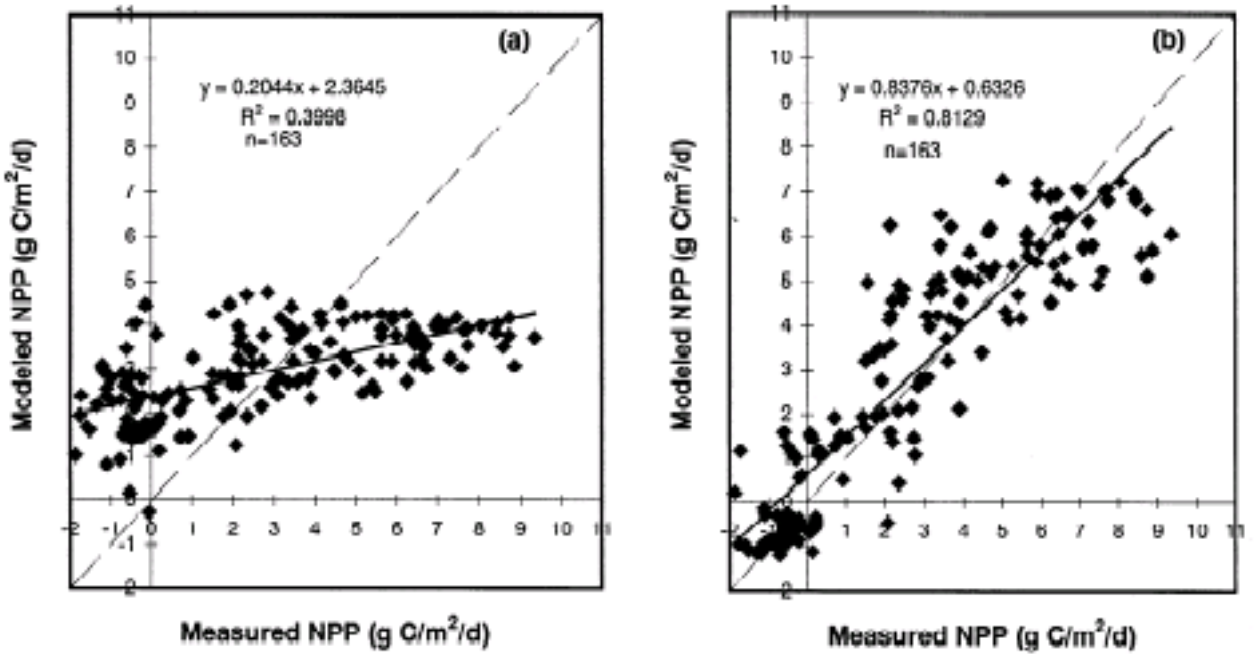
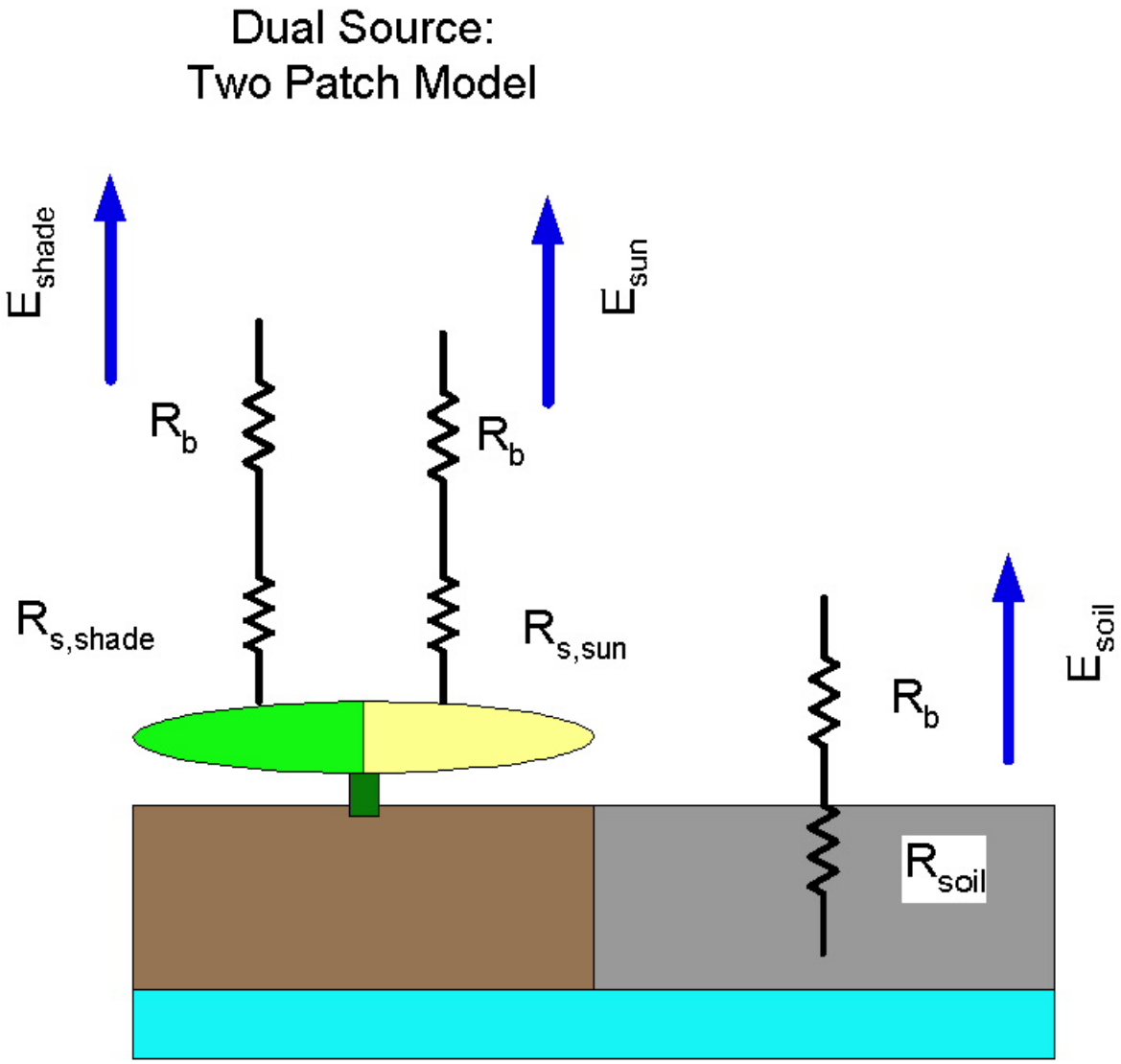
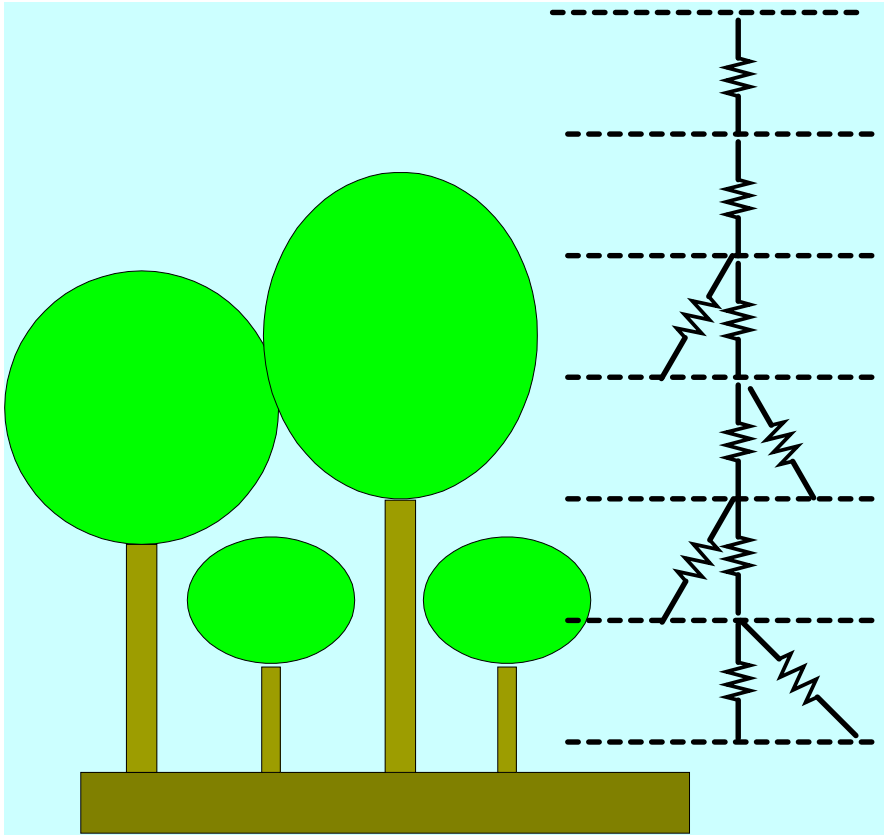


Fig. 9. One-to-one comparison of the measured NPP with the modeled NPP for a mature aspen stand. (a) big-leaf model, and (b) daily integrated model with sunlit–shaded leaf separation.


Dual Source:
Two Patch Model
E shade
E sun
R b
R b
R s,shade
R s,sun
R b
E soil
R soil

Multi-Layer Models



Quantifying Sources and Sinks

$$\frac{\partial F}{\partial z} = S(C,z) = - a(z) \frac{(C(z) - C_i)}{r_b(z) + r_s(z)}$$

- Biology:
  - Leaf area density: a(z);
  - Internal Concentration: C_i;
  - Stomatal Resistance, r_s
- Physics:
  - Boundary Layer Resistance, r_b;
  - Atmospheric Concentration, C(z)

Weight Source/Sink by Fraction of Sunlit and Shaded Leaves and Their Environment

$$S(C,z) = f(I_{sun}, T_{sun}, q_{sun}, C_{sun}) \cdot p_{sun}(z) + f(I_{shade}, T_{shade}, q_{shade}, C_{shade}) \cdot p_{shade}$$

Dual Source Model: Discrete Form

Whole Canopy Surface Conductance,
Wt function of sun and shade leaf areas

$$G_{sfc} = L_{sun} G_{sun} + L_{sh} G_{sh}$$

$$L_{sun} = (1 - \exp(-kL)) / k$$

Sunlit leaf area

$$L_{sh} = L - L_{sun}$$

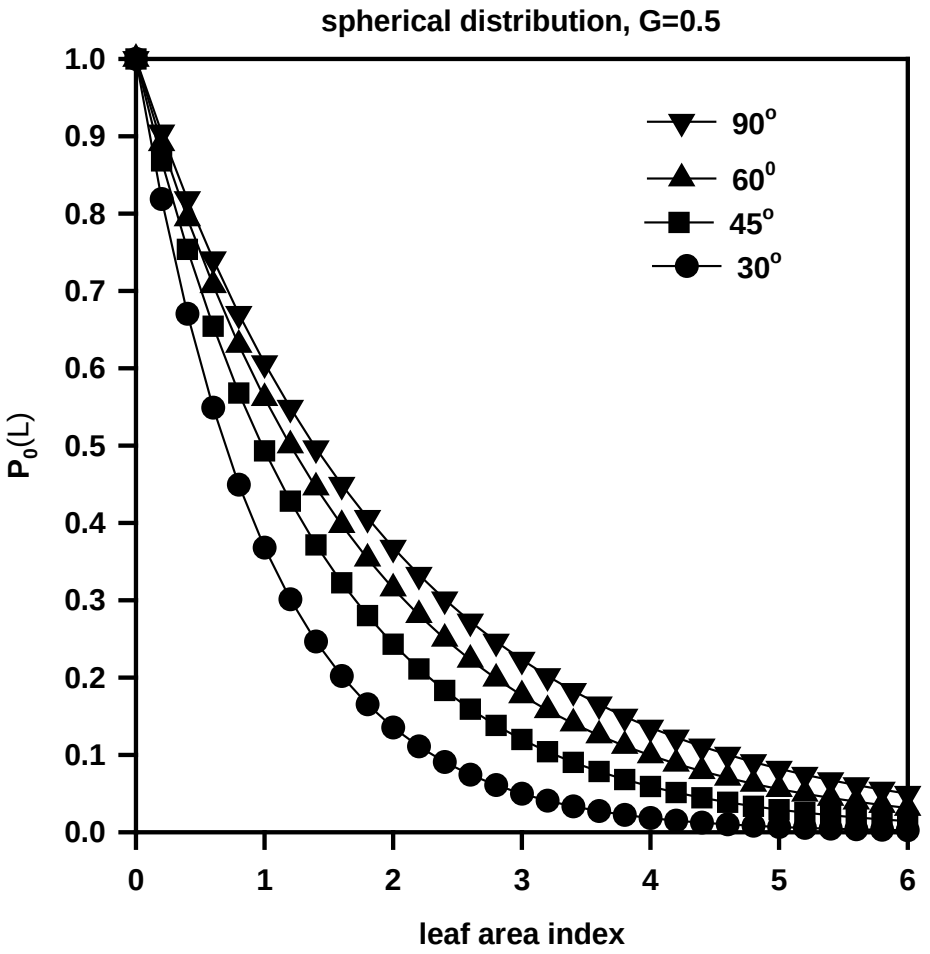
Shaded leaf area

Probability of Sunlit (Beam) and Shaded Leaves

$$P_b = -\frac{\sin\beta}{G}\frac{dP_0}{dL}$$

$$P_{sh} = 1 - P_b$$

Sun Angles and the probability of beam penetration, P_0



Beer's Law

$$P_0 = \exp(-kL)$$

$$P_0 = \exp(-\frac{LG}{\cos\theta_{sun}}) = \exp(-\frac{LG}{\sin\beta_{sun}})$$

L: Leaf area Index
G: direction cosine, leaf normal vs solar zenith angle

Random Spatial Distribution: Poisson Prob Distr.

Prob of Beam Penetration

$$P_0 = \exp(-\frac{L\,G}{\sin\beta})$$

Prob of Sunlit Leaf

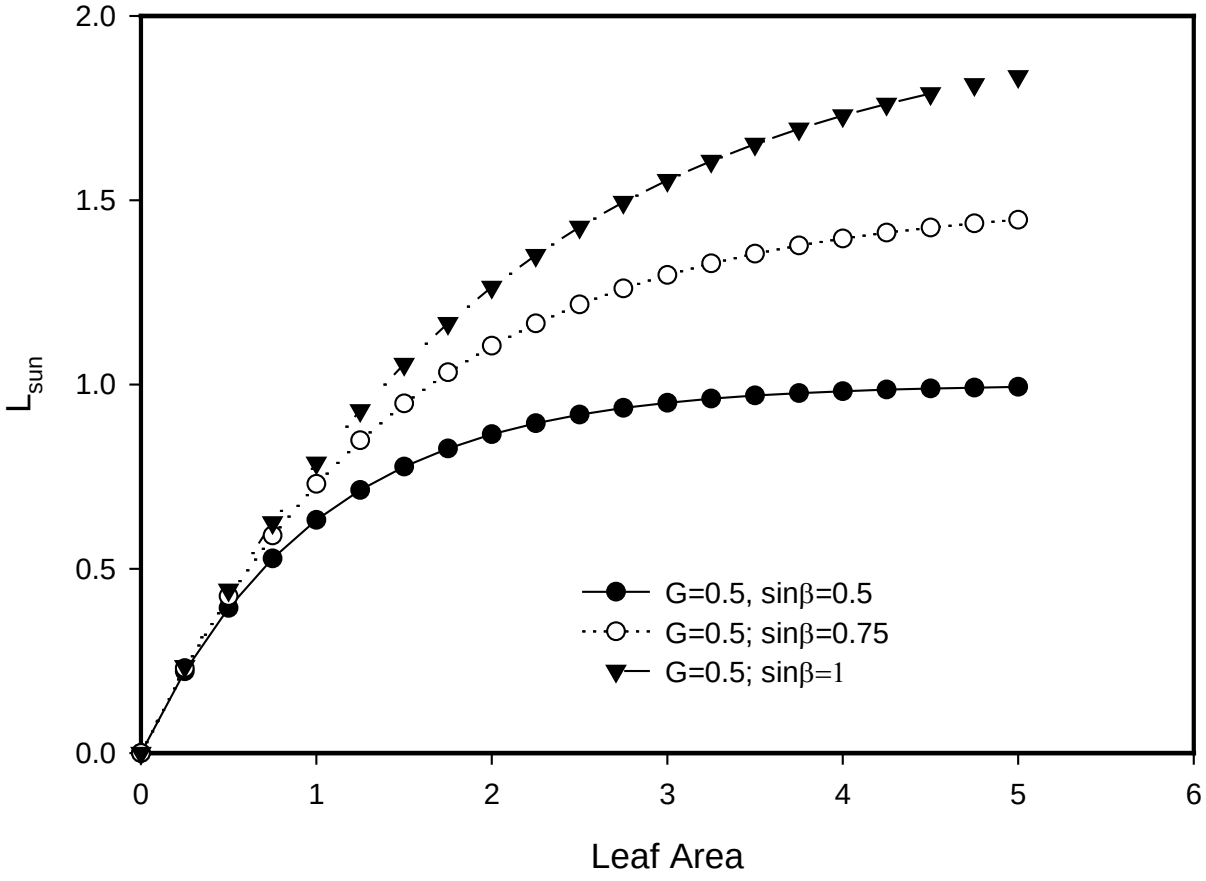
$$P_b = -\frac{\sin\beta}{G}\frac{dP_0}{dL} = \exp(-\frac{L\,G}{\sin\beta})$$

Sunlit Leaf Area

$$L_{sun} = \int_0^L p_b(l)dl$$

$$L_{sun} = \frac{\sin\beta}{G}(1 - \exp(-\frac{GL}{\sin\beta})$$

Sunlit Leaf Area



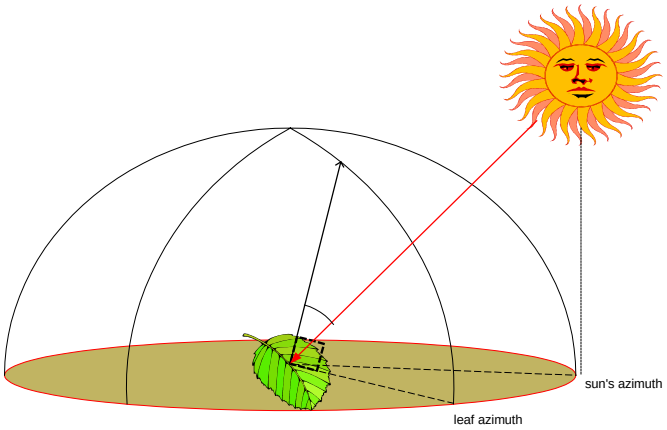
Sunlit Leaf Area, clumped Leaves

$$L_{sun} = \int_{L}^{0} \Omega \exp(-\frac{\Omega G L}{\sin \beta}) dL$$

$$\int a \exp(-bx) dx = -\frac{a}{b} \exp(-bx)$$

$$L_{sun} = \frac{\sin \beta}{GL}(1 - \exp(-\frac{\Omega G L}{\sin \beta})$$

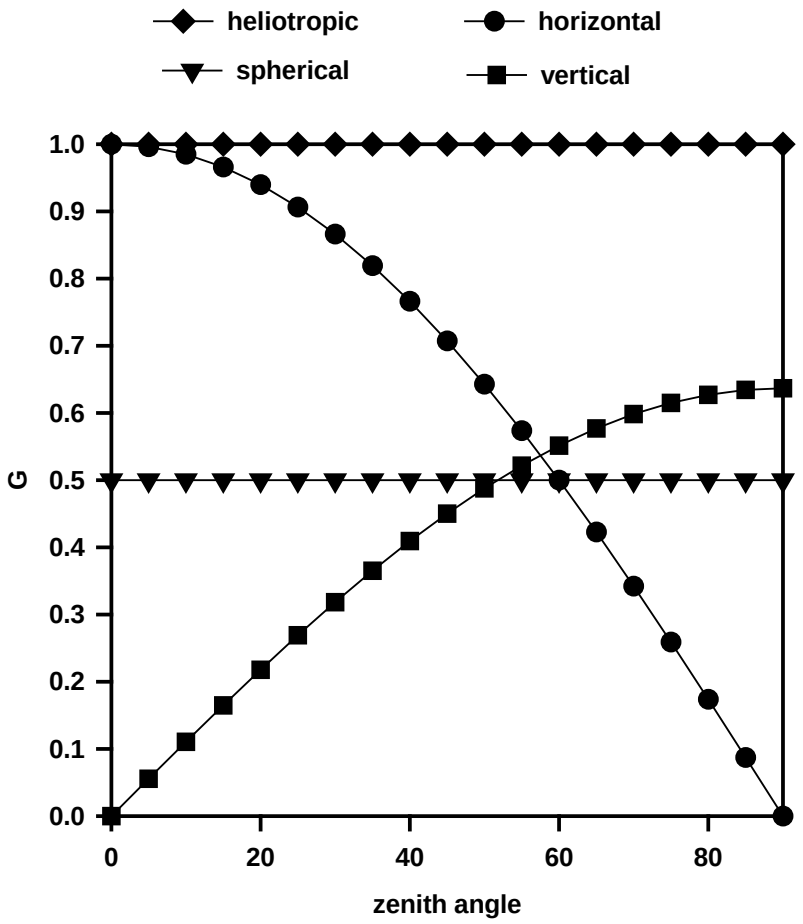
G Function, the relation between leaf normals and the sun



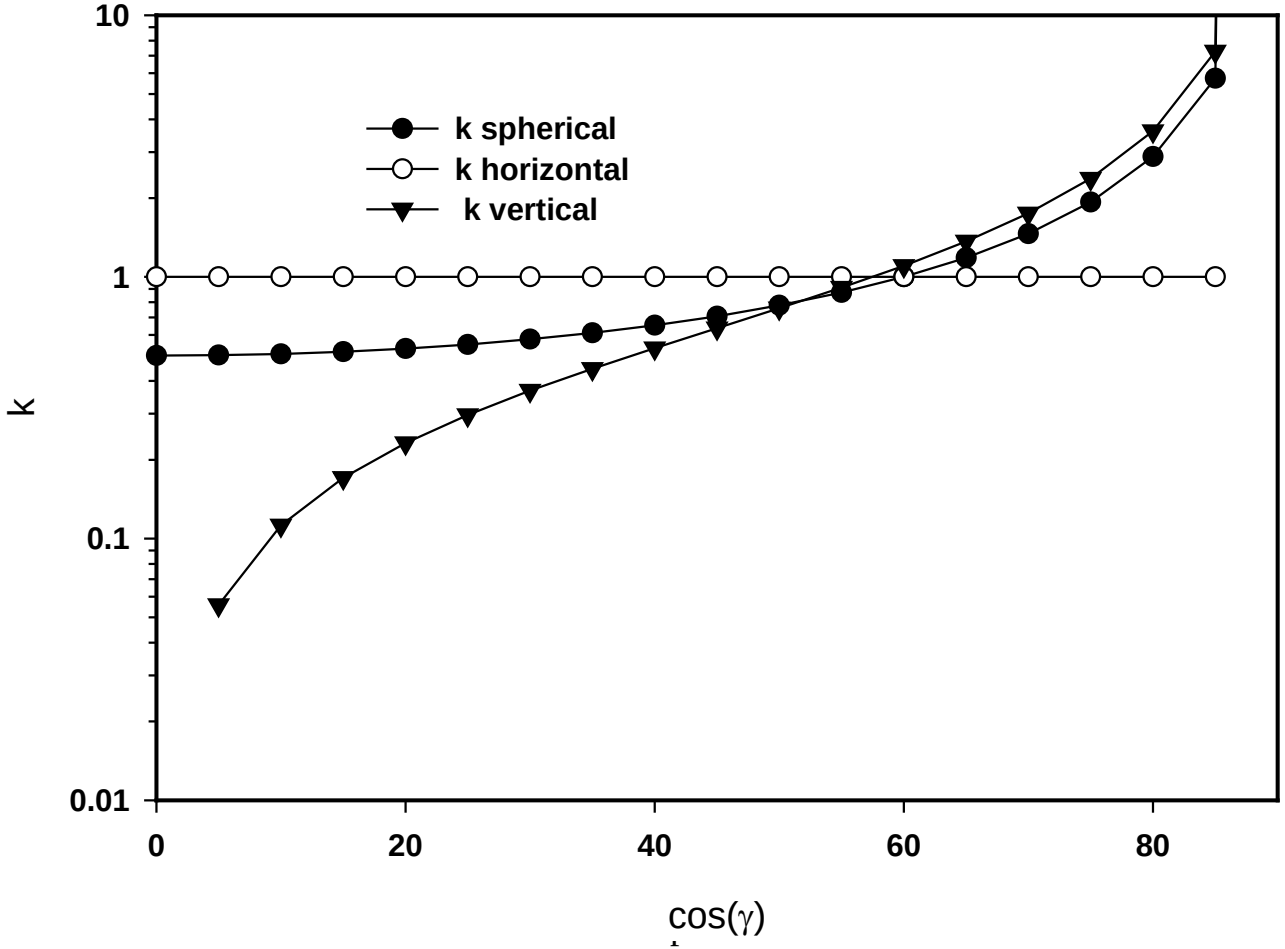
$$G(\theta,\varphi) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \int_0^{\pi/2} g(\theta_{leaf},\varphi_{leaf})\left|\cos(nn_{leaf}\right|\sin\theta_{leaf}\, d\theta_{leaf}$$

$$\cos(nn_{leaf}) = \cos\theta\cdot\cos\theta_{leaf} + \sin\theta\cdot\sin\theta_{leaf}\cos(\varphi-\varphi_{leaf})$$

G functions for different leaf inclination angle distributions



Extinction coefficients, k, with different solar zenith angles

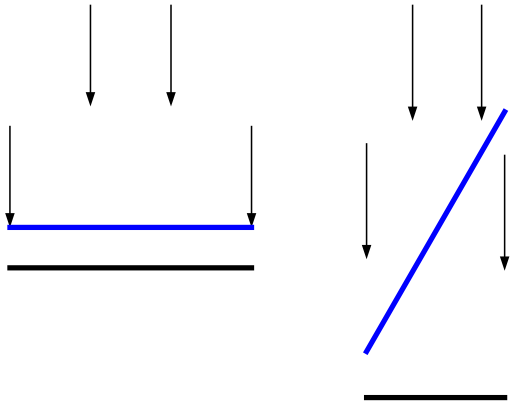


The extinction coefficient, k, equals the fraction of hemi-surface leaf area (*A*) that is **projected onto the horizontal** (*A_h*), from a particular zenith angle.

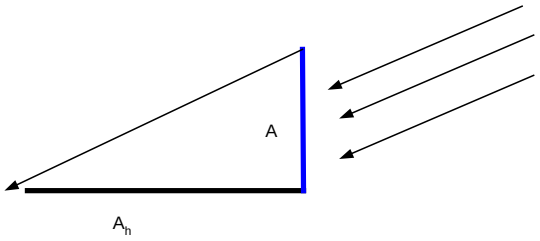
$$k = \frac{A_h}{A}$$

Light interception by Inclined leaves $k = \frac{A_h}{A}$

k= A_h/A; it equals 1
As A_h and A equal
One another



k goes to zero as
A_h goes to zero



k goes to infinity
As A_h goes to
infinity

$$\frac{A_{horiz}}{A_{leaf}} = \frac{\cos\alpha}{\sin\beta_{sun}} = \kappa = \frac{G}{\sin\beta_{sun}} = \frac{G}{\cos\theta_{sun}}$$

Leaf Angle Distribution	G, direction cosine	K, extinction coefficient
Horizontal	cos(θ)	1
Vertical	2/π sin(θ)	2 tan(θ/π)
Conical	cos(θ) cos(θ_l)	cos(θ)
Spherical or random	0.5	1/(2 cos(θ))
Heliotropic	1	1/ cos(θ)
Ellipsoidal	*	**

Define K in terms of Sun and Leaf Inclination Angles

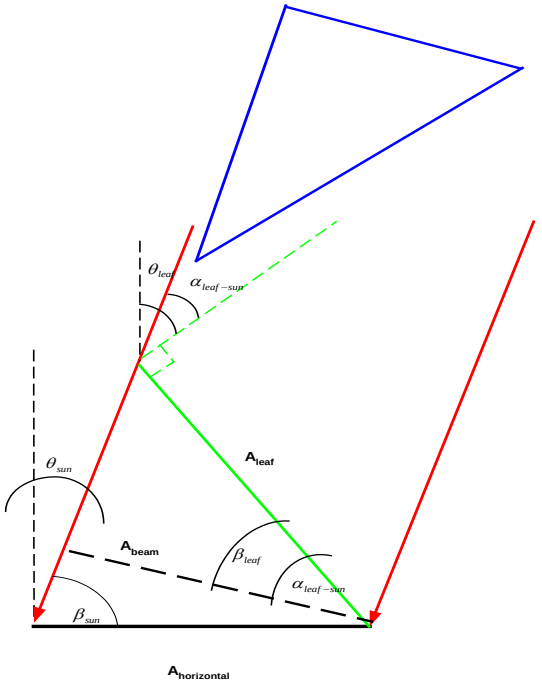
$$\frac{A_{horiz}}{A_{leaf}} = \frac{\cos\alpha}{\sin\beta_{sun}} = \kappa = \frac{G}{\sin\beta_{sun}} = \frac{G}{\cos\theta_{sun}}$$

α,angle between leaf normal And solar zenith

β, solar elevation angle

k, extinction coefficient

G, G-function or direction cosine



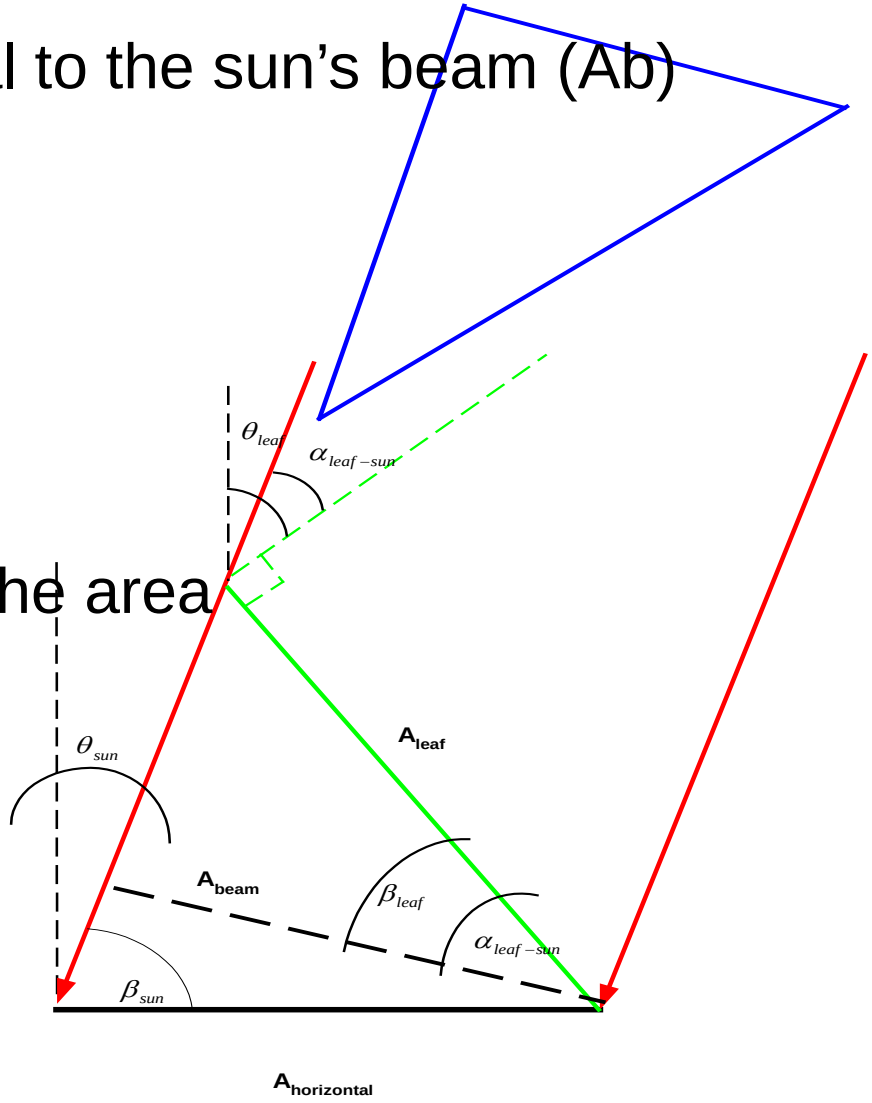
$\beta_{leaf} = \theta_{leaf}$

Project the area of a leaf normal to the sun's beam (Ab) onto the horizontal (Ah).

$$\frac{A_b}{A_h} = \sin\beta = \cos\theta$$

Project the area of a leaf onto the area normal to the solar beam

$$\frac{A_{beam}}{A_{leaf}} = \cos\alpha$$



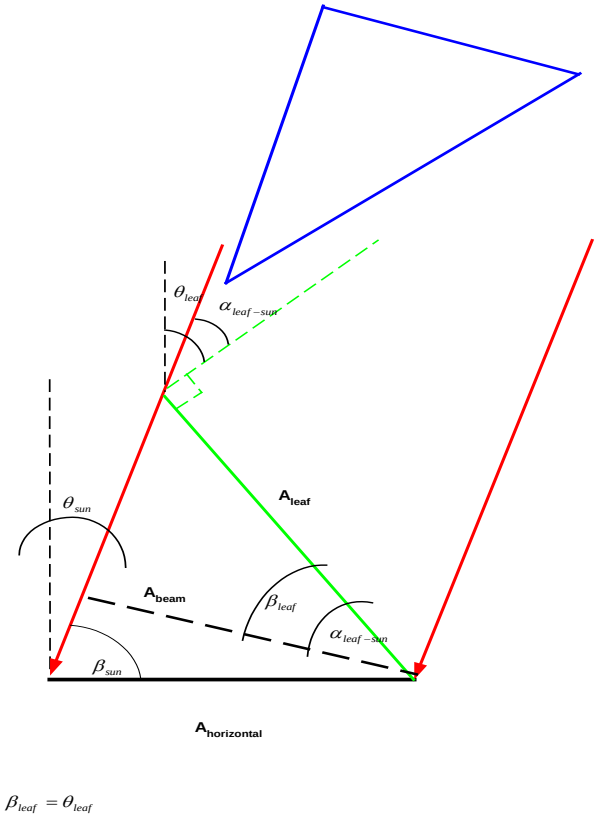
$\beta_{leaf} = \theta_{leaf}$

$$A_{beam} = A_{leaf} \cos\alpha$$

$$A_{leaf} = \frac{A_{beam}}{\cos\alpha}$$

$$\frac{A_{beam}}{A_{horiz}} = \sin\beta_{sun} = \frac{A_{leaf}\cos\alpha}{A_{horiz}} = \cos\theta_{sun}$$

$$\frac{A_{leaf}}{A_{horiz}} = \frac{\sin\beta_{sun}}{\cos\alpha} = \frac{\cos\theta_{sun}}{\cos\alpha}$$

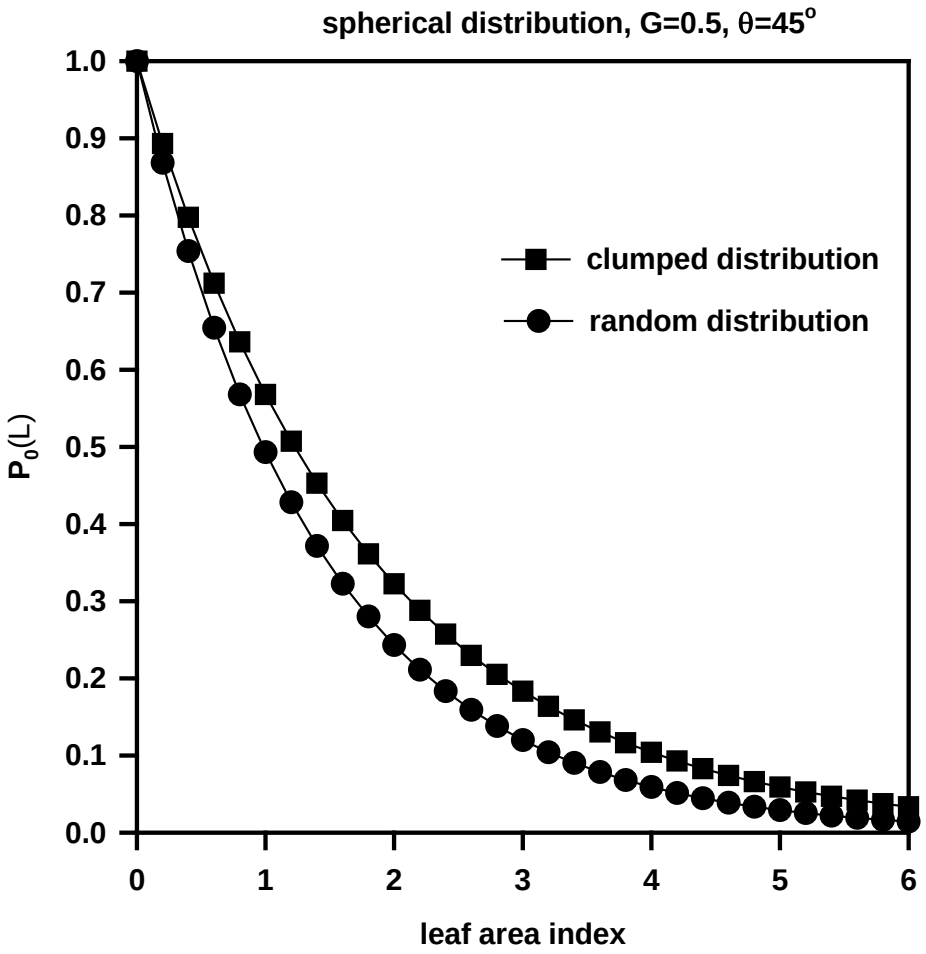


$\beta_{leaf} = \theta_{leaf}$

Voila'

$$\kappa = \frac{G}{\sin\beta_{sun}} = \frac{G}{\cos\theta_{sun}}$$

Probability of beam penetration with clumped and randomly distributed foliage



Beer's Law

$$P_0 = \exp(-kL)$$

$$P_0 = exp(-\frac{L\,G\Omega}{sin\,\beta})$$

Ω, clumping coef

ɔmet and

Micromet

Random Spatial Distribution: Poisson Prob Distr.

Prob of Beam Penetration

$$P_0 = \exp(-\frac{L\,G}{\sin\beta})$$

Prob of Sunlit Leaf

$$P_b = -\frac{\sin\beta}{G}\frac{dP_0}{dL} = \exp(-\frac{L\,G}{\sin\beta})$$

Clumped Leaves

$$P_0 = exp(-\frac{L\,G\Omega}{sin\,\beta})$$

$$P_b = -\frac{\sin\beta}{G}\frac{dP_0}{dL} = \Omega \cdot \exp(-\frac{L\,G\Omega}{\sin\beta})$$

Sunlit leaves are illuminated by direct and diffuse light

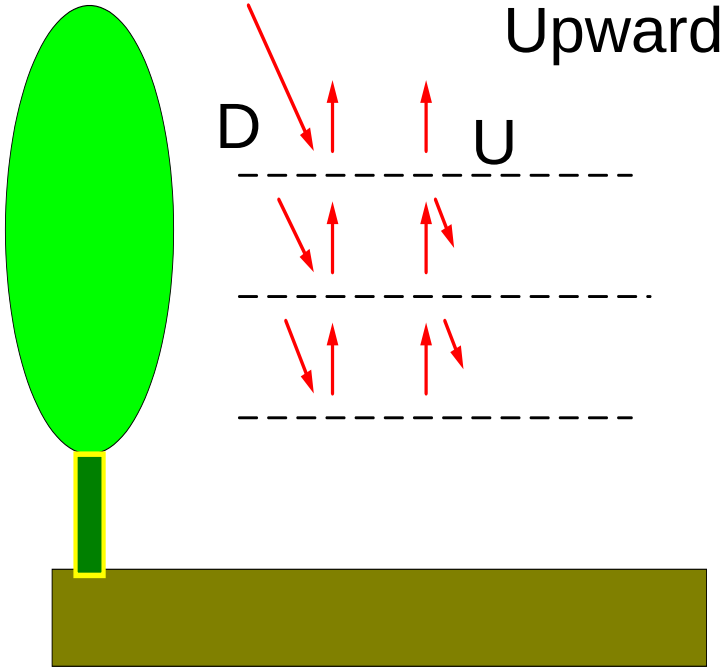
$$I_{sun} = \frac{I_{beam} \cdot G}{\sin \beta} + I_{shade}$$

Direct Light is Directional
Diffuse Light is Isotropic and Hemispherical

Radiative Transfer Scheme

Downward Diffuse $D_i = R_l \cdot U_i + T_n D_{i+1}$

Upward Diffuse $U_{i+1} = R_u \cdot D_{i+1} + T_n U_i$



$$T_n = exp(\frac{-\Delta f \cdot G \cdot \Omega}{\sin \beta}) + (1 - exp(\frac{-\Delta f \cdot G \cdot \Omega}{\sin \beta}))\tau$$

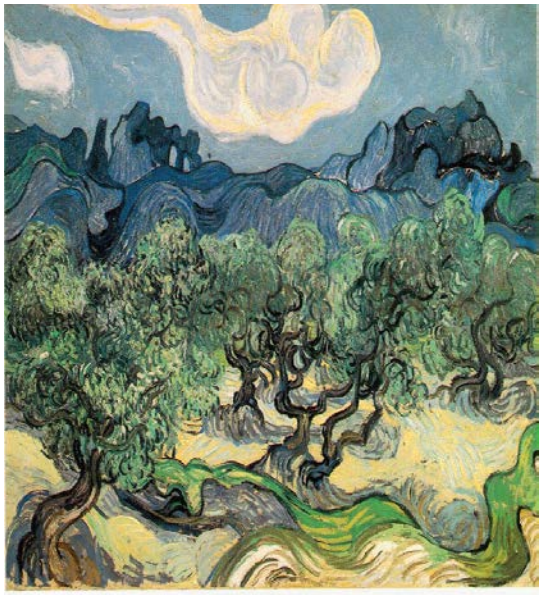
$$R_l = (1 - exp(\frac{-\Delta f \cdot G \cdot \Omega}{\sin \beta}))\rho_l$$

$$R_u = (1 - exp(\frac{-\Delta f \cdot G \cdot \Omega}{\sin \beta}))\rho_u$$

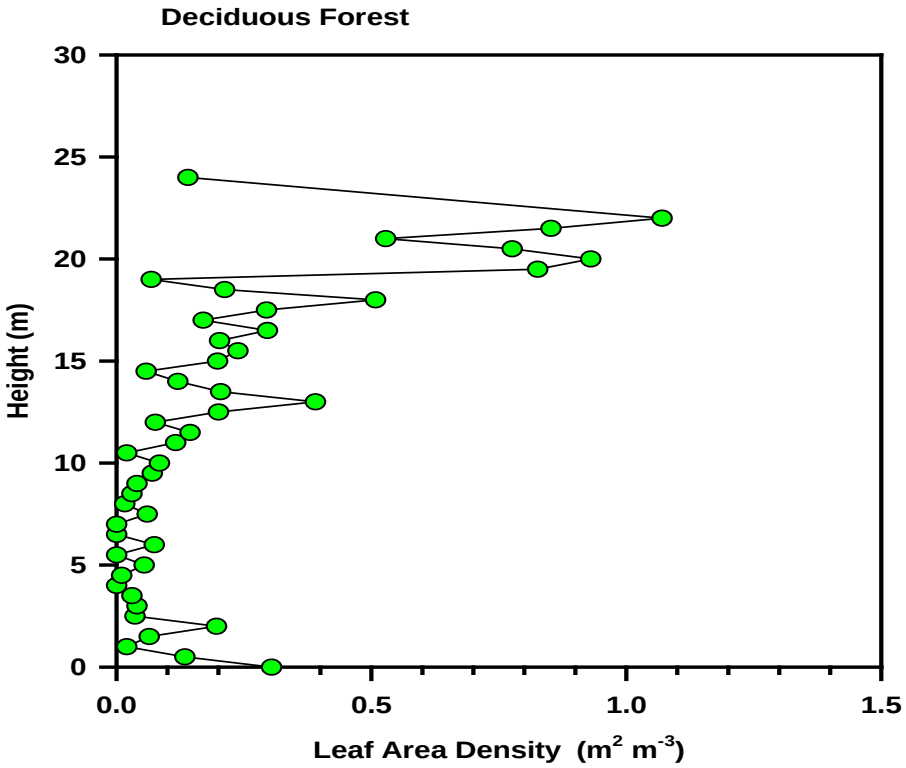
After Norman, 1979

Sources of Spatial Heterogeneity

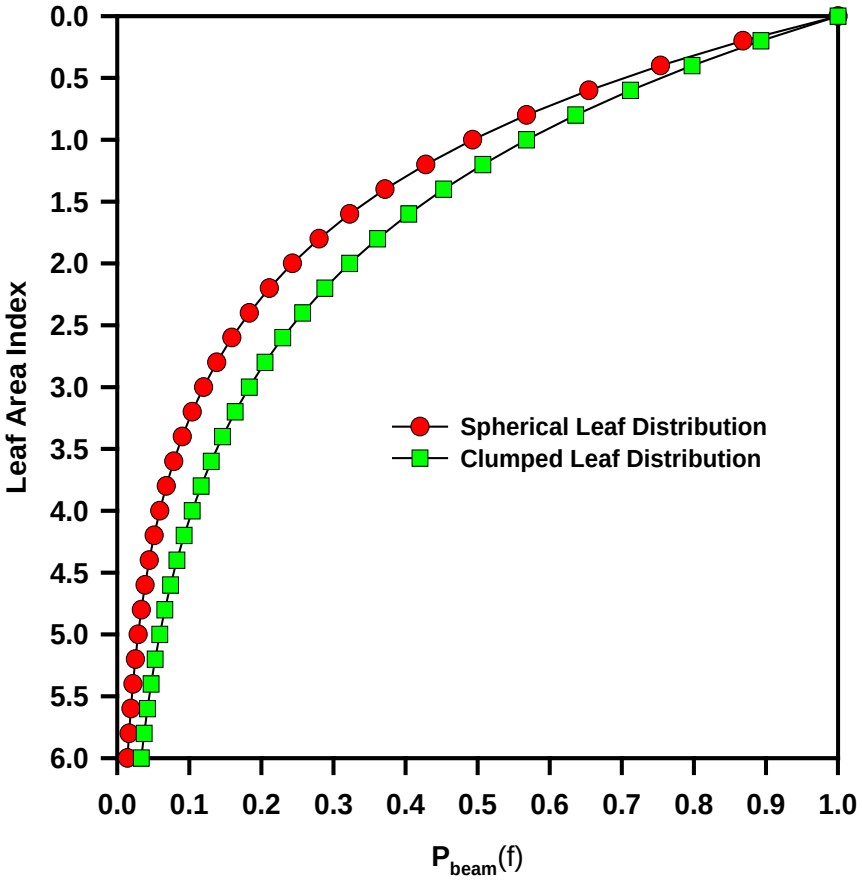
- Vertical Variations in:
  - Leaf area index
  - Leaf inclination angles
  - Leaf Clumping
  - Leaf N + photosynthetic capacity
  - Stomatal conductance
  - Light, Temperature, Wind, Humidity, CO_2

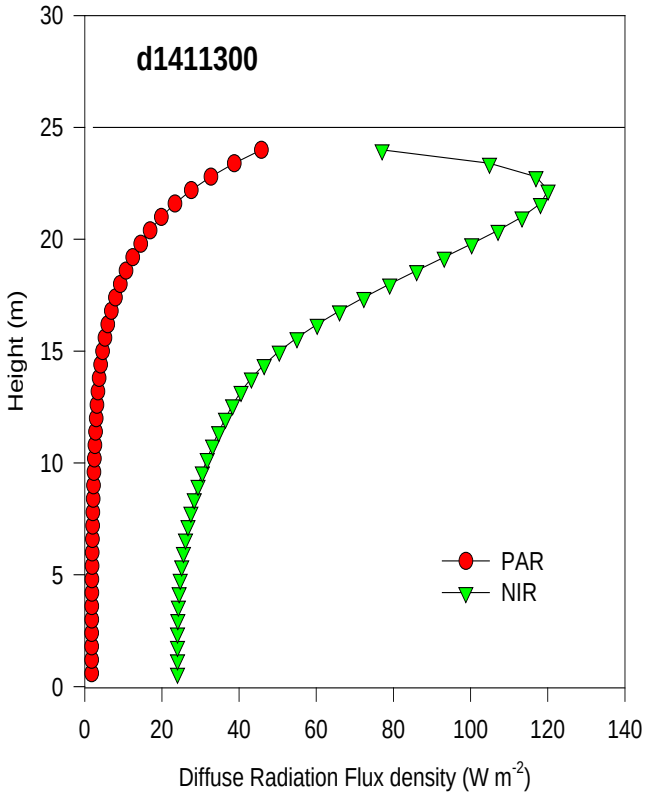


Vertical Profiles in Leaf Area



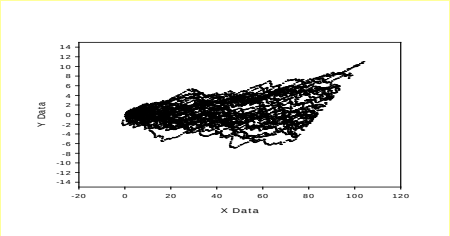
Vertical Variation in Sunlight





Turbulence Closure Schemes

- Lagrangian



- Eulerian
  - Zero Order, c(z)=constant
  - First Order, F=K dc/dz
  - Second Order and ++ (dc/dt, dw'c'/dt)

Higher Order Closure Equations and Unknowns

Order of Closure	Turbulence Budget Equations	Unknowns	Scalar Budget Equations $(\frac{\partial c}{\partial t})$	Unknowns	Closure Scheme
zero		$\overline{u}, \overline{w}$		$\overline{T}, \overline{q}, \overline{C}$	$\overline{c} = f(t,x,y,z)$
First Order	$\overline{u}$	$\overline{u'u'}, \overline{w'w'}, \overline{w'u'}$	$\overline{T}, \overline{q}, \overline{C}$	$\overline{T'^2}, \overline{q'^2}, \overline{C'^2}, \overline{w'T'}$ $\overline{w'q'}, \overline{w'C'}$	$\overline{w'c'} = -K\frac{\partial c}{\partial z}$
Second Order	$\overline{u'u'}, \overline{w'w'}, \overline{w'u'}$ $\overline{v'v'}$	$\overline{u'u'u'}, \overline{w'w'w'}$, $\overline{w'u'u'}, \overline{u'w'w'}$	$\overline{T'^2}, \overline{q'^2}, \overline{w'T'}$, $\overline{w'q'}, \overline{T'q'}, \overline{q'T'}$	Numerous third order moments	$\overline{w'w'c'} = -K\frac{\partial \overline{w'c'}}{\partial z}$
Third Order	$\overline{w'w'u'}, \overline{w'w'v'}$ $\overline{w'u'u'}, \overline{w'v'v'}$		$\overline{w'w'T'}, \overline{w'T'q'}$, $\overline{u'w'T'}, \overline{w'T'T'}$, $\overline{w'w'q'}$	Numerous fourth order moments	$\overline{w'w'w'w'} = 3\overline{w'w'} \cdot \overline{w'w'}$ quasi-Gaussian approximation

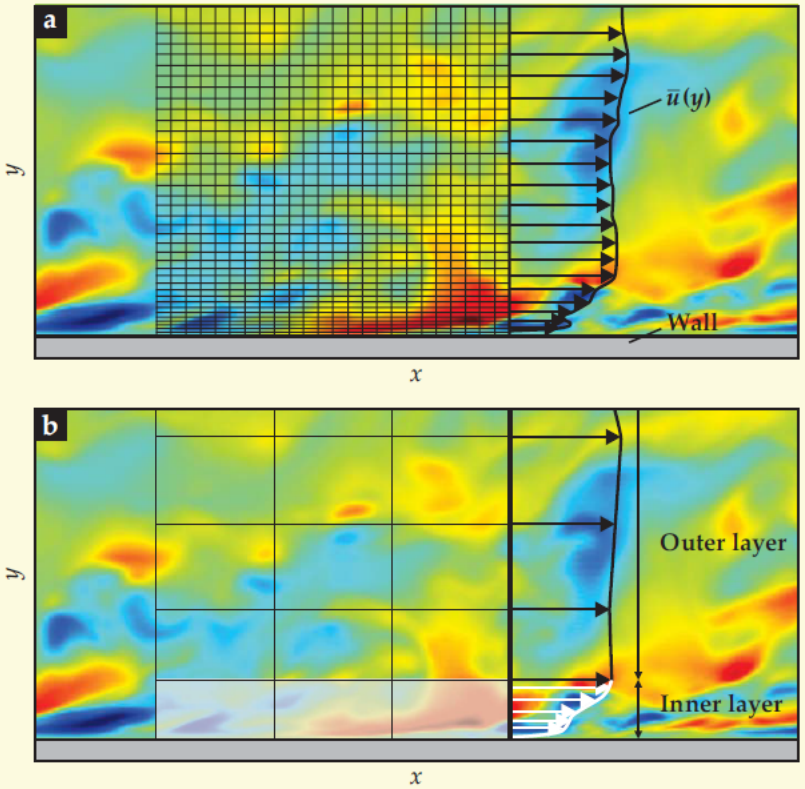


Figure 5. The grid spacing in a large eddy simulation must be fine enough to resolve all but the smallest length scales in a turbulent flow. In this simulated boundary-layer flow, red and blue areas indicate eddies, and the arrows indicate the mean streamwise velocity $\bar{u}$ at various distances y from the wall. **(a)** For standard large eddy simulation, the necessary grid spacing is exceedingly fine due to the very small scales in the near-wall region. **(b)** A coarser grid can be used if the inner layer near the wall, shaded white, is described instead by an empirical model. (Adapted from ref. 7.)

Smits and Maruvic 2013 Physics Today

Scalar Conservation Budget Equations: What the Terms Mean

$$\frac{\partial \overline{u}}{\partial t} = 0 = -\frac{\partial \overline{u'w'}}{\partial z} - \frac{\overline{\partial p'}}{\rho \partial x} - \frac{\partial \overline{p}}{\rho \partial x} + \upsilon \frac{\partial^2 \overline{u}}{\partial z \partial z}$$

$$\frac{\partial \overline{q}}{\partial t} = 0 = -\frac{\partial \overline{w'q'}}{\partial z} + S_q$$

Flux Divergence

Time Rate of Change

Source/Sink

Pressure Fluctuation is a function of the drag coefficient

$$\overline{\frac{\partial p'}{\partial x_i}} = C_d a(z) \overline{u_i}^2$$

$$\frac{\partial \overline{u'w'}}{\partial z} = C_d a(z) \overline{u_i}^2$$

$$\overline{u(z)} = u_h \exp(-\alpha(1 - \frac{z}{h}))$$

K Theory in the Surface Layer

$$K_m(z) = \frac{\overline{w'u'}(z)}{\rho \, \partial \bar{u} / \partial z}$$

Short vegetation

$$K_m(z) = \frac{u_*^2}{\partial \bar{u} / \partial z} = \frac{u_*^2}{u_* / k\, z} = u_* k\, z$$

Tall vegetation

$$K_m(z) = \frac{u_*^2}{\partial \bar{u} / \partial z} = \frac{u_*^2}{u_* / k(z-d)} = u_* k(z-d)$$

K Theory in the Plant Canopy

$$K_m(z) = \frac{\overline{w'u'}(z)}{\rho \, \partial \bar{u} / \partial z}$$

$$K_m(z) \approx \tau_l(z)\sigma_w^2(z)$$

Stanley Corrsin (1974) wrote that several conditions must hold to apply K-theory:

• the length scales of the turbulent transfer must be less than the length scales associated with the curvature of the concentration gradient of the scalar.

• the turbulent length scale must be constant over the distance where the concentration gradient changes significantly.

$$\overline{w'c'} = \tau\left(\overline{w'^2}\,\frac{\partial \bar{c}}{\partial z} + \frac{\partial \overline{w'w'c'}}{\partial z}\right)$$

$$\overline{w'c'} \sim K_c\,\frac{\partial \bar{c}}{\partial z} + TT$$

2nd Order Equation, General Form

$$\frac{\partial \overline{u_i' u_k'}}{\partial t} + \overline{u}_j \frac{\partial \overline{u_i' u_k'}}{\partial x_j} + \overline{u_k' u_j'} \frac{\partial \overline{u_i}}{\partial x_j} + \overline{u_i' u_j'} \frac{\partial \overline{u_k}}{\partial x_j} + \frac{\partial \overline{u_i' u_k' u_j'}}{\partial x_j} =$$

$$-\left[\frac{\overline{\partial u_k' p'}}{\partial x_i} + \frac{\overline{\partial u_i' p'}}{\partial x_k} \right] + \left[\overline{u}_k \frac{\overline{\partial p'}}{\partial x_i} + \overline{u}_i \frac{\overline{\partial p'}}{\partial x_k} \right] + \overline{p' \left[\frac{\partial u_k'}{\partial x_i} + \frac{\partial u_i'}{\partial x_k} \right]} + \frac{g}{T} \left[\overline{\theta' u_i'} \delta_{k3} + \overline{\theta' u_k'} \delta_{i3} \right] + \upsilon \frac{\partial^2 \overline{u_i' u_k'}}{\partial x_j \partial x_j} - 2\upsilon \overline{\frac{\partial u_i'}{\partial x_j} \frac{\partial u_k'}{\partial x_j}}$$

Examples of 2nd Order Budget Equations

$$\frac{\partial \overline{u'u'}}{\partial t} = 0 = -2\overline{w'u'}\frac{\partial \bar{u}}{\partial z} - \frac{\partial \overline{w'u'u'}}{\partial z} - 2\frac{\overline{u'\partial p'}}{\rho \partial x} - 2\frac{\overline{u}\overline{\partial p'}}{\rho \partial x} - \frac{2}{3}\varepsilon$$

$$\frac{\partial \overline{w'w'}}{\partial t} = 0 = -\frac{\partial \overline{w'w'w'}}{\partial z} - 2\frac{\overline{w'\partial p'}}{\rho \partial z} - 2\frac{g}{\theta}\overline{w'\theta_v'} - \frac{2}{3}\varepsilon$$

$$\frac{\partial \overline{u'w'}}{\partial t} = 0 = -\overline{w'w'}\frac{\partial \bar{u}}{\partial z} - \frac{\partial \overline{w'u'u'}}{\partial z} + \left(\frac{\overline{p'\partial u'}}{\partial z} + \frac{\overline{p'\partial w'}}{\partial x}\right)$$

$$\frac{\partial \overline{w'q'}}{\partial t} = 0 = -\overline{w'w'}\frac{\partial \bar{q}}{\partial z} - \frac{\partial \overline{w'w'q'}}{\partial z} - \frac{\overline{q'\partial p'}}{\partial z} + g\beta\overline{\theta'_v q'}$$

Flux Conservation Budget: What the Terms Mean

$$\frac{\partial \overline{w'q'}}{\partial t} = 0 = -\overline{w'w'}\frac{\partial \overline{q}}{\partial z} - \frac{\partial \overline{w'w'q'}}{\partial z} - \frac{\overline{q'\partial p'}}{\partial z} + g\beta\overline{\theta'_v q'}$$

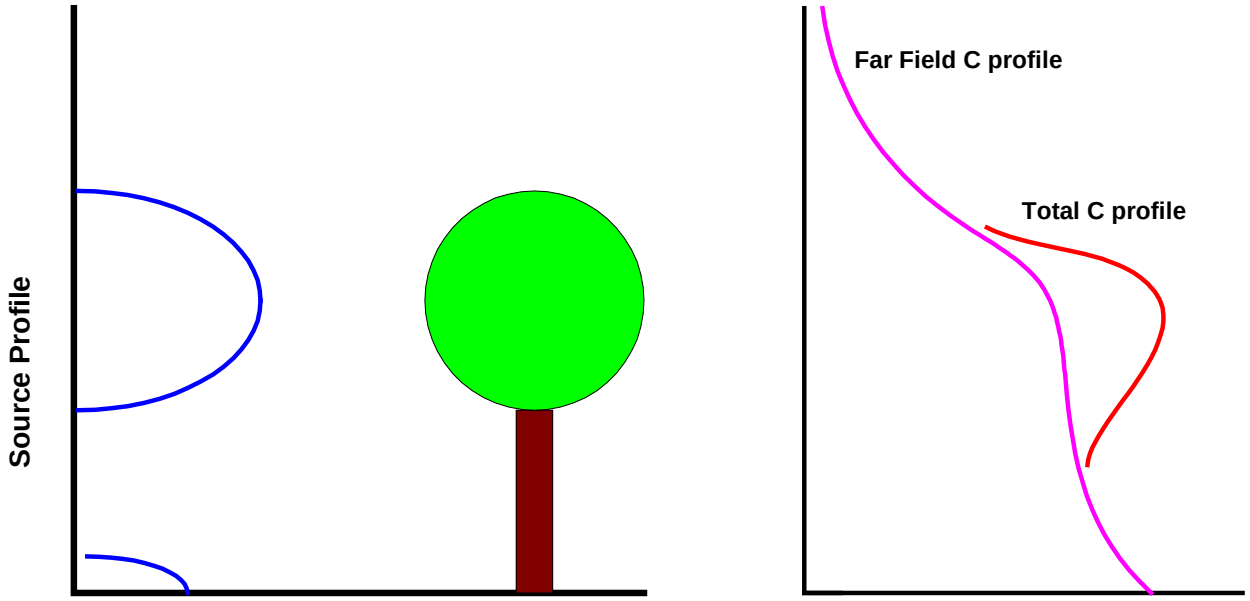
Non-local Transport

Buoyancy prod

Shear Prod

Pressure Interactions

Lagrangian Near- and Far-Field Theory



$$C(z) = C_n(z) + C_f(z)$$

$$C(r,t) = \frac{n(r,t)}{V}$$

$$c(z,t) = \int_0^t \int_0^z P(z,t|z_o,t_o)\, S(z_o,t_o)\, dz_o \; dt_o$$

Concentration is function of conditional probability and Source Strength

Form of Langevin's Equation for Heterogeneous turbulence

$$dw = -a_1(z,t,w)dt + b(z,t,w)\xi(t)dt$$

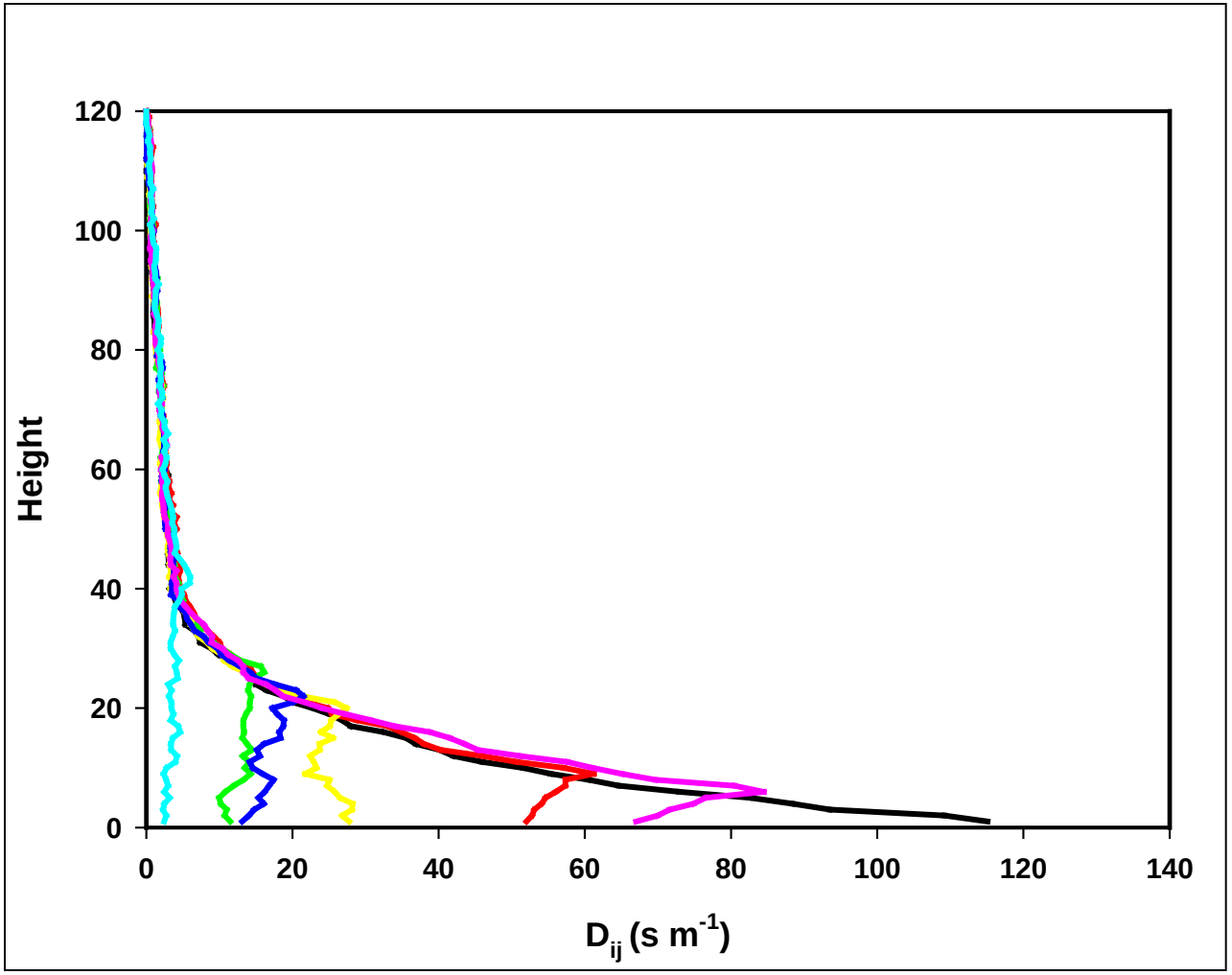
$$dw_L = (-\frac{w_L}{T_L} + \frac{1}{2}\left[1 + \frac{{w_L}^2}{\sigma_w^2}\right]\frac{\partial\sigma_W^2}{\partial z})dt + \sqrt{\frac{2\sigma_W^2}{T_L}}\xi(t)dt$$

Dispersion Matrix

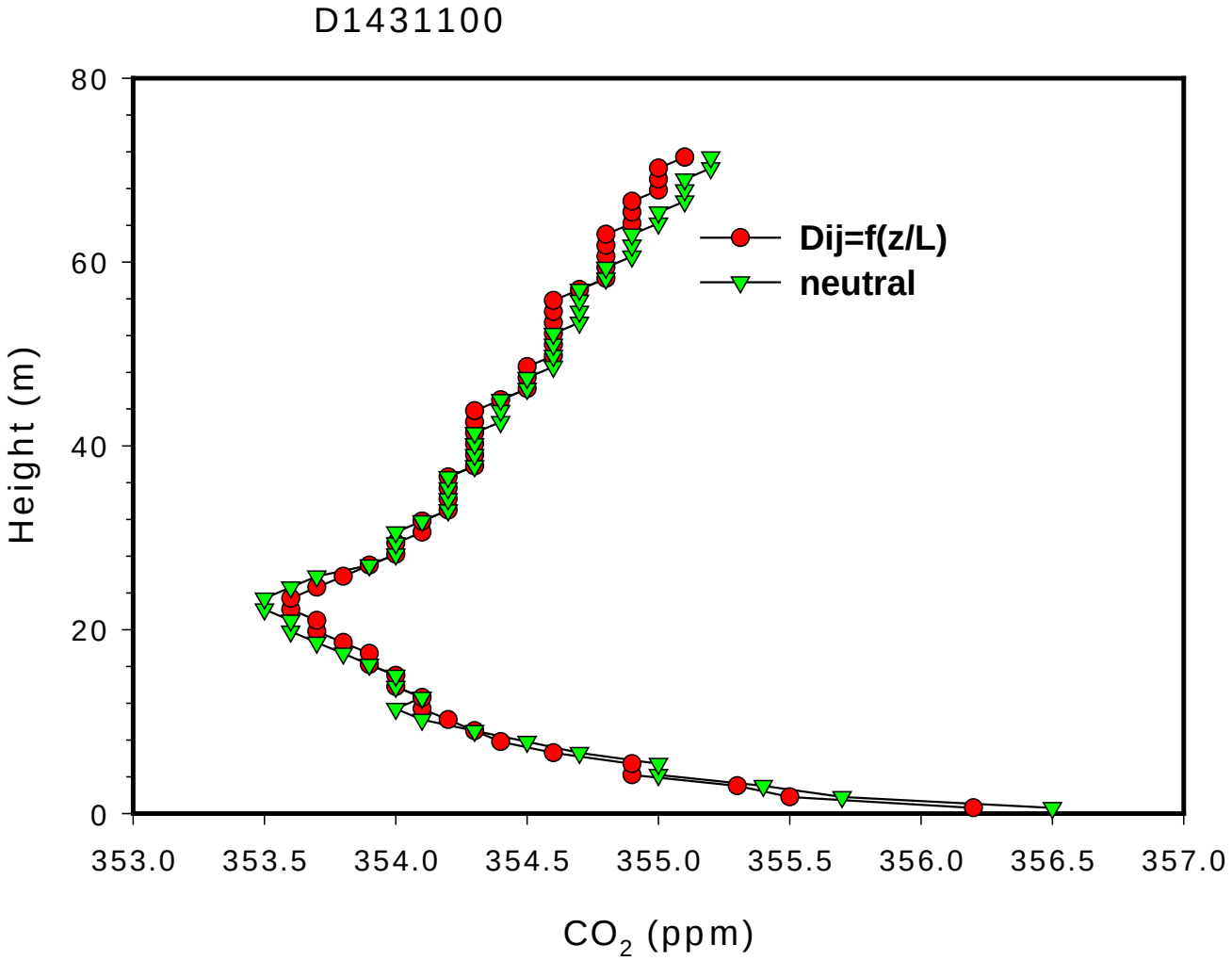
$$c_i - c_r = \sum_{j=1}^{N} S_j(c_j) D_{i,j} \Delta z_j$$

$$D_{ij} = \frac{C_i - C_r}{S_j \Delta z_j}$$

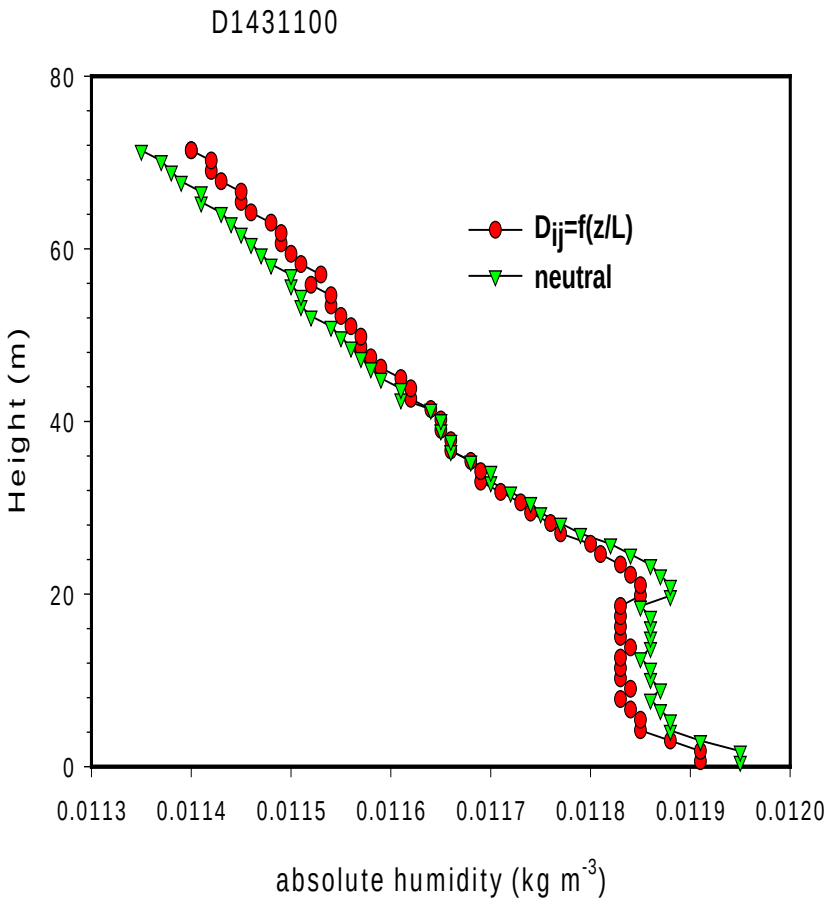
Turbulent Mixing

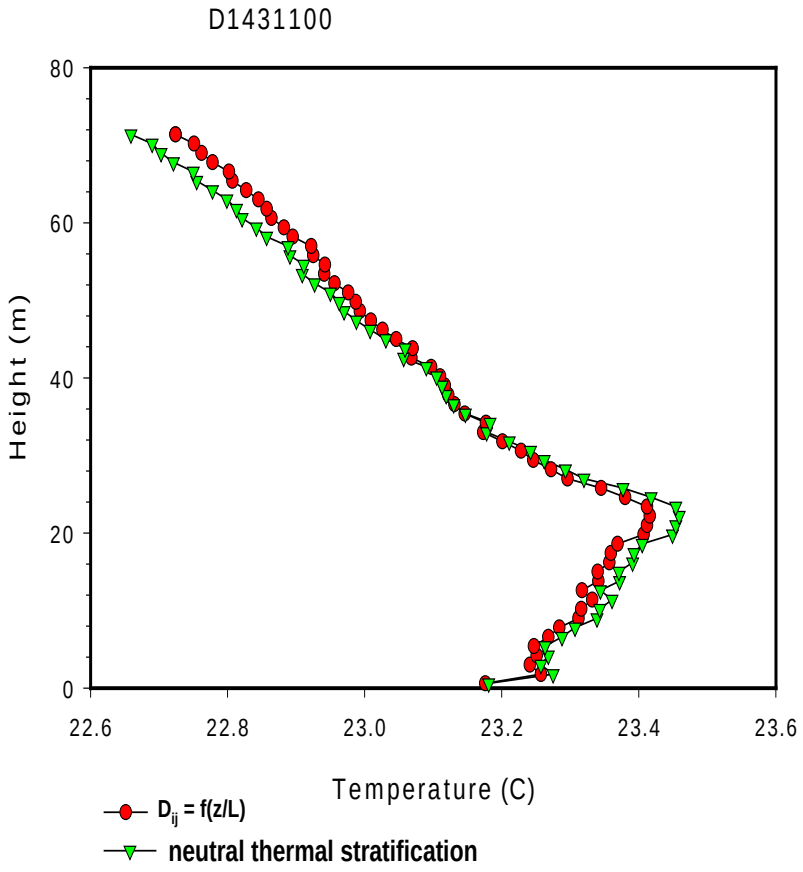


Vertical Gradients in CO_2

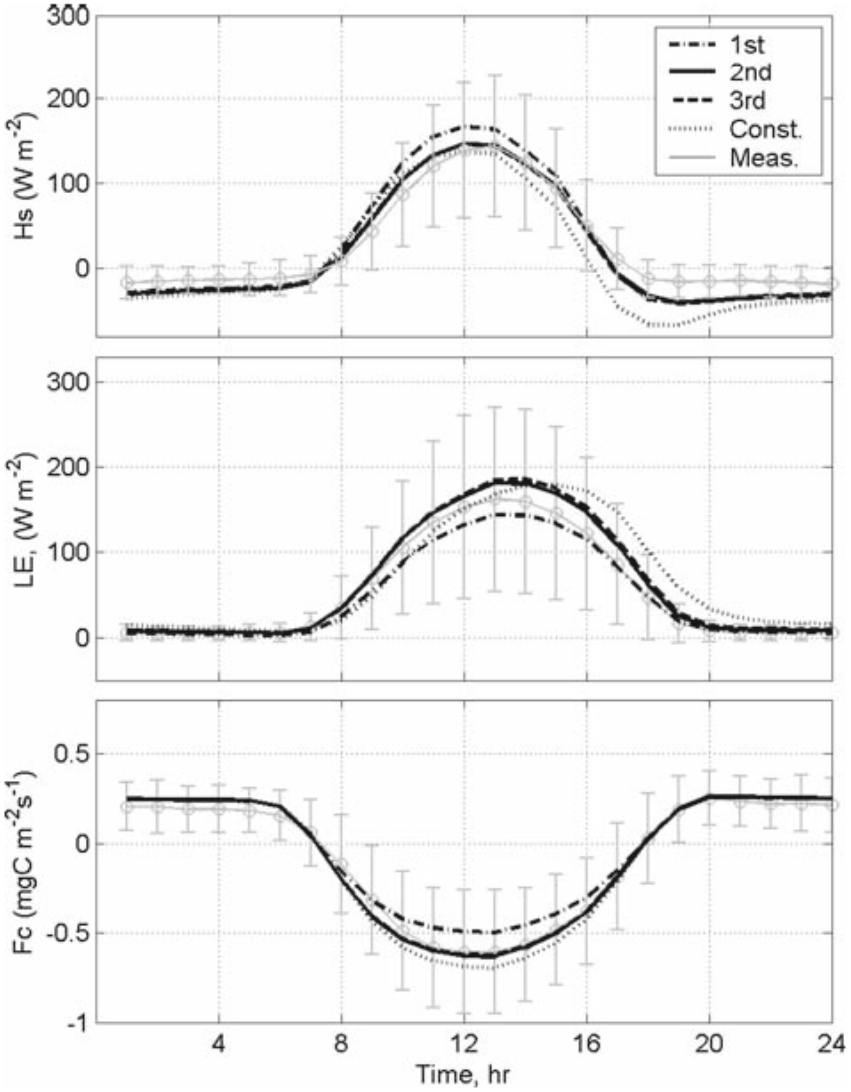


Vertical Gradients in q and T





Model Hierarchy

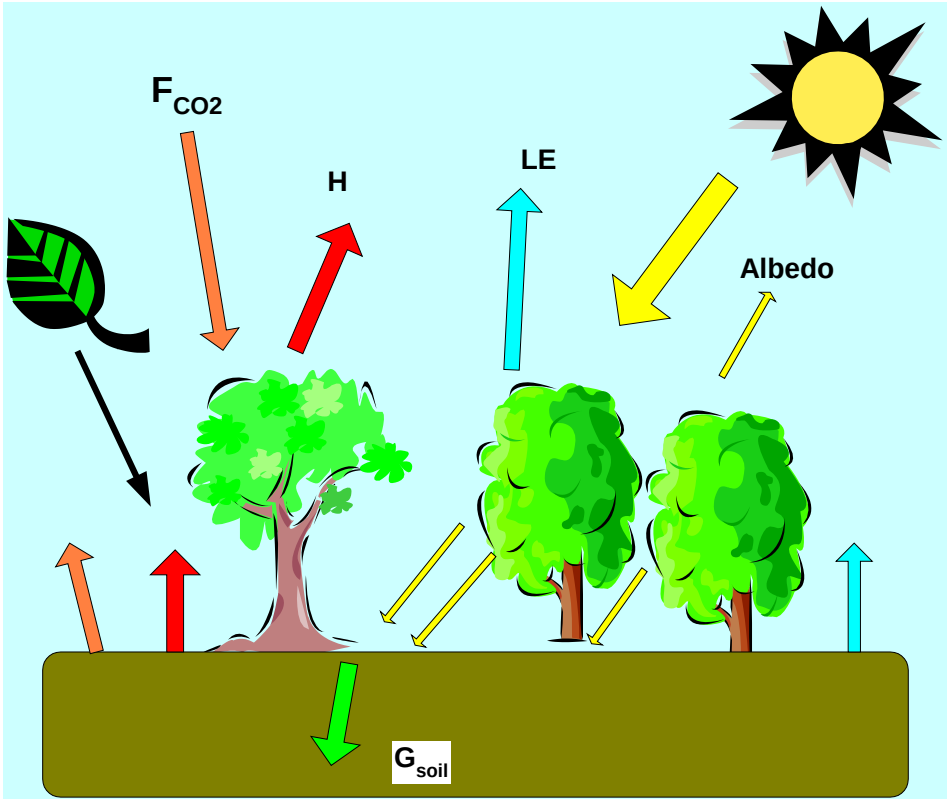


Juang et al 2008 BLM

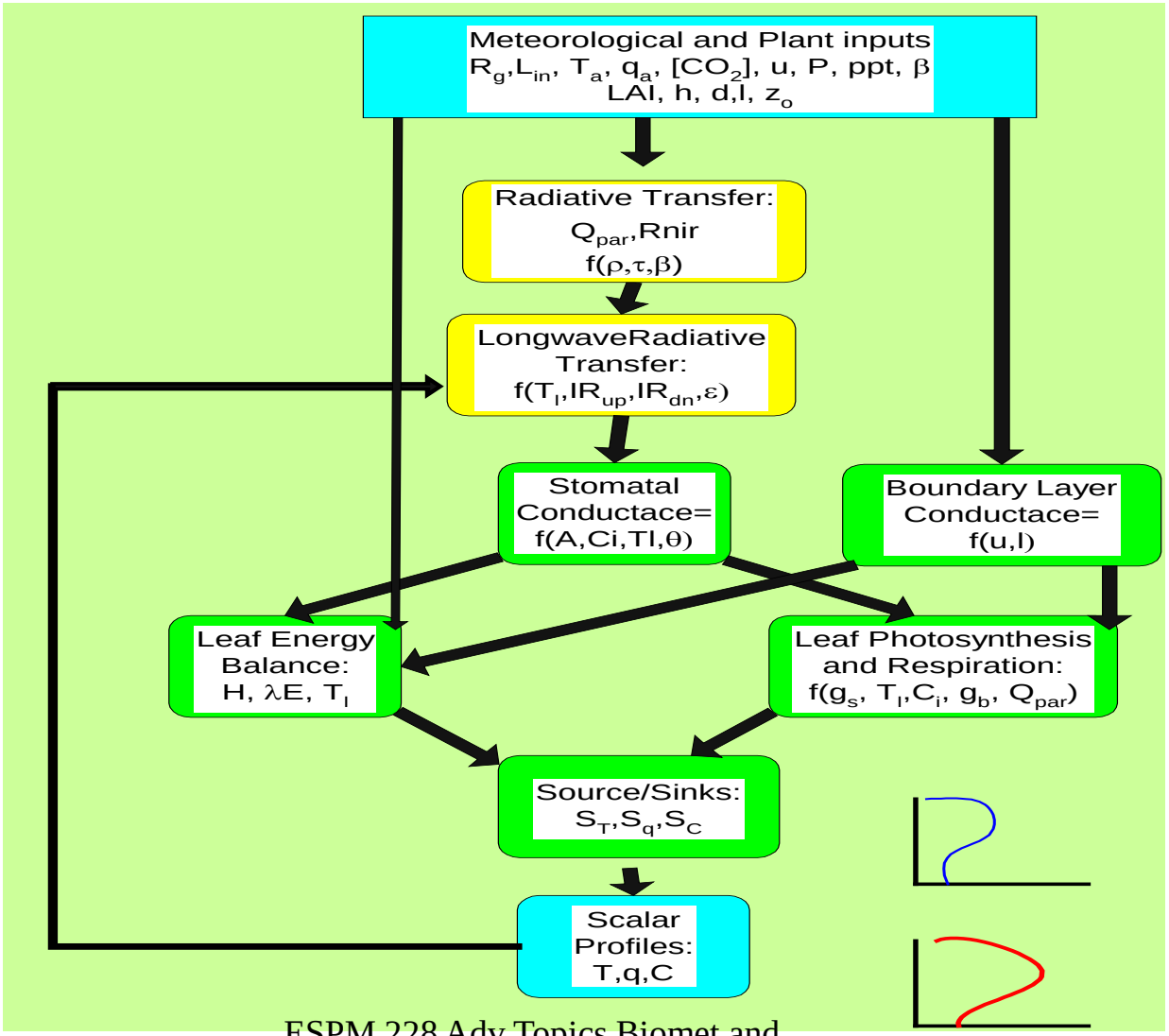
CANOAK MODEL

Physiology
Photosynthesis
Stomatal Conductance
Transpiration

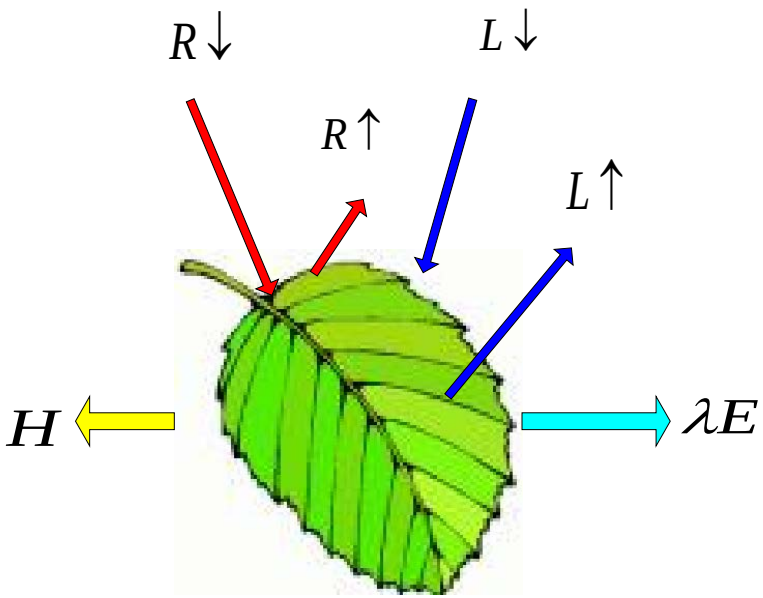
Micrometeorology
Leaf/Soil Energy Balance
Radiative Transfer
Lagrangian Turbulent Transfer



CANOAK Schematic



Leaf Energy Balance



- R: is shortwave solar energy, W m^{-2}
- L: is Longwave, terrestrial energy, W m^{-2}
- λE: Latent Heat Flux Density, W m^{-2}
- H: Sensible Heat Flux Density, W m^{-2}

Leaf Energy Balance, Wet, Transpiring Leaf

$$R_n = H + \lambda E$$

Net Radiation is balanced by the sum of
Sensible and Latent Heat exchange

$$Q = (1-\rho)R\downarrow + \varepsilon L\downarrow = \varepsilon\sigma T_l^4 + H + \lambda E$$

Derivation

1: Leaf Energy Balance

$$R_n = H + \lambda E$$

2: Resistance Equations for H and λE

$$\lambda E = \frac{(m_v / m_a)\lambda \rho_a g_w (e_s(T_l) - e_a)}{P}$$

$$H = \rho_a C_p (T_l - T_a) g_h$$

3: Linearize T^4 and $e_s(T)$

$$e_s(T_l) - e_a = D + e_s'(T_l - T_a) = \frac{\lambda E \cdot P}{\rho_a \lambda (m_v / m_a) g_w}$$

$$\varepsilon \sigma T_l^4 = \varepsilon \sigma T_a^4 + 4 \varepsilon \sigma T_a^3 (T_l - T_a)$$

Linearize with 1st order Taylor's Expansion Series

$$f(x) \sim f(x_0) + (x - x_0)\frac{df}{dx}$$

$$\varepsilon\sigma T_l^4 = \varepsilon\sigma T_a^4 + 4\varepsilon\sigma T_a^3 (T_l - T_a)$$

Linearize the Saturation Vapor Pressure function

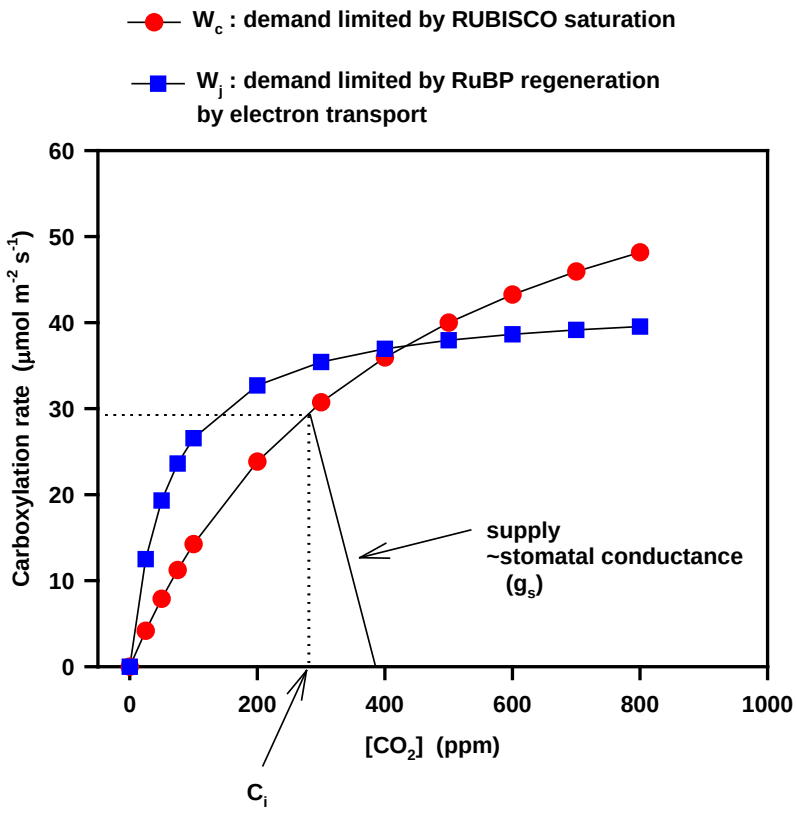
$$e_s(T_l) = e_s(T_a) + e_s'(T_l - T_a) \qquad e_s(T)' = \frac{de_s(T)}{dT}$$

$$e_s(T_l) = e_x(T_a) + e_s'(T_l - T_a) + \frac{e_s''}{2}(T_l - T_a)^2 \qquad e_s(T)'' = \frac{d^2 e_s(T)}{dT^2}$$

$$V_c - 0.5V_o = V_c\left(1 - \frac{\Gamma^*}{C_c}\right) = \min[W_c, W_j, W_p]\left(1 - \frac{\Gamma^*}{C_c}\right)$$

- W_c, the rate of carboxylation when ribulose bisphosphate (RuBP) is saturated
-
- W_j, the carboxylation rate when RuBP regeneration is limited by electron transport.

- W_p carboxylation rate with triose phosphate utilization



Analytical Equation for Leaf Photosynthesis

Table 1 List of equations and unknowns for solving coupled photosynthesis-stomatal conductance model (after Baldocchi, 1994)

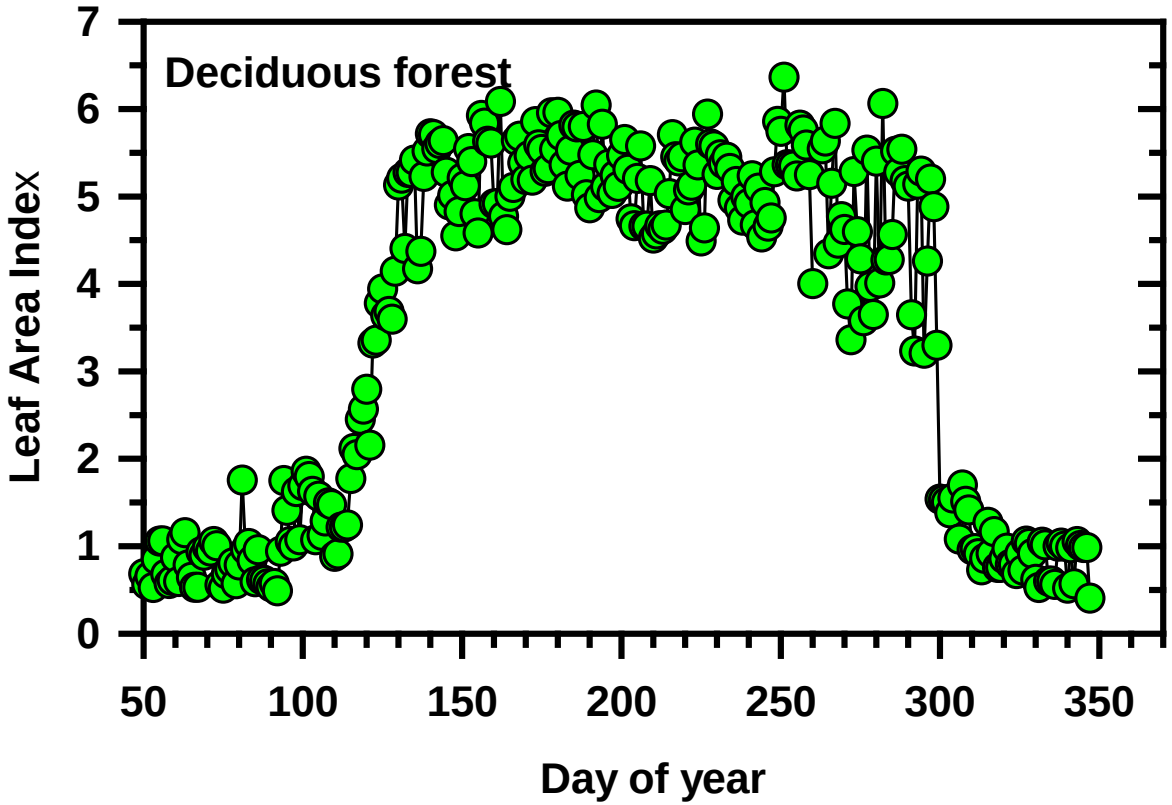
Unknowns	Equation
C_s	$C_a - \frac{A}{g_b}$
C_i	$C_s - \frac{A}{g_s}$
g_s	$\frac{m A rh}{C_s} + g_0$
$A+R_d$	$V_c - 0.5 V_o = \min[W_c, W_j](1 - \frac{\Gamma}{C_i})$
W_j, W_c	$\frac{a C_i - ad}{e C_i + b}$

Baldocchi 1994 Tree Physiology

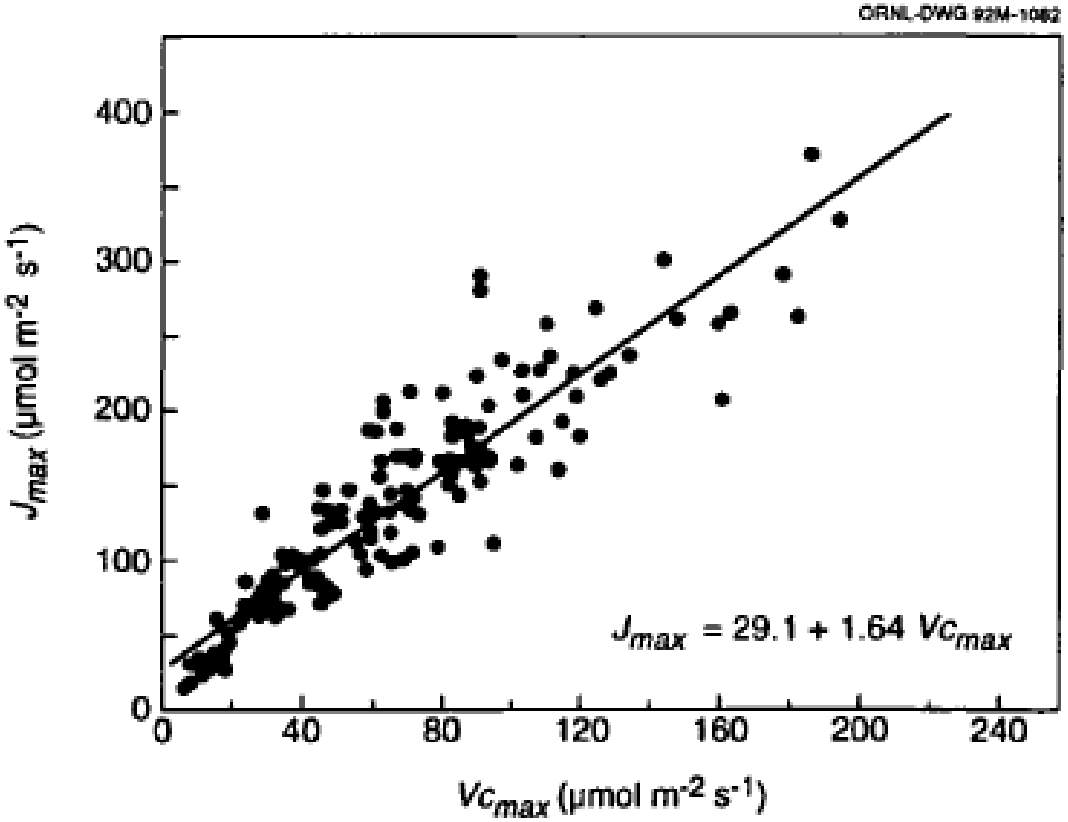
Model Parameters

- Leaf Area Index
- Photosynthetic Capacity, J_{max}, V_{cmax}
- Kinetics
- Basal Respiration, leaf/soil

Seasonality in LAI, Deciduous Forests

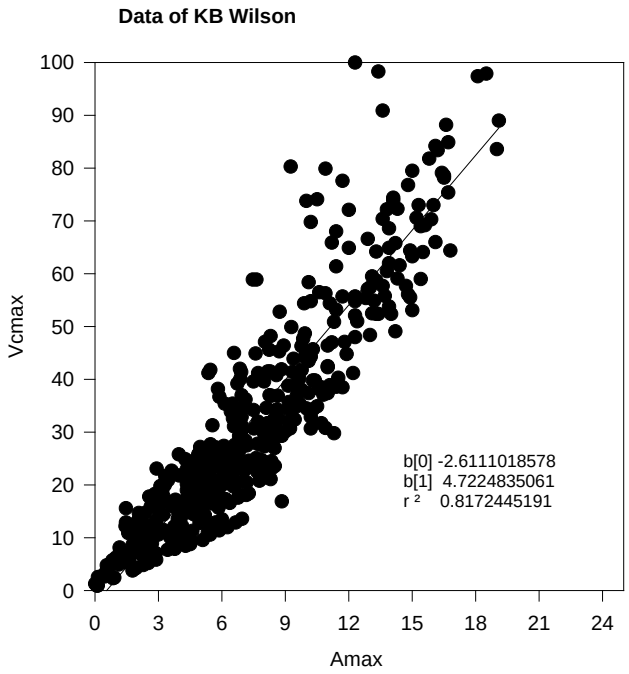


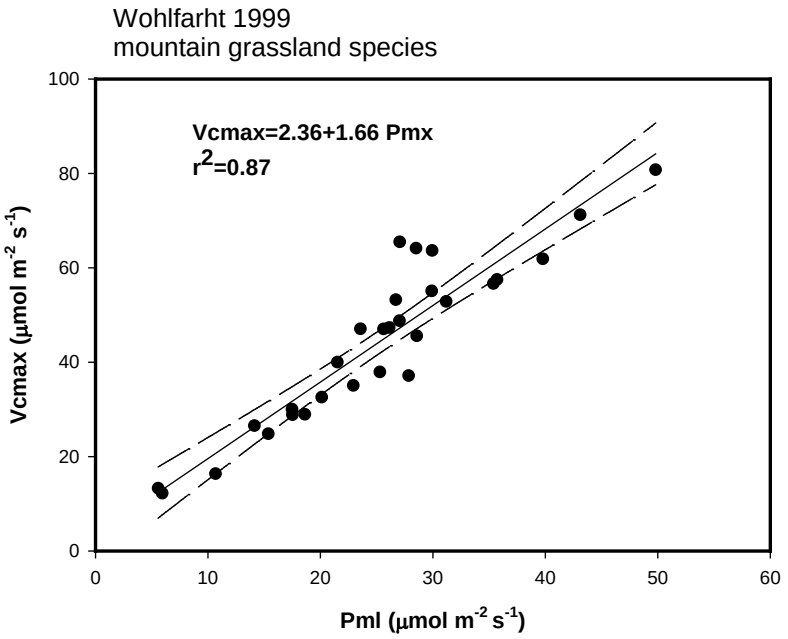
J_{max} and V_{cmax} scale with one another



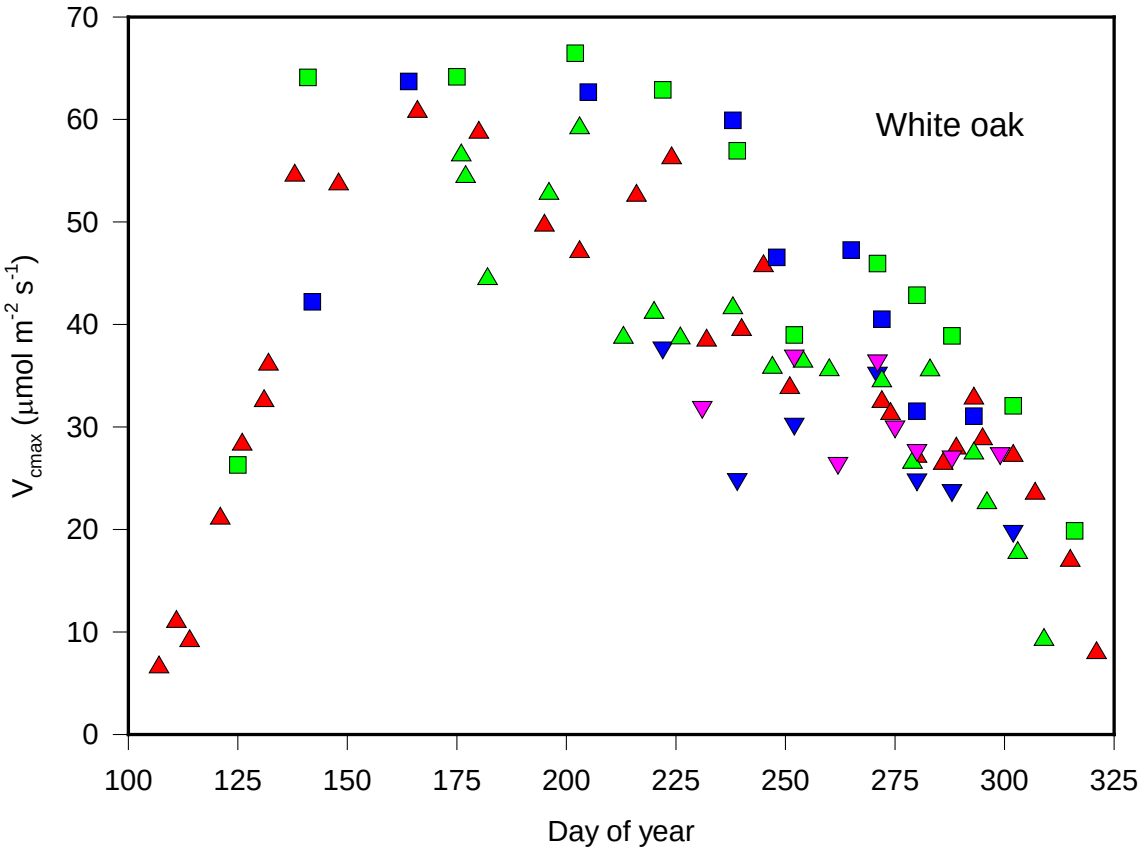
Wullschleger, 1993 J Expt Bot

Practical Assessment for Vcmax in sites with many species and spatial variability



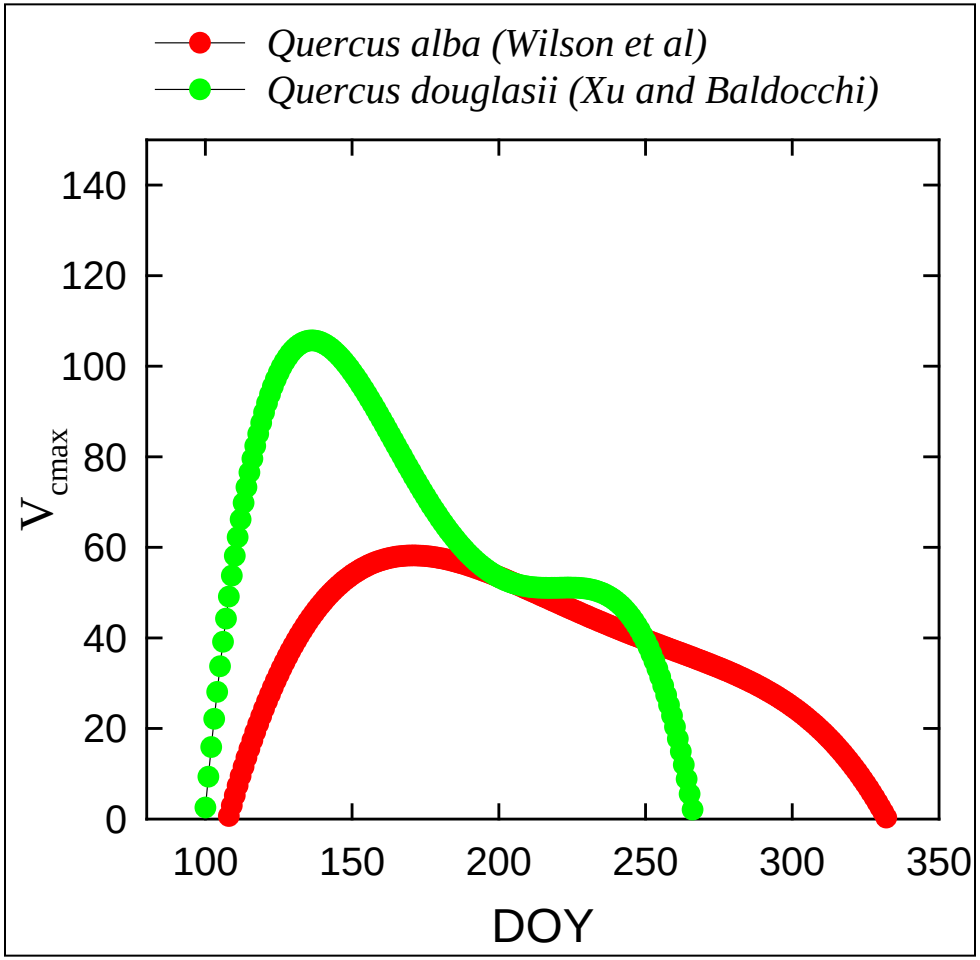


Seasonality in V_{cmax}



Wilson et al. 2001 Tree Physiol

High V_{cmax} must be Achieved in Seasonally- Droughted Ecosystems to attain Positive Carbon Balance

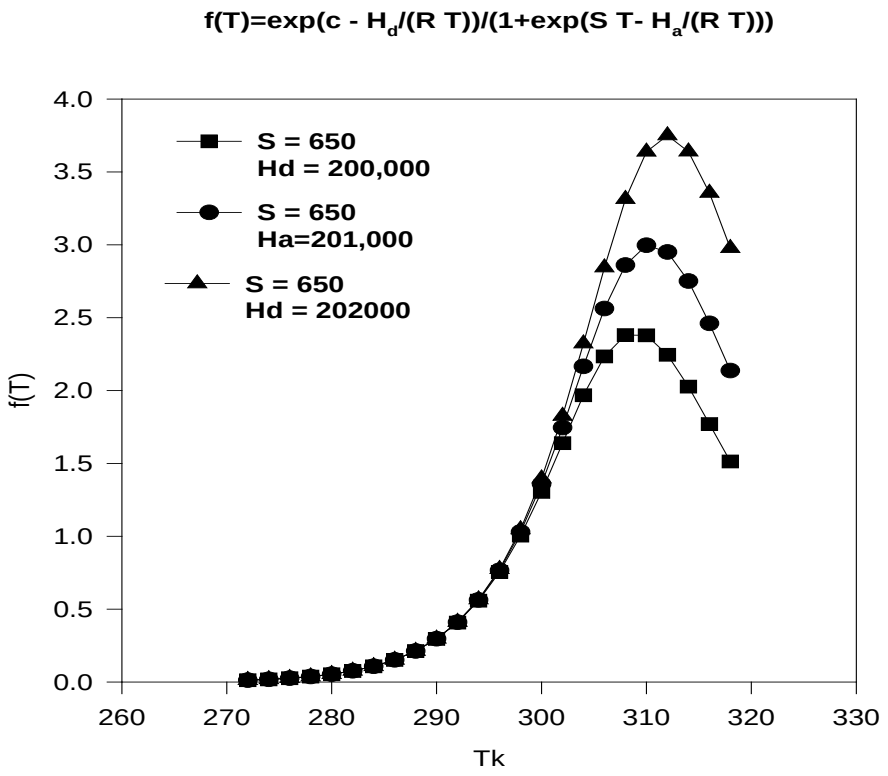


Area under the Curves are Similar

Temperature Response Curve

$$f(T) = f(T_{298}) \frac{\exp(c - \frac{\Delta H_a}{RT})}{1 + \exp(sT_K - \frac{\Delta H_d}{RT_K})}$$

$$f(T) = \frac{\exp\left(E_a \cdot (T_l - T_{opt}) / (R \cdot T_l \cdot T_{opt})\right)}{1 + \exp\left(\frac{s \cdot T_l - \Delta H_d)}{R \cdot T_l}\right)}$$



E_a or H_a activation energy
s: change in entropy
H_d: change in deactivation enthalpy
R: Universal gas constant
T: temperature, K

Harley and Tenhunen; Bernacchi et al.

Today, We Know Parameters have Uncertainty

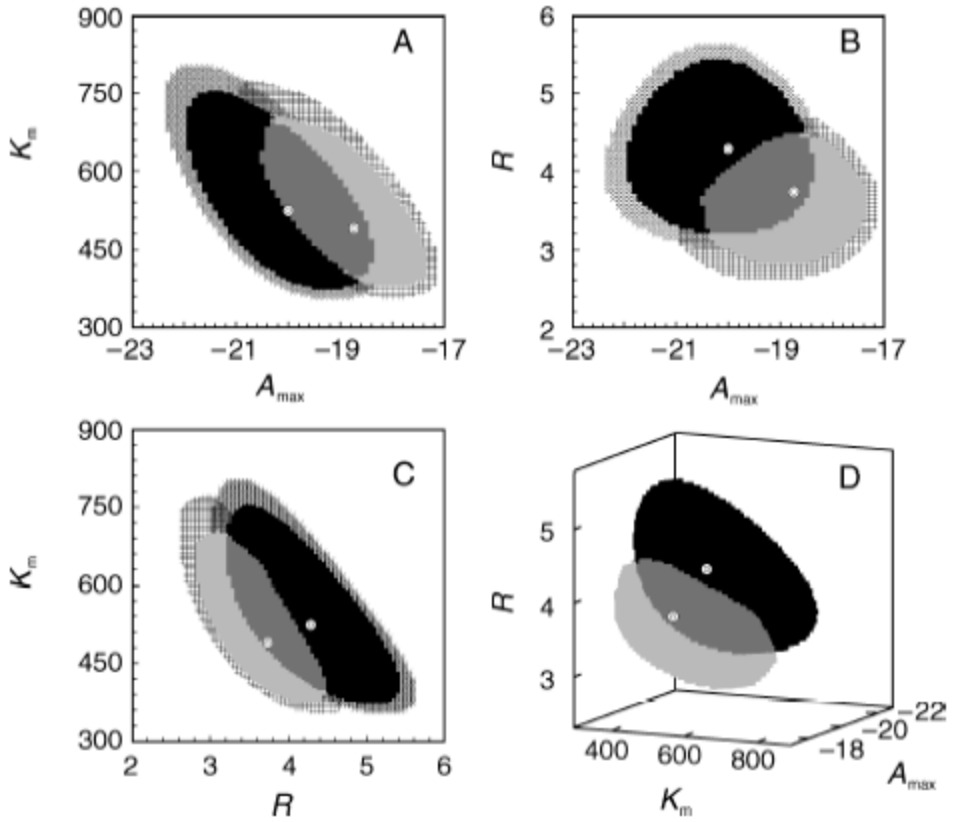


Figure 6. Parameter estimates for a Michaelis-Menten model of leaf photosynthesis ($= A_{max} I/(K_m + I) + R$) determined from June 2000 carbon dioxide (CO_2) flux data. The black region represents the 95% uncertainty limits of parameter triplets assuming Gaussian uncertainties with $\sigma = 2.7$ μmol m^{-2} s^{-1}, and the gray indicates the corresponding 95% uncertainty region assuming the double exponential probability density function with $\sqrt{2}\beta = 2.5$ μmol m^{-2} s^{-1}. The cross-hatched areas indicate the 99% uncertainty regions. The first three panels (A–C) represent different 2-D projections of the parameter sets and the final panel (D) shows a 3-D representation. Abbreviations: A_{max} = maximum rate of uptake; K_m = half-saturation constant; I = incident PPFD; and R = ecosystem respiration. Units for A_{max} and R are μmol CO_2 m^{-2} s^{-1}, and for K_m are μmol PPFD m^{-2} s^{-1}.

Hollinger and Richardson 2005 Tree Physiol

Part 2, Upscaling from Landscapes to the Globe

'*Space: The final frontier … To boldly go where no man has gone before*'

Captain James Kirk, Starship Enterprise

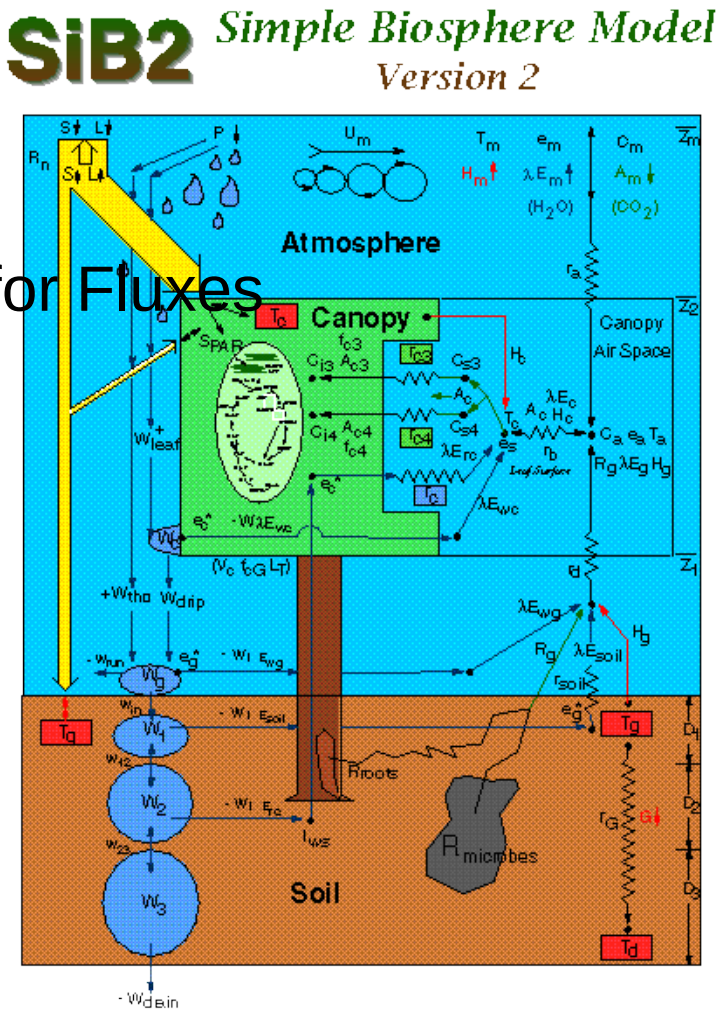
Big Picture Question Regarding Predicting and Quantifying the 'Breathing of the Biosphere':

- **How can We Be 'Everywhere All the Time?'**

Big-Leaf Model

Ohm's Law Analog for Fluxes

$$F = \frac{V}{\Sigma R}$$



- Motivation
  - Current Global-Scale Remote Sensing Products tend to rely on
    - Highly-Tuned Light Use Efficiency Approach
      - GPP=PAR*fPAR*LUE (since Monteith 1960's)
    - Empirical, Data-Driven Approach (machine learning technique)
    - Some Forcings come from Satellite Remote Sensing Snap Shots, at fine Spatial scale (< 1 km)
    - Other Forcings come from coarse reanalysis data (several tens of km resolution)
  - Hypothesis, We can do Better by:
    - Applying the Principles taught in Biometeorology 129 and Ecosystem Ecology 111 which Reflect Intellectual Advances in these Fields over the past Decade
    - Merging Vast Environmental Databases
    - Utilizing Microsoft Cloud Computational Resources

Lessons Learned from the CanOak Model

25+ years of Developing and Testing a Hierarchy of Scaling Models with Flux Measurements at Contrasting Oak Woodland Sites in Tennessee and California

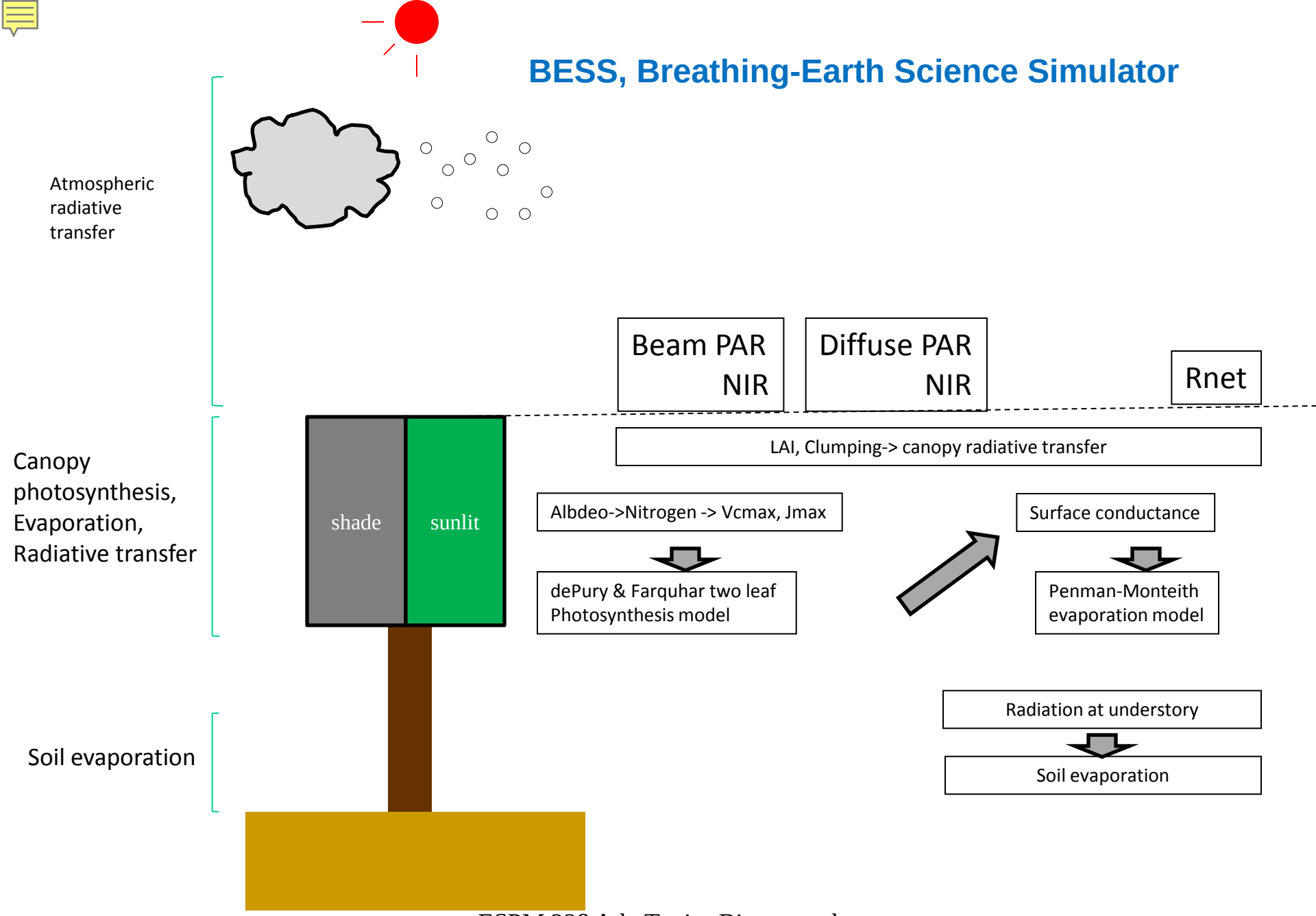
We Must:

- Couple Carbon and Water Fluxes
- Assess Non-Linear Biophysical Functions with Leaf-Level Microclimate Conditions
- Consider Sun and Shade fractions separately
- Consider effects of Clumped Vegetation on Light Transfer
- Consider Seasonal Variations in Physiological Capacity of Leaves and Structure of the Canopy

Necessary Attributes of Global Biophysical ET Model: Applying Lessons from the Berkeley Biomet Class and CANOAK

- Treat Canopy as Dual Source (Sun/Shade), Two-Layer (Vegetation/Soil) system
  - Treat Non-Linear Processes with Statistical Rigor (Norman, 1980s)
- Requires Information on Direct and Diffuse Portions of Sunlight
  - Monte Carlo Atmospheric Radiative Transfer model (Kobayashi + Iwabuchi,, 2008)
- Light transfer through canopies MUST consider Leaf Clumping
  - Apply New Global Clumping Maps of Chen et al./Pisek et al.
- Couple Carbon-Water Fluxes for Constrained Stomatal Conductance Simulations
  - Photosynthesis and Transpiration on Sun/Shade Leaf Fractions (dePury and Farquhar, 1996)
  - Compute Leaf Energy Balance to compute Leaf Saturation Vapor Pressure and Respiration Correctly
  - Photosynthesis of C_3 and C_4 vegetation Must be considered Separately
- Use Emerging Ecosystem Scaling Rules to parameterize models, based on remote sensing spatio-temporal inputs
  - Vcmax=f(N)=f(albedo) (Ollinger et al; Hollinger et al;Schulze et al.; Wright et al.)
  - Seasonality in Vcmax is considered (Wang et al.)

BESS, Breathing-Earth Science Simulator



Challenge for a Computationally-Challenged Biometeorology Lab: Extracting Data Drivers from Global Remote Sensing to Run the Model

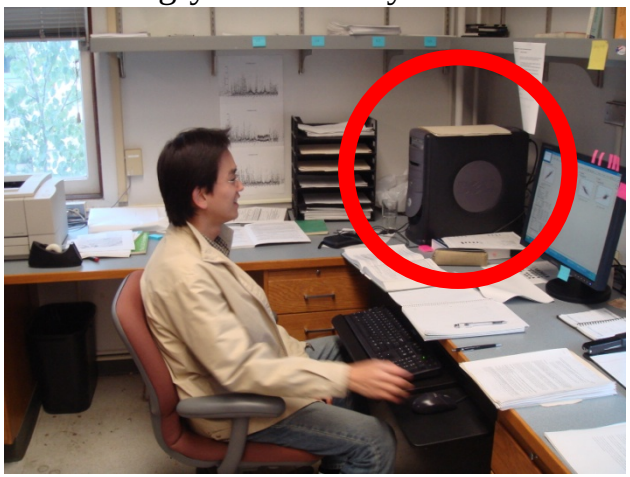
MOD04	aerosol
MOD05	Precipitable water
MOD06	cloud
MOD07	Temperature, ozone
MCD43	albedo
MOD11	Skin temperature
MOD15	LAI
POLDER	Foliage clumping

Atmospheric radiative transfer

Net radiation

Canopy radiative transfer

Youngryel was lonely with 1 PC



Size and Number of Candidate Data Sets is Enormous

	#Source Files	Source Size	# Result Files	Result Size
USA (18)	21850	238 GB	27375	261 GB
FluxTower (3)	80670	993 GB	58400	210 GB
Global (3)	152670	2414 GB	352225	630 GB

US: 15 tiles

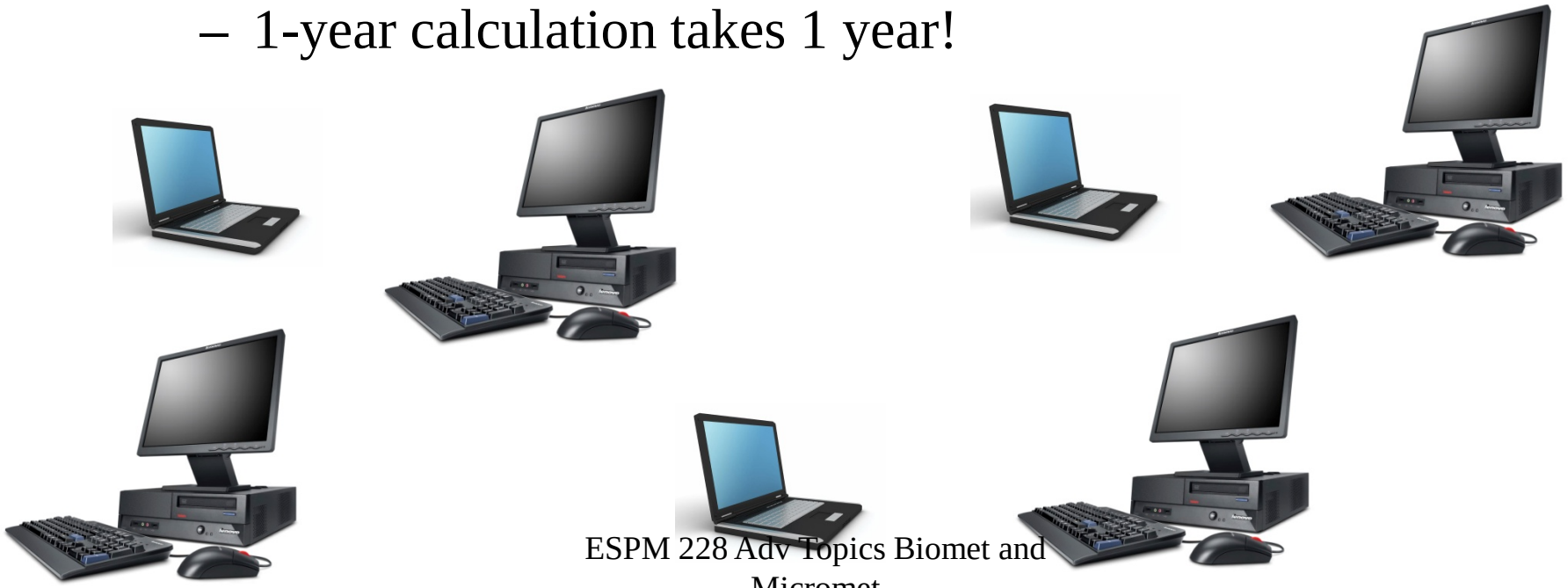
FluxTower: 32 tiles

Global: 193 tiles

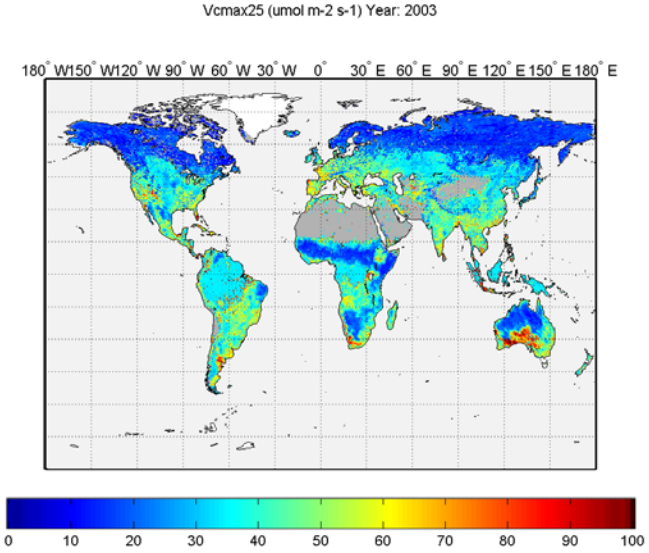
1. **Global 1-year source data: 2.4 TB (10 yr: 24 TB)**
2. **How to know which source files are missed among >0.1 million files**

Barriers to Global Remote Sensing by the Berkeley Biometeorology Lab

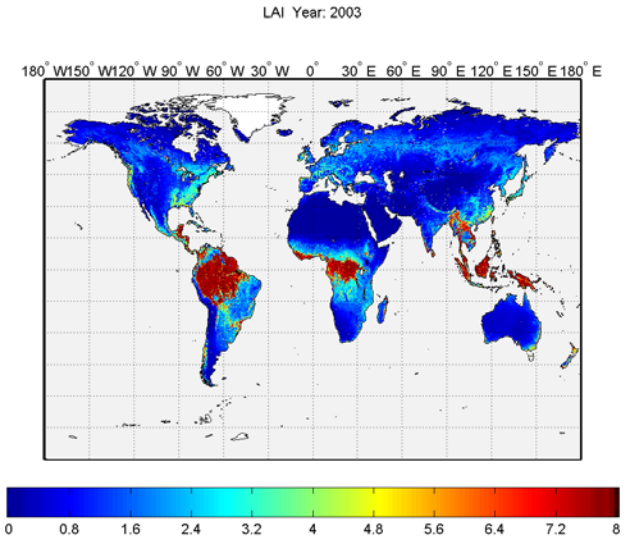
- Data processing
  - Global 1-year calculation: 9000 CPU hours
  - That is, 375 days.
  - 1-year calculation takes 1 year!



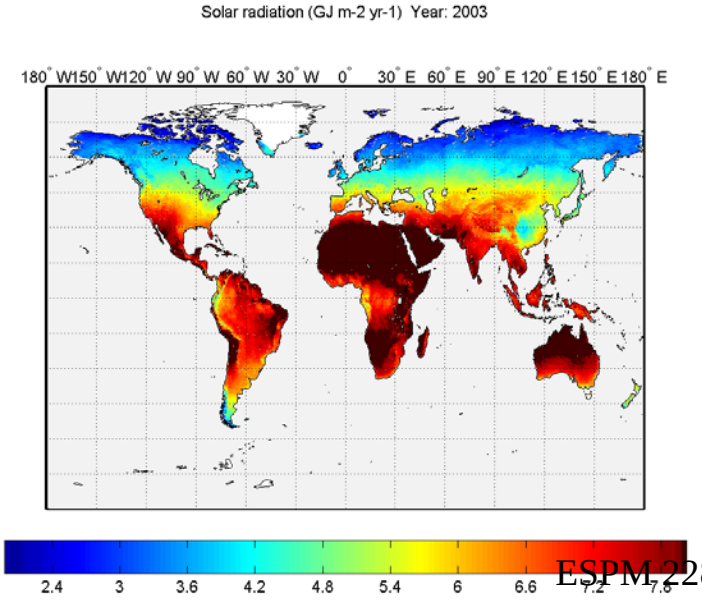
Photosynthetic Capacity



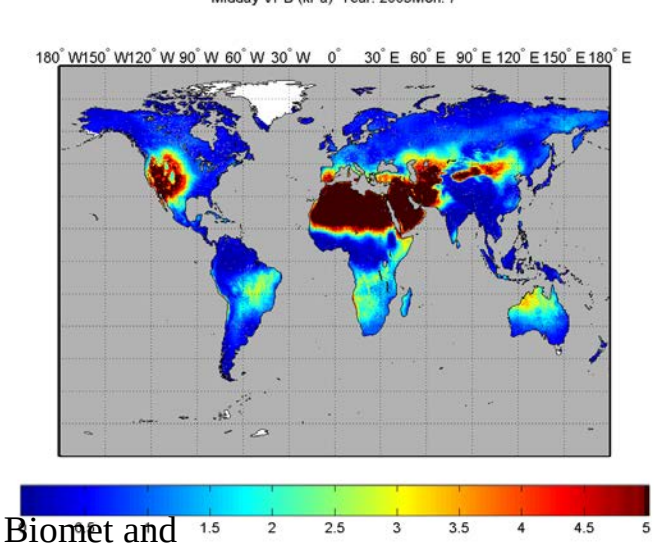
Leaf Area Index



Solar Radiation



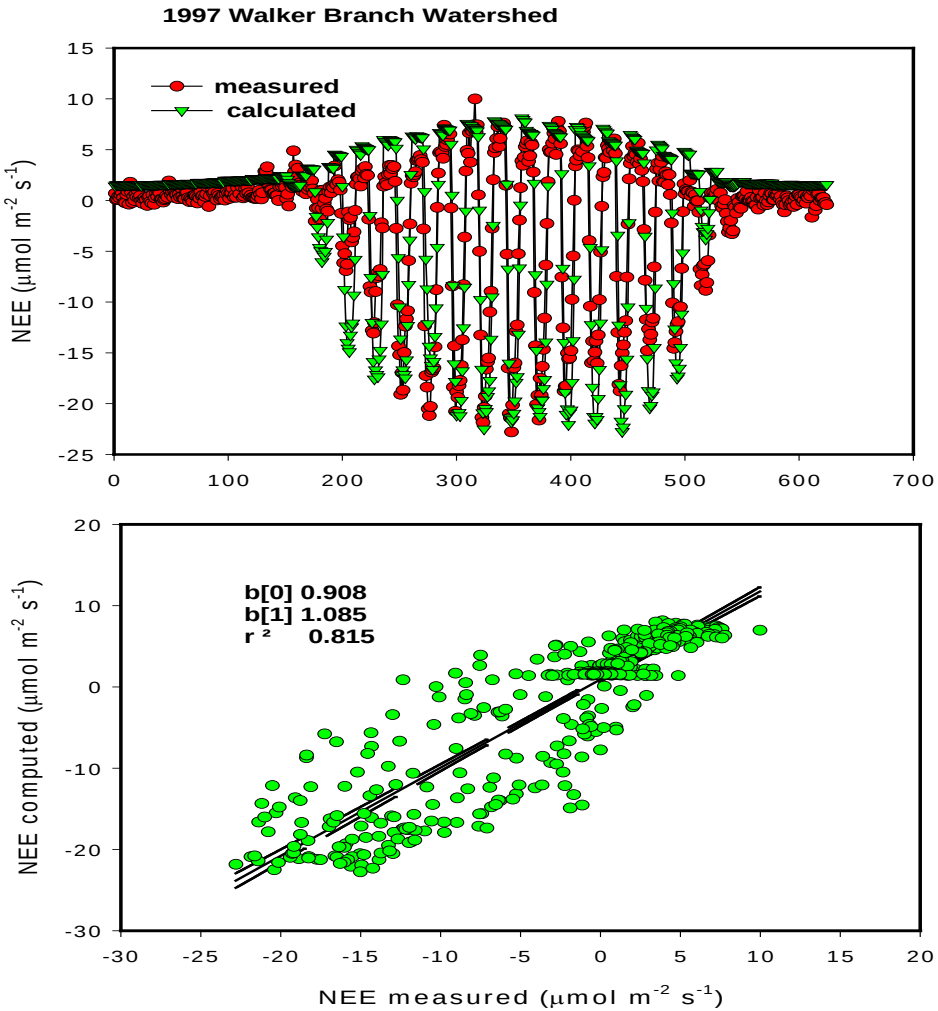
Humidity Deficits



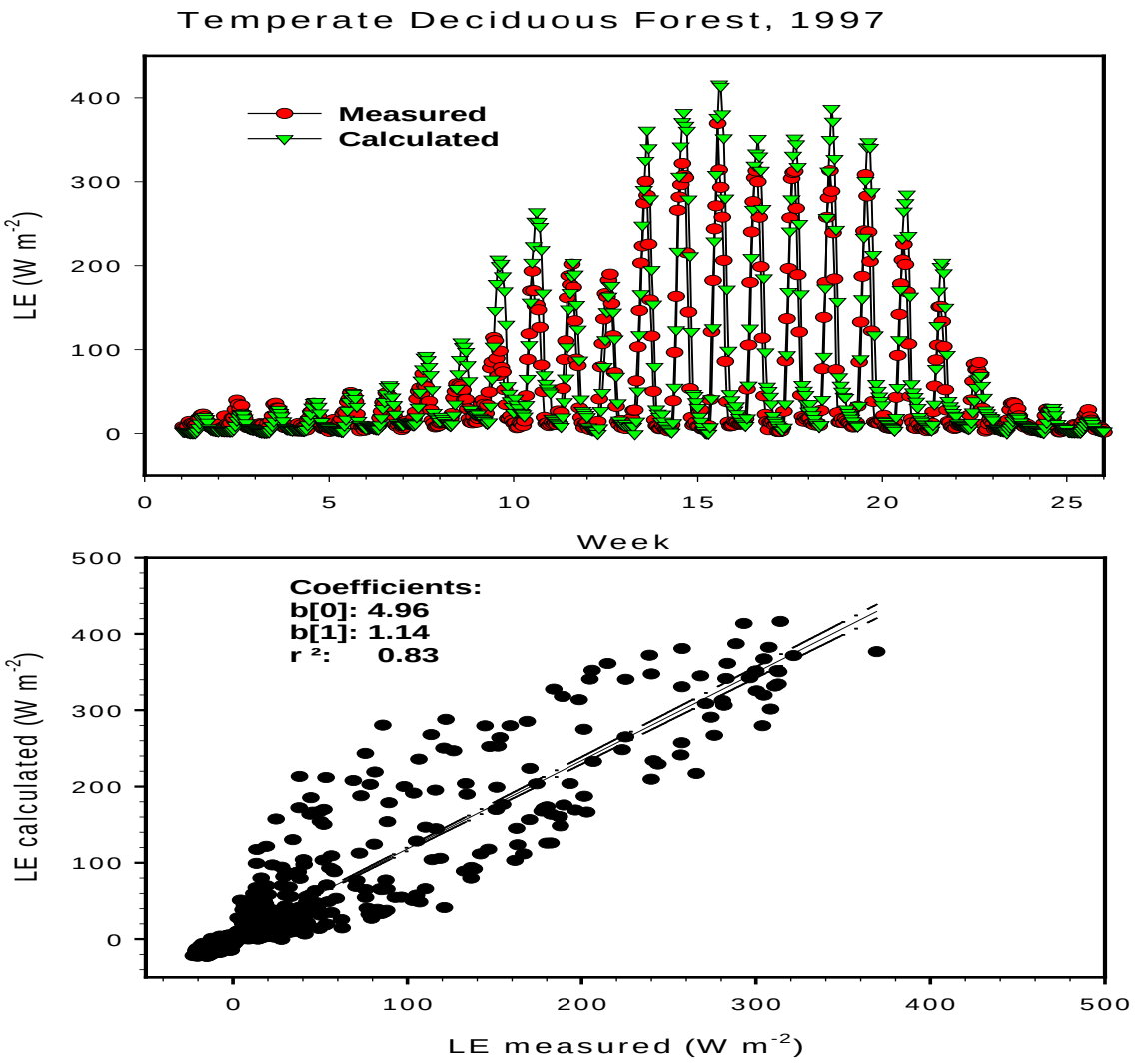
Results and Discussion

P1. Validation and Testing

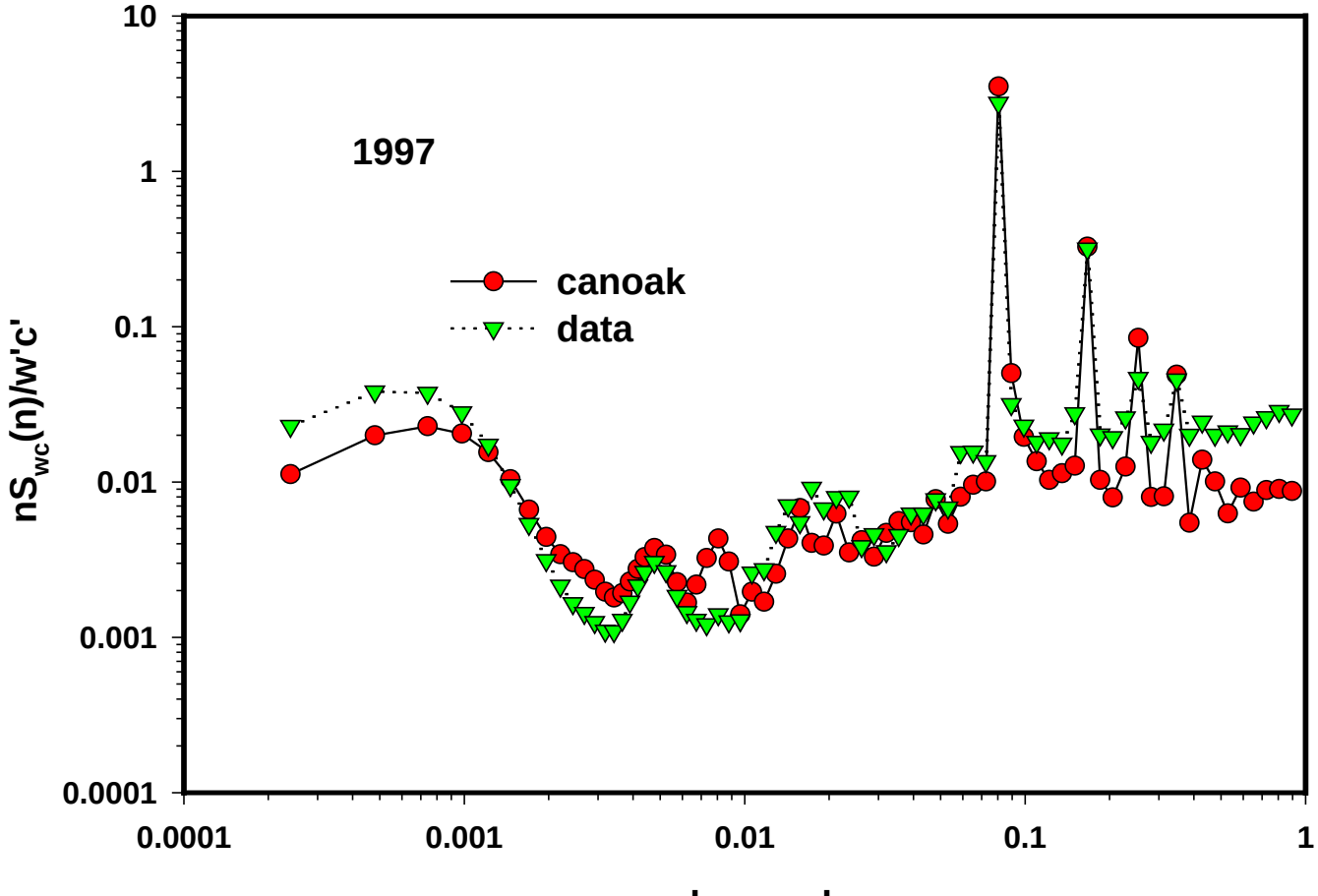
Model Test: Hourly to Annual Time Scale



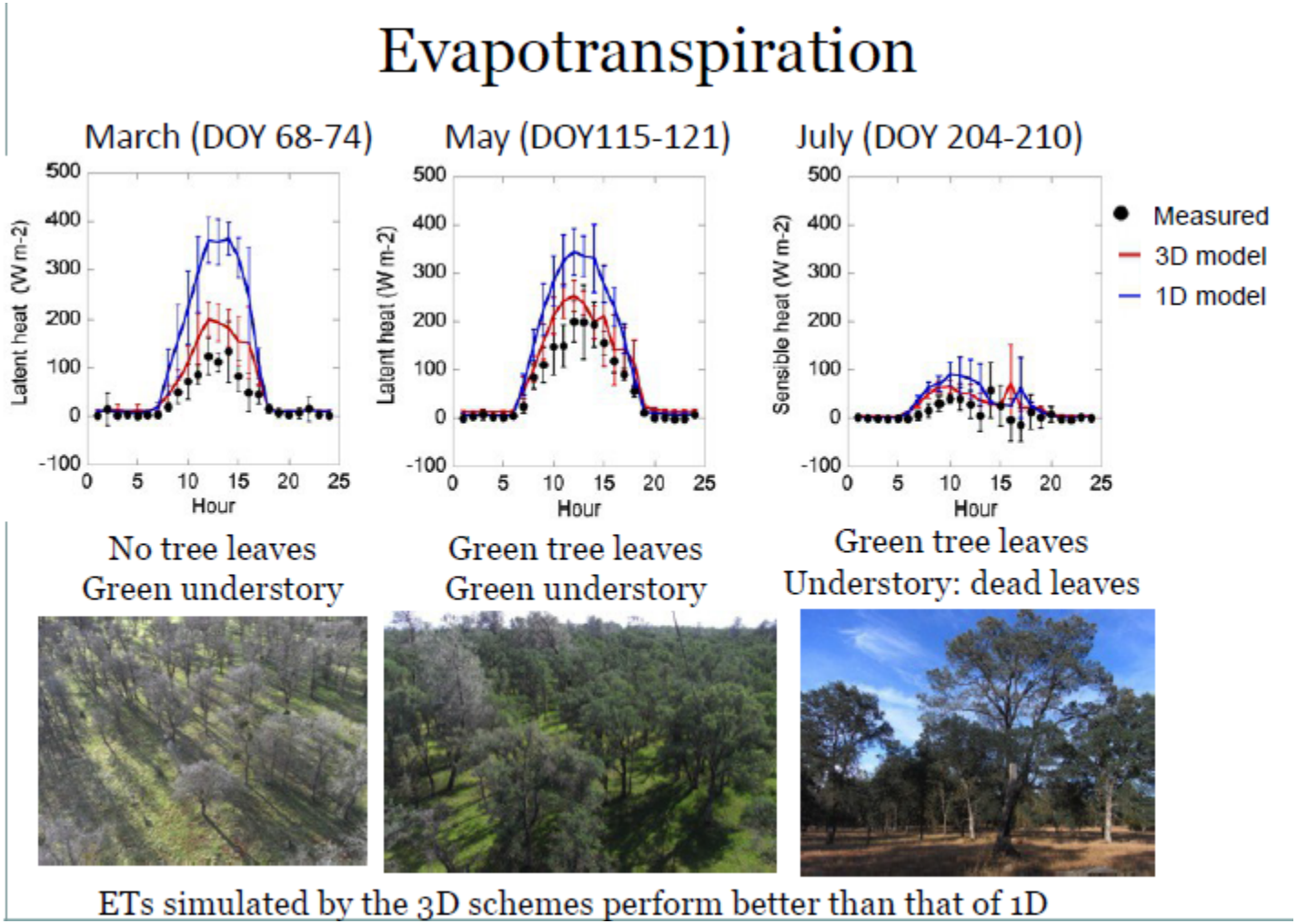
Model Test: Hourly Data



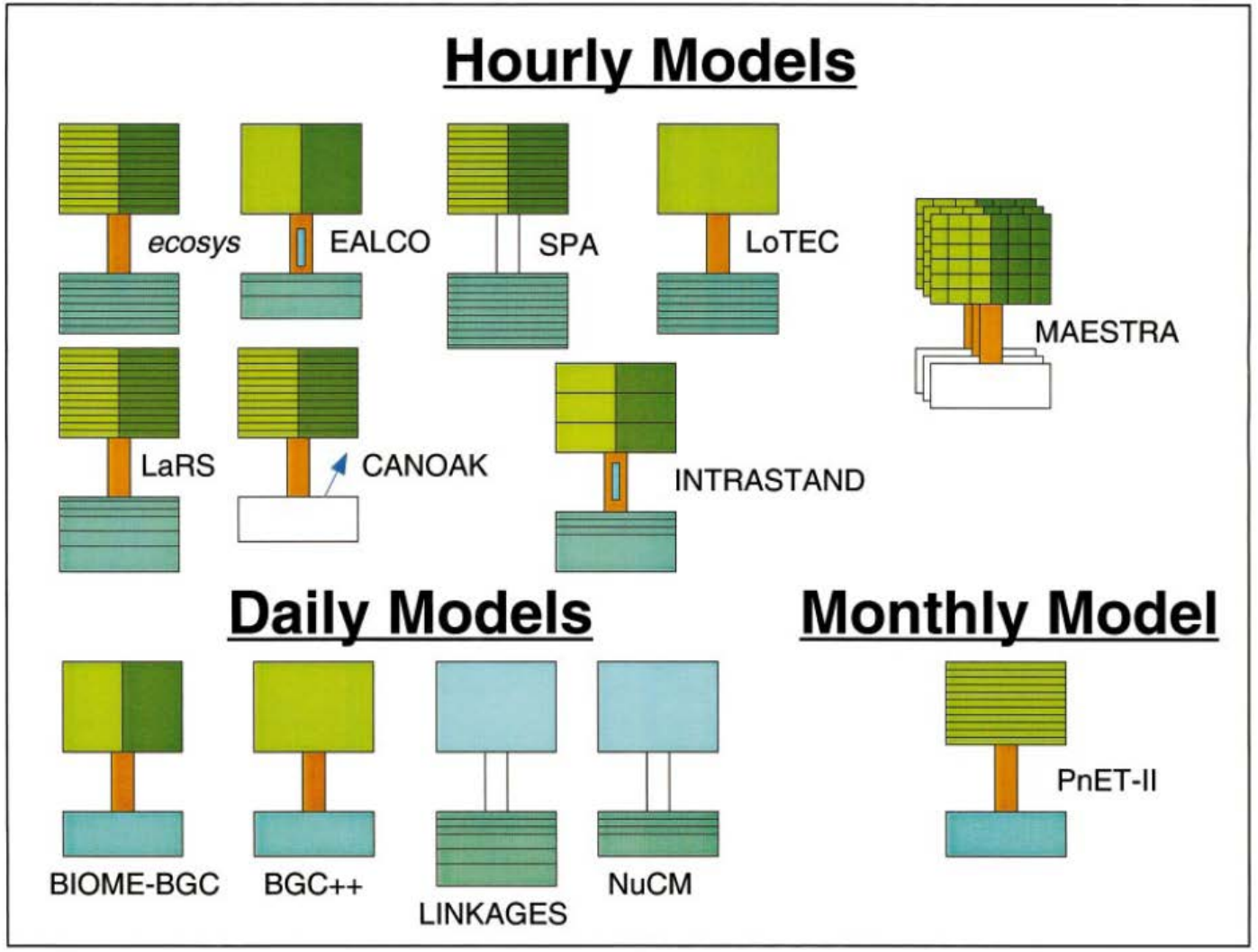
Time Scales of Interannual Variability
are recreated forcing model withi weather and seasonal changes in LAI and Vcmax



Importance of Model Hierarchy Testing

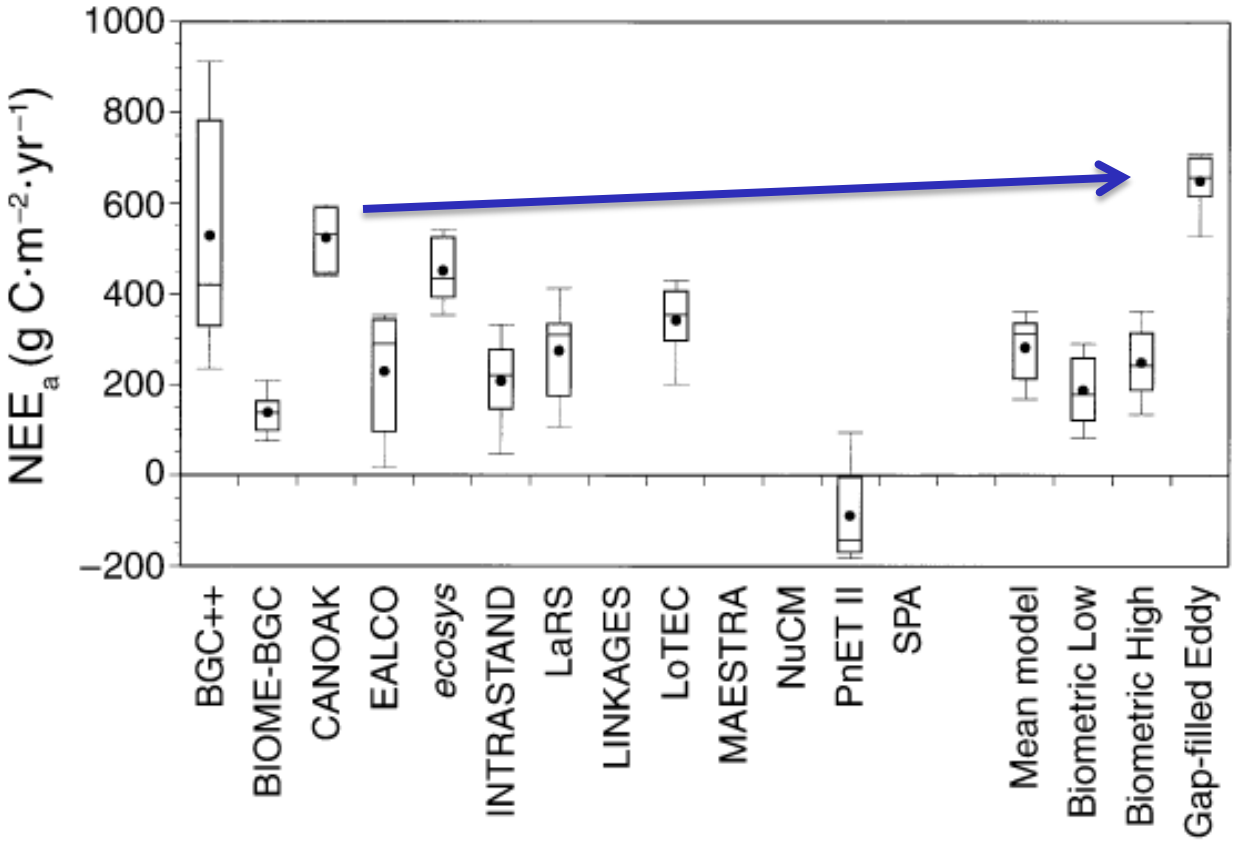


Kobayashi et al



Hanson et al. 2004. Ecol Mono

Model Validation:
Who is Right and Wrong, and Why?
How Good is Good Enough?



Hansen et al, 2004 Ecol Monograph

Monte Carlo Model parameterization

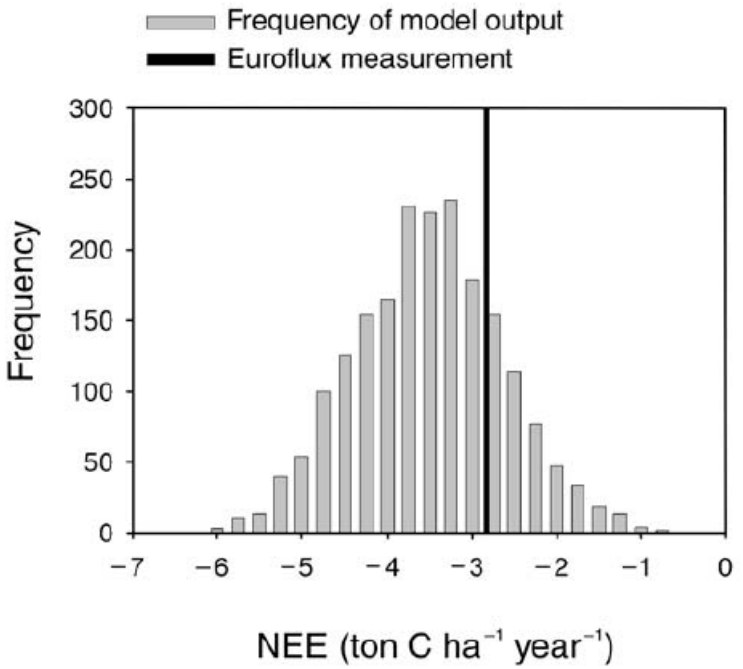
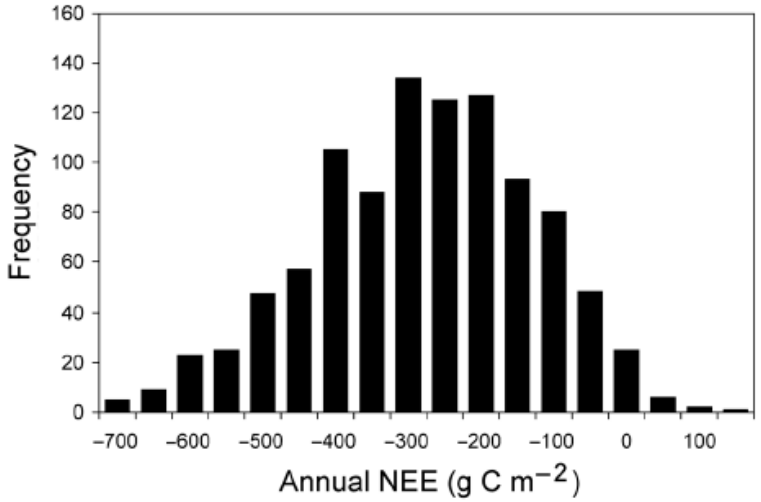


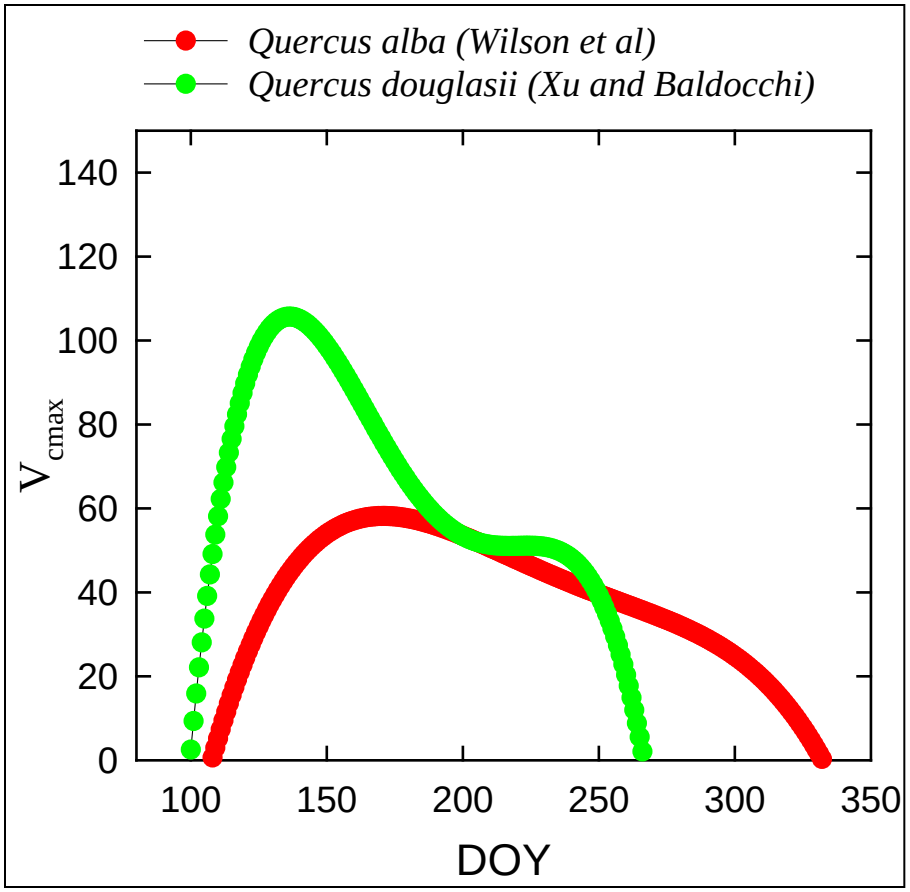
Figure 2. Distribution of the total net ecosystem exchange (NEE; Mg C ha^{-1} year^{-1}) in 1997 for the Hesse forest in France. The calculation of this distribution is based on 2000 Monte Carlo simulations. Only the uncertainty of ten key parameters was taken into account. The black bar above shows the measured (Euroflux) NEE value and does

Verbeek et al 2006 Tree Physiol



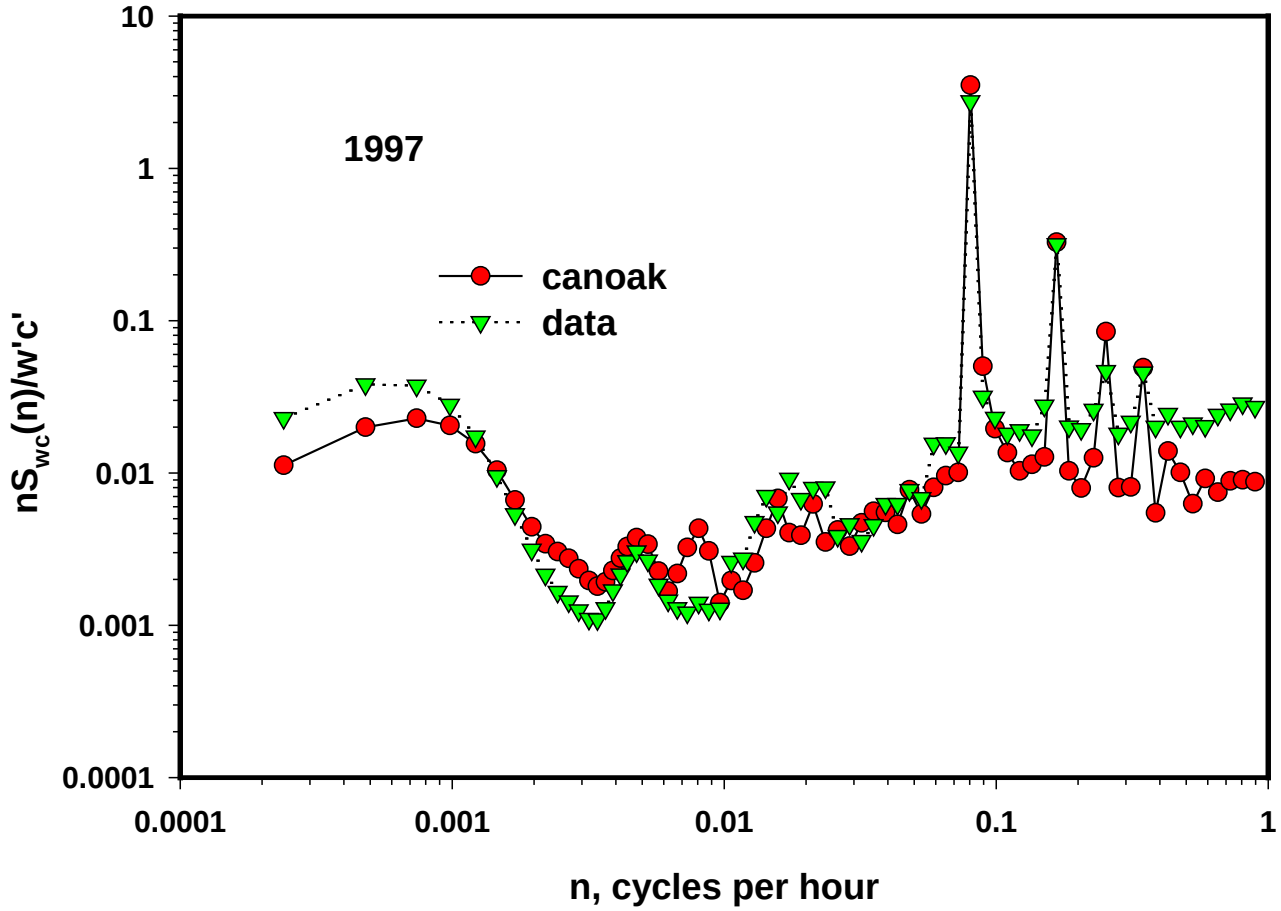
Medlyn et al 2005 Tree Physiol

Seasonality of Model Parameters: e.g. Photosynthetic Capacity



Live Fast, Die Young
In Stressed Environments

Measured and Modeled CO2 Flux Spectra



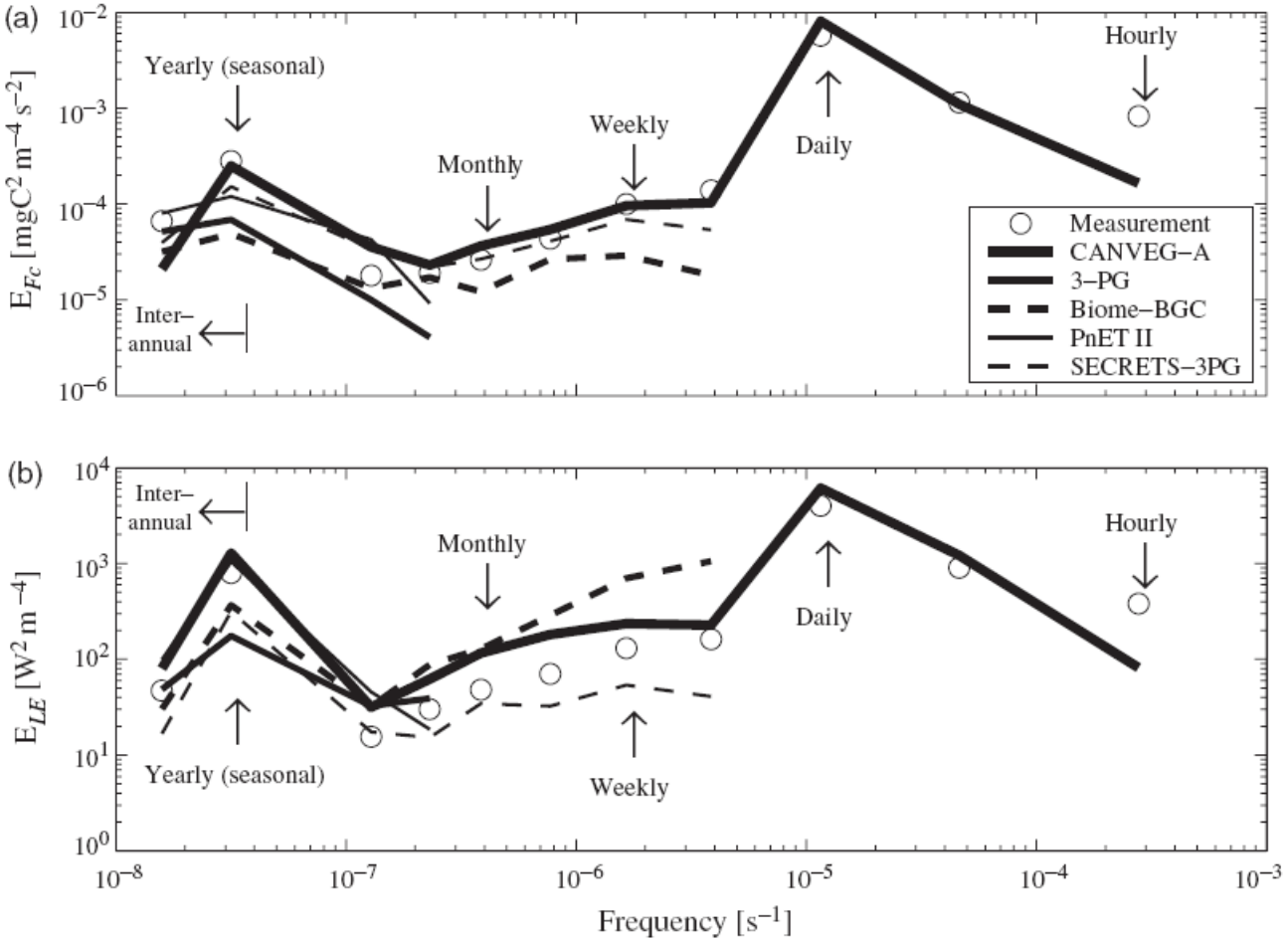
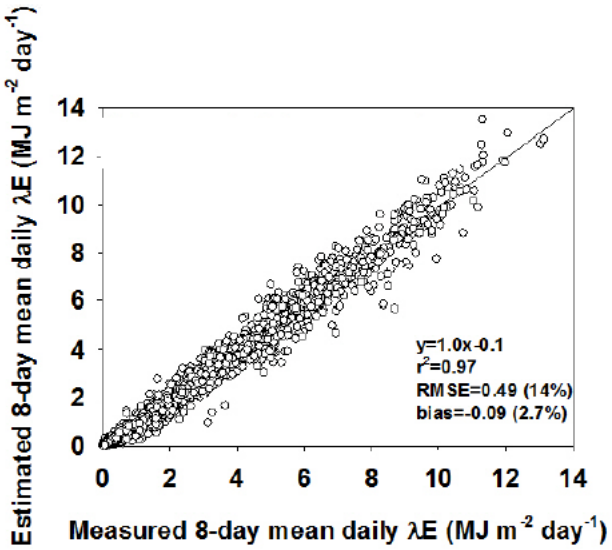
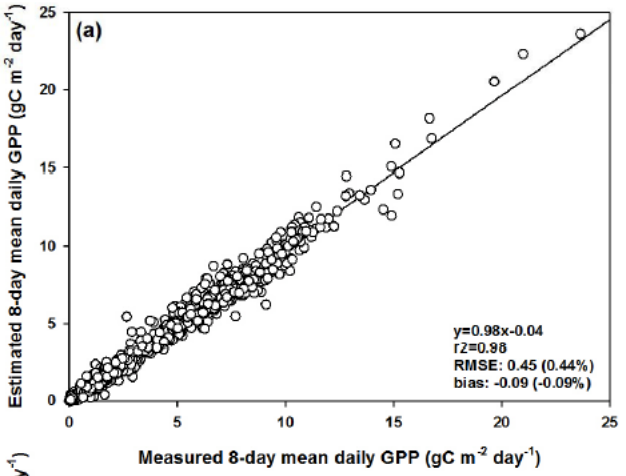


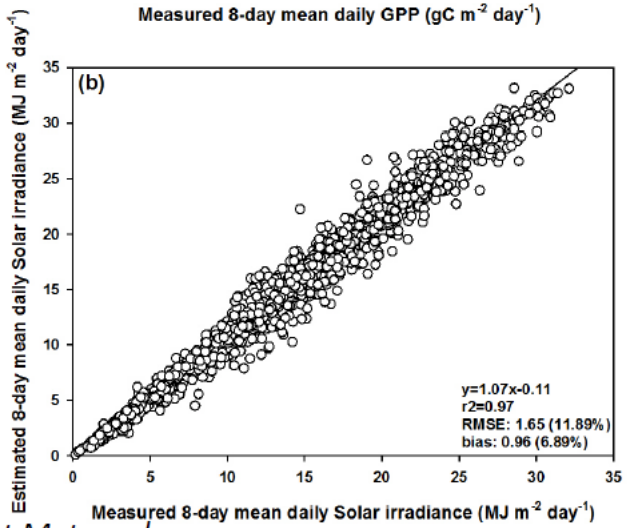
Fig. 4 Measured and modeled power spectra for the CO_2 flux *Fc* [panel (a)] and latent heat flux *LE* [panel (b)].

Test of BESS Model with Flux Towers

Tested the scheme using 33 flux tower data from the Arctic to the Tropics

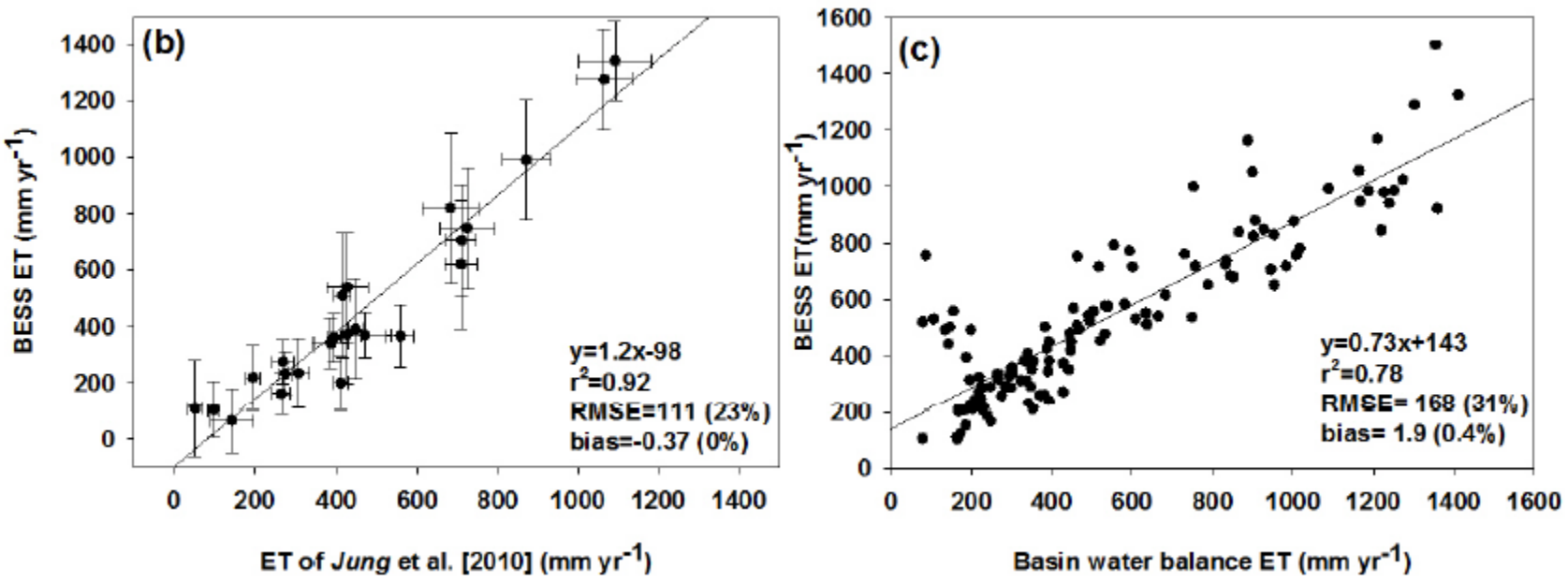






Ryu et al (in minor revision) *Agricultural and Forest Meteorology*

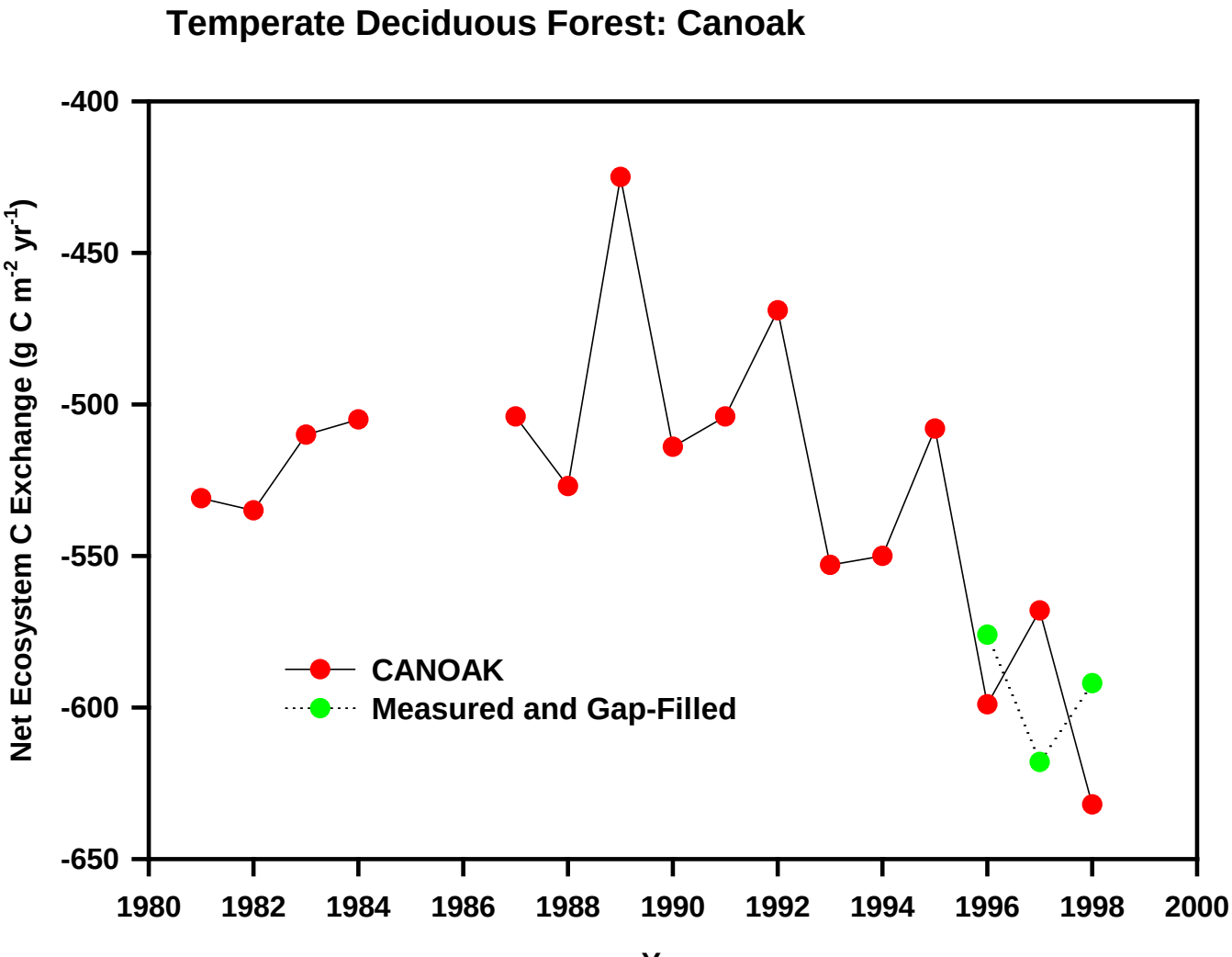
Test of BESS model with Data-Driven Model (Jung et al.) and Basin Water Balance



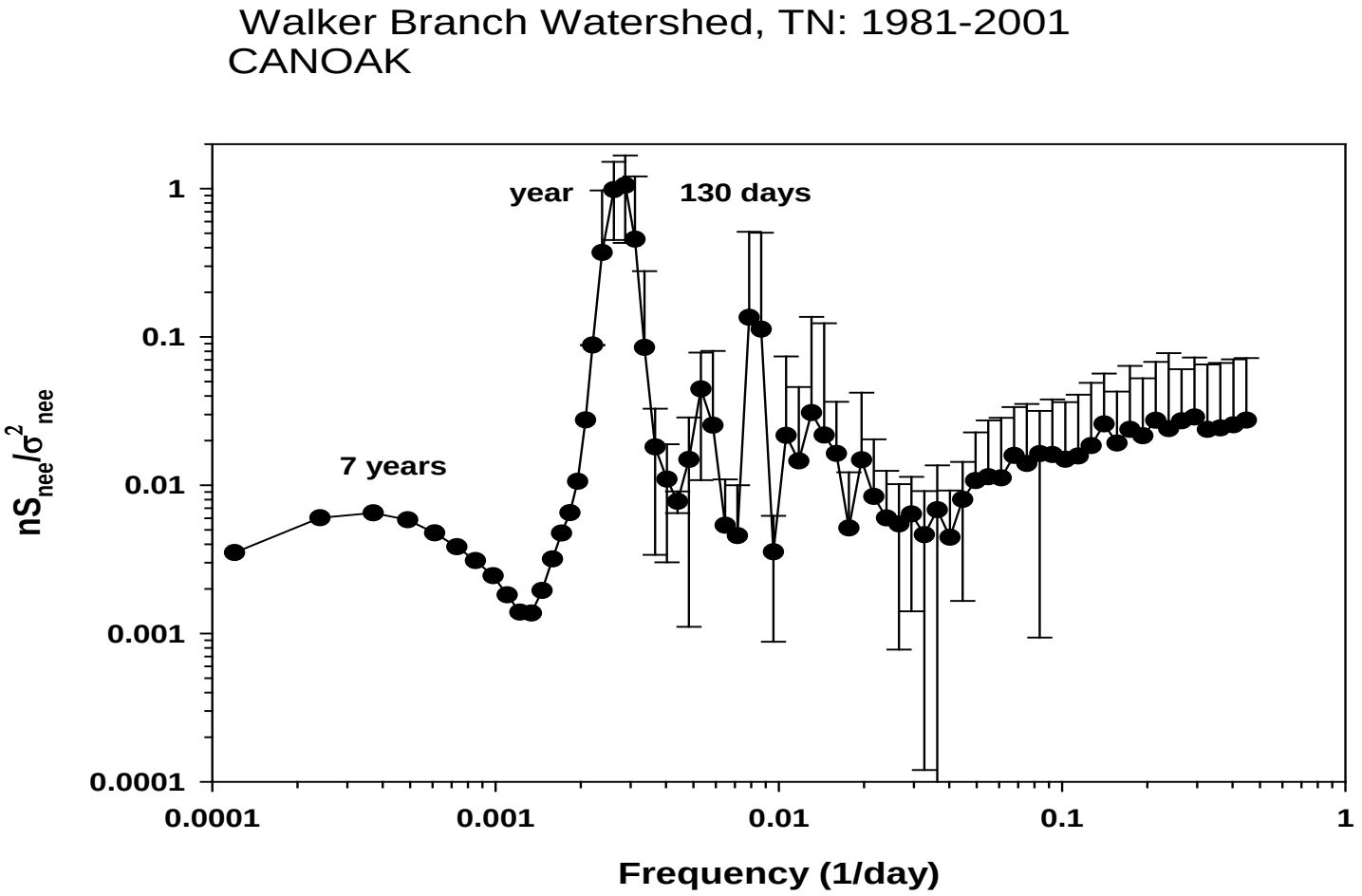
Ryu et al 2012 GBC

P2. Sensitivity and Science Questions f(Time, space, Parameters & Processes)

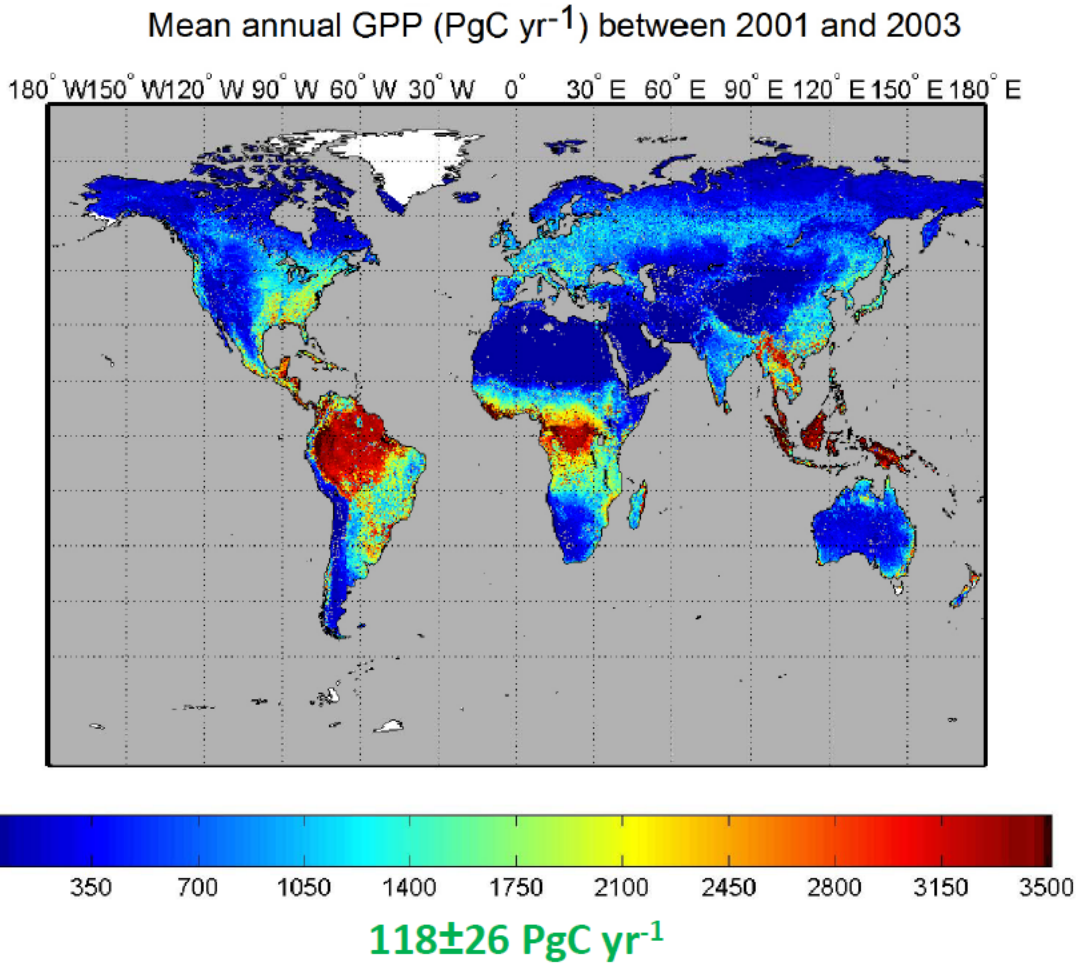
What is Interannual Variability, beyond the measurement record?



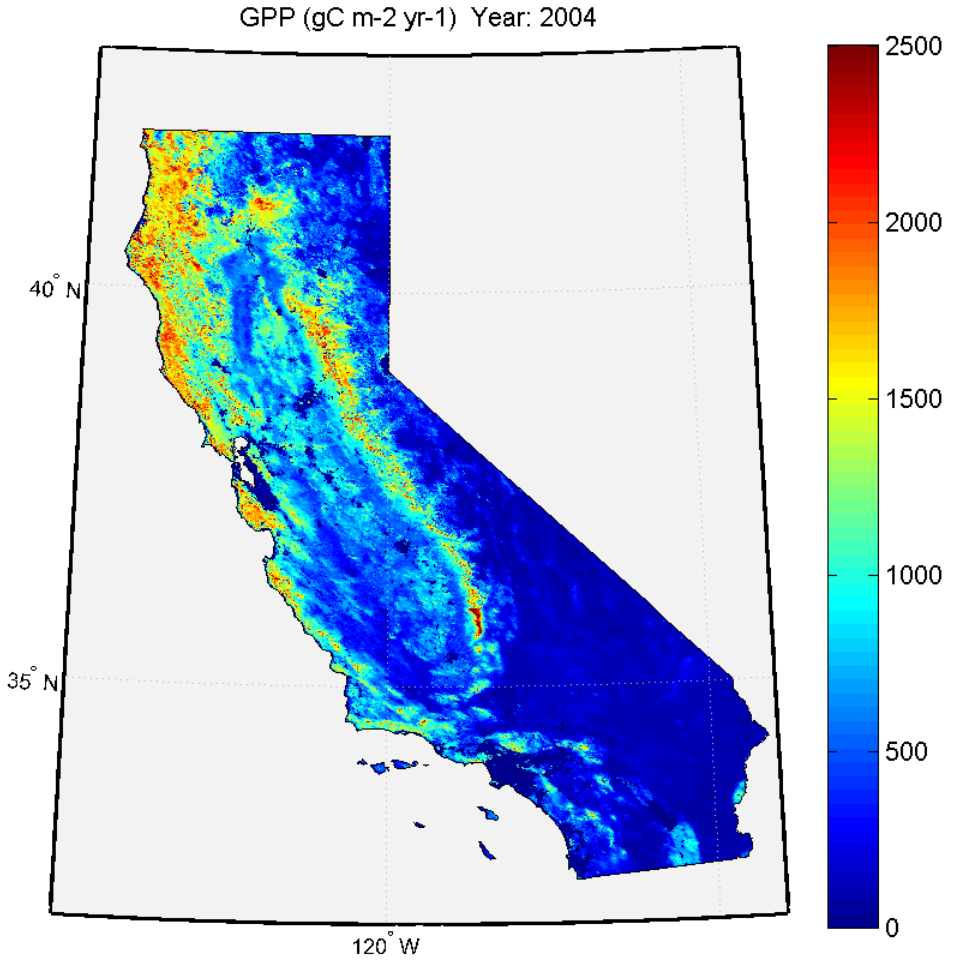
Decadal Scales of Variability, Information exists at Long time scales



What is Globally Integrated GPP?

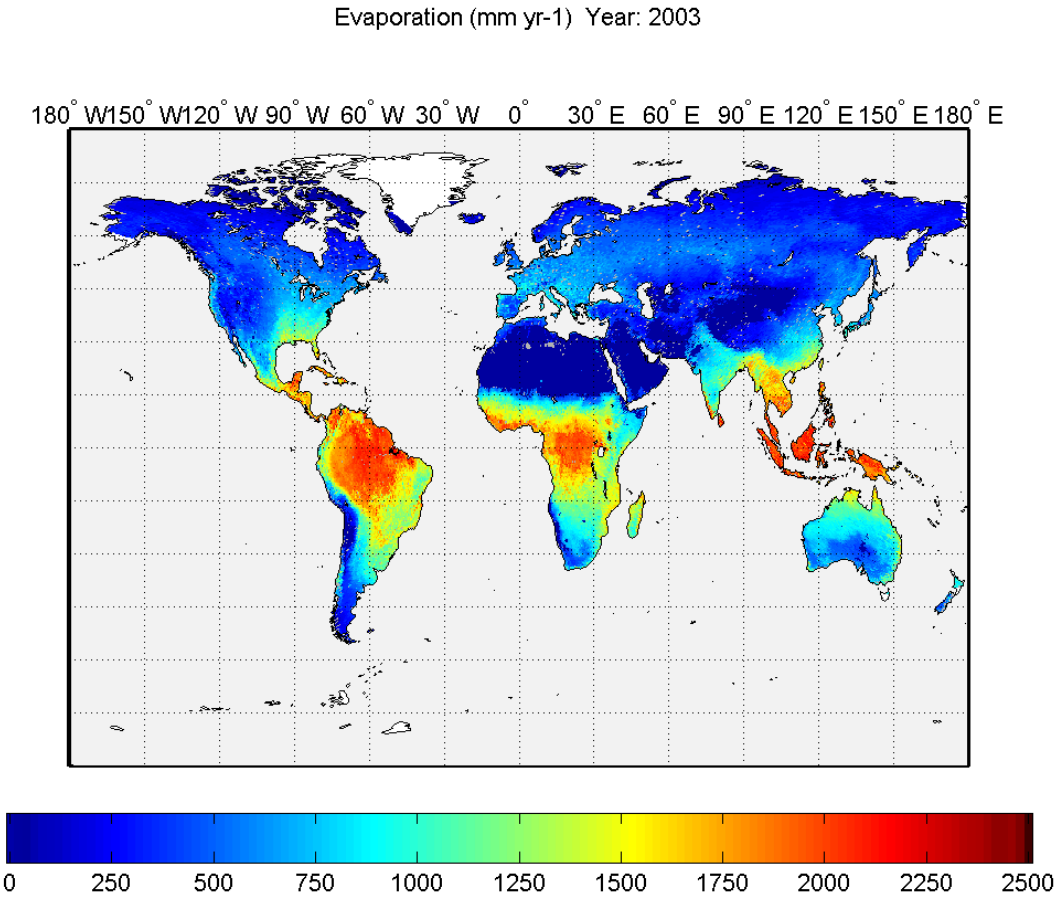


UpScaling GPP Regionally with Sun-Shade Coupled Energy Balance Photosynthesis Model



Ryu et al. unpublished

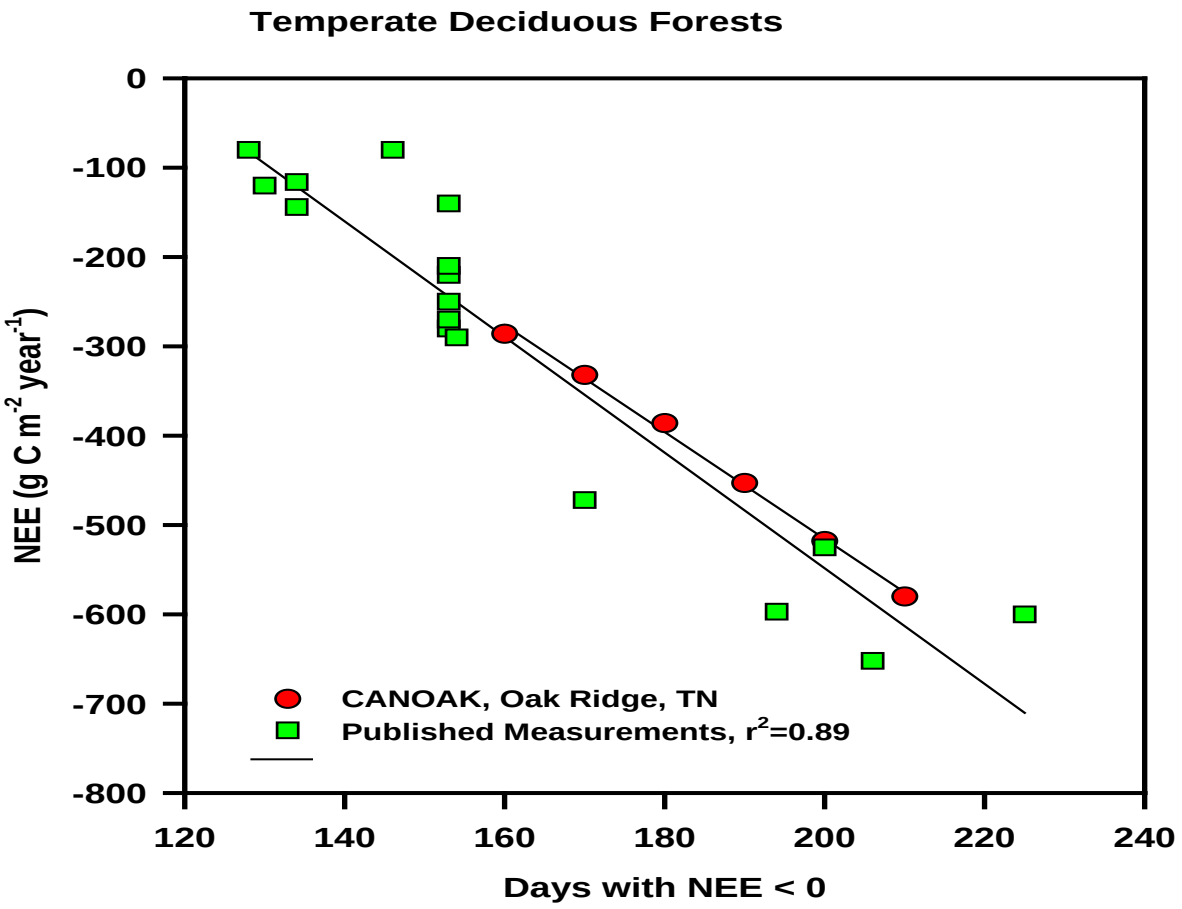
Global Evaporation at 1 to 5 km scale



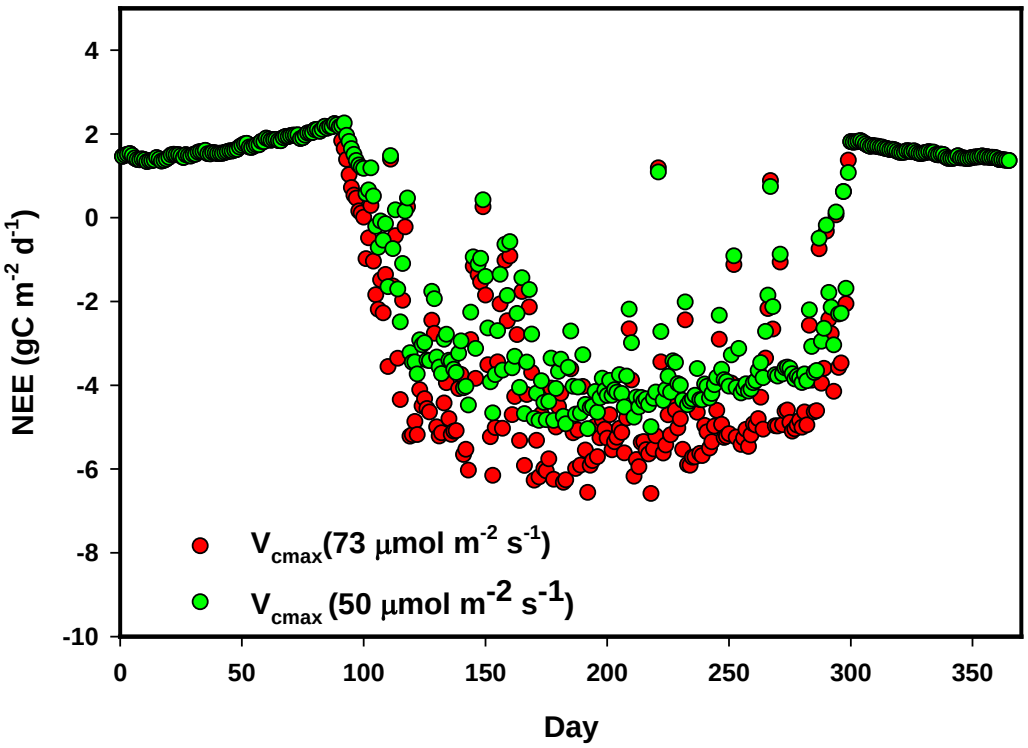
<ET> = 503 mm/y == 6.5 10^{13} m^3/y

An Independent, Bottom-Up Alternative to Residuals
based on the Global Water Balance, ET = Precipitation - Runoff

NEE and Growing Season Length

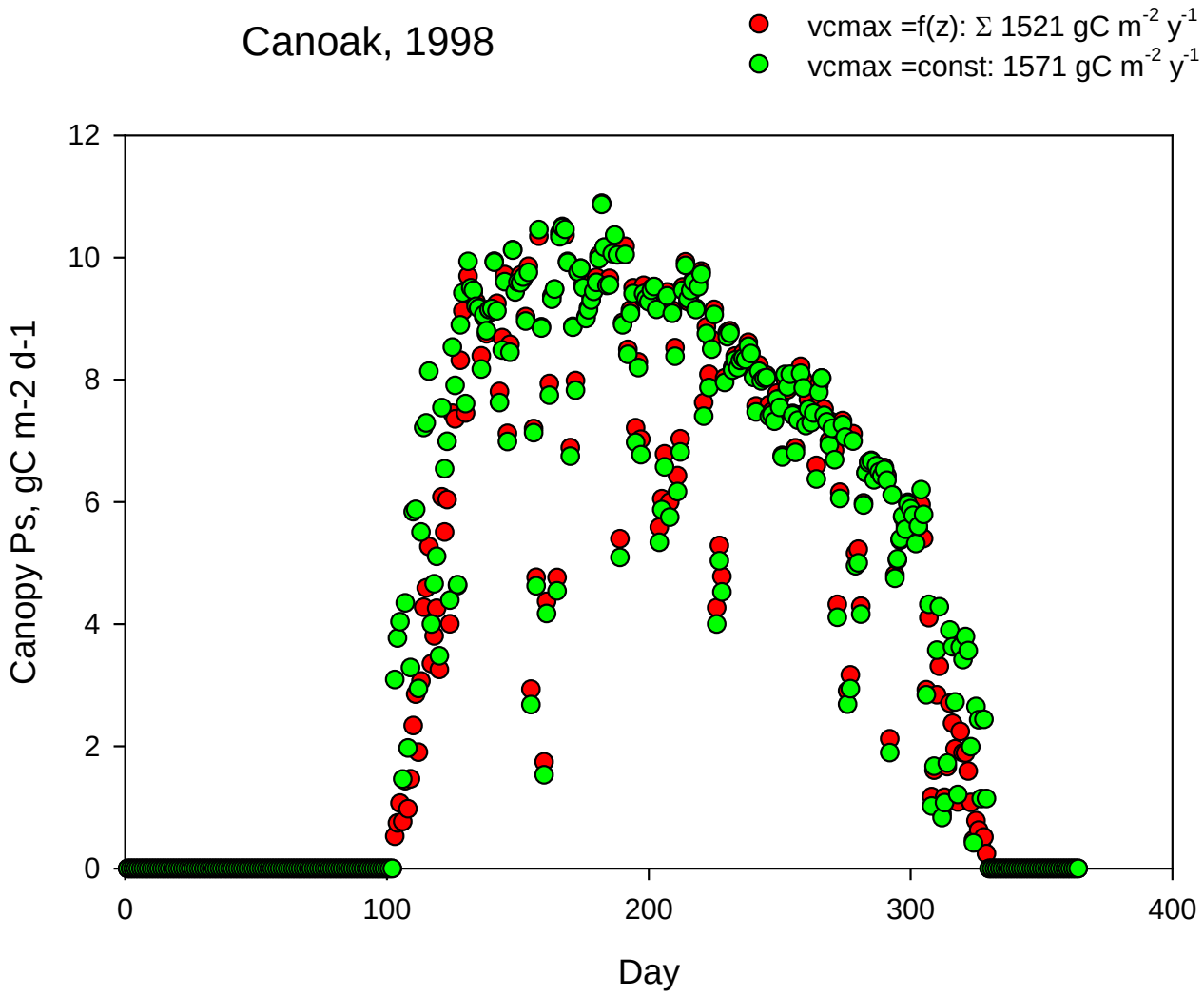


Importance of Vcmax



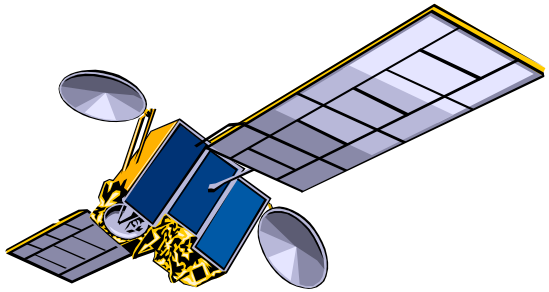
	$V_{cmax}(73)$	$V_{cmax}(50)$	% difference
NEE (gC m-2 a-1)	-577	-454	-21.3
λE (MJ m^{-2} a^{-1})	1690	1584	-6.3
H (MJ m^{-2} a^{-1})	1096	1199	9.3

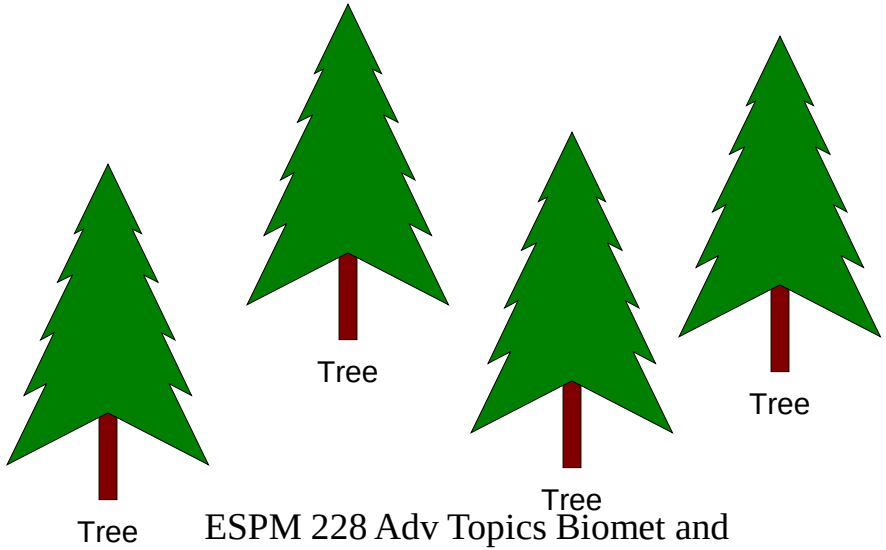
Vertical Variations in Vcmax, are they needed?



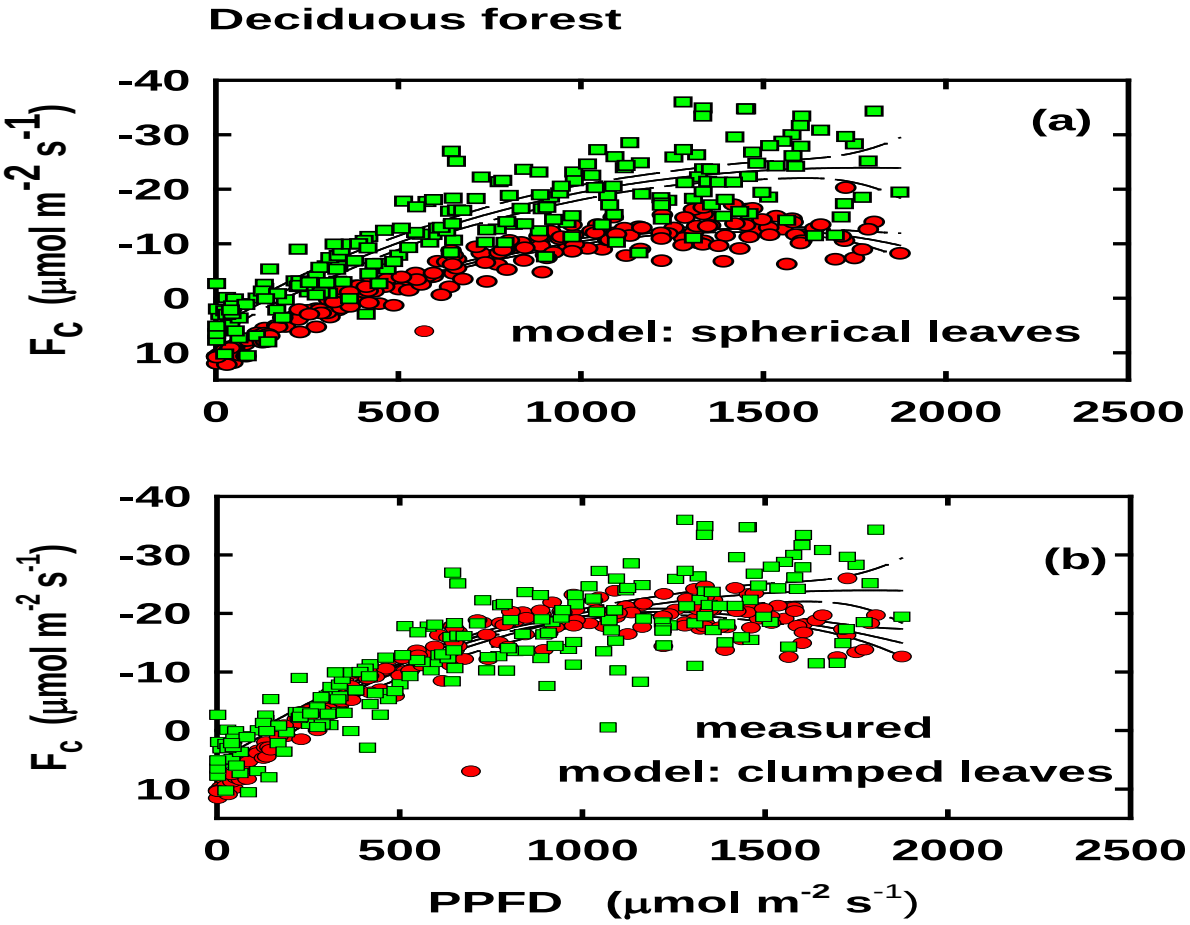
Light Use Efficiency and Net Primary Productivity

$$NPP = \varepsilon \, f \, Q_p$$

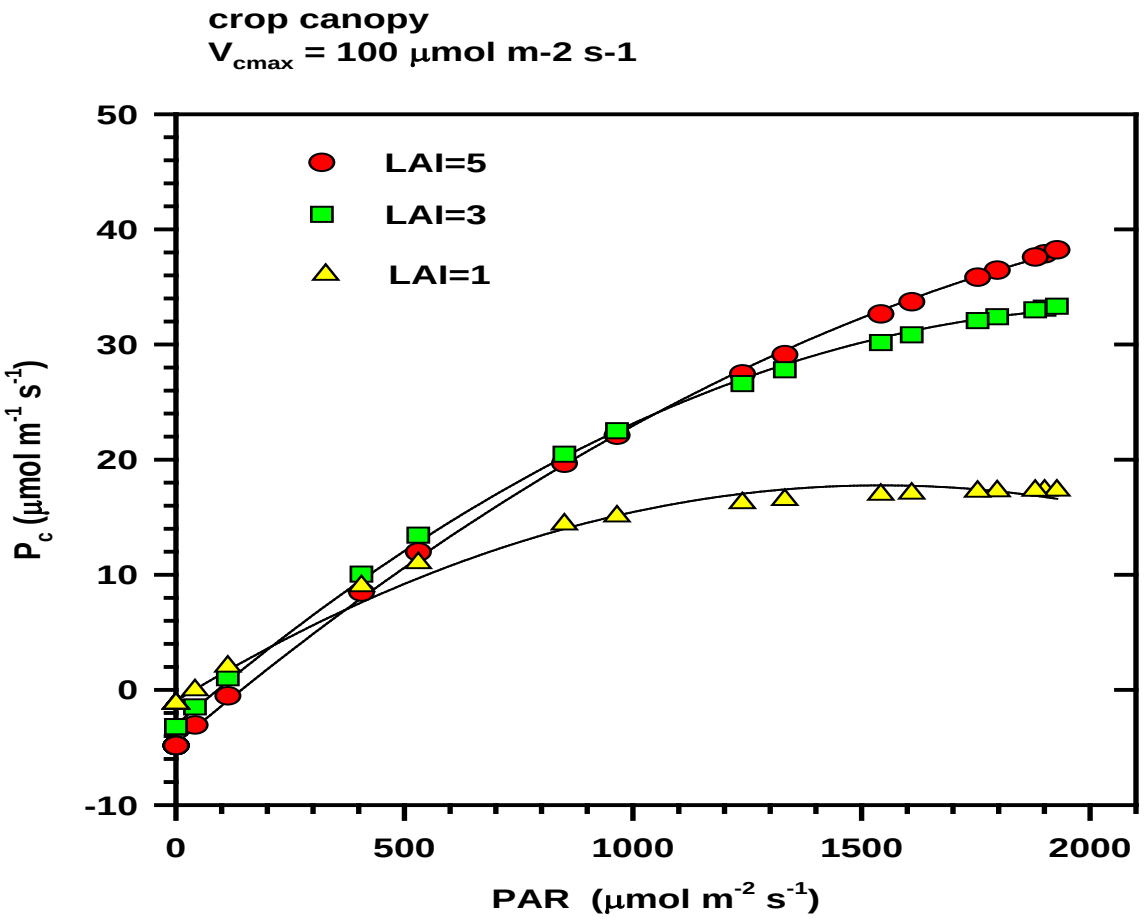




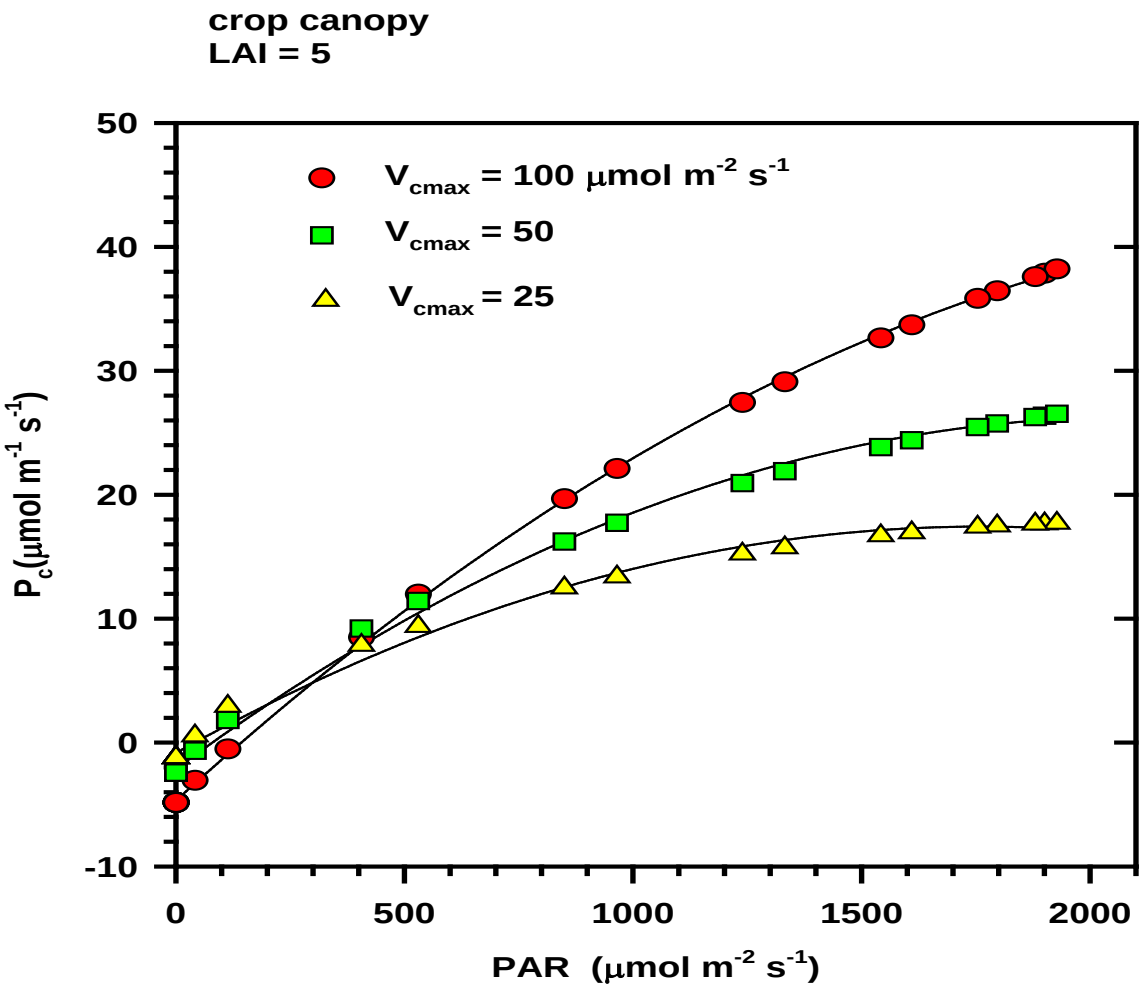
Emergent Processes: Impact of Leaf Clumping on Canopy Light Response Curves



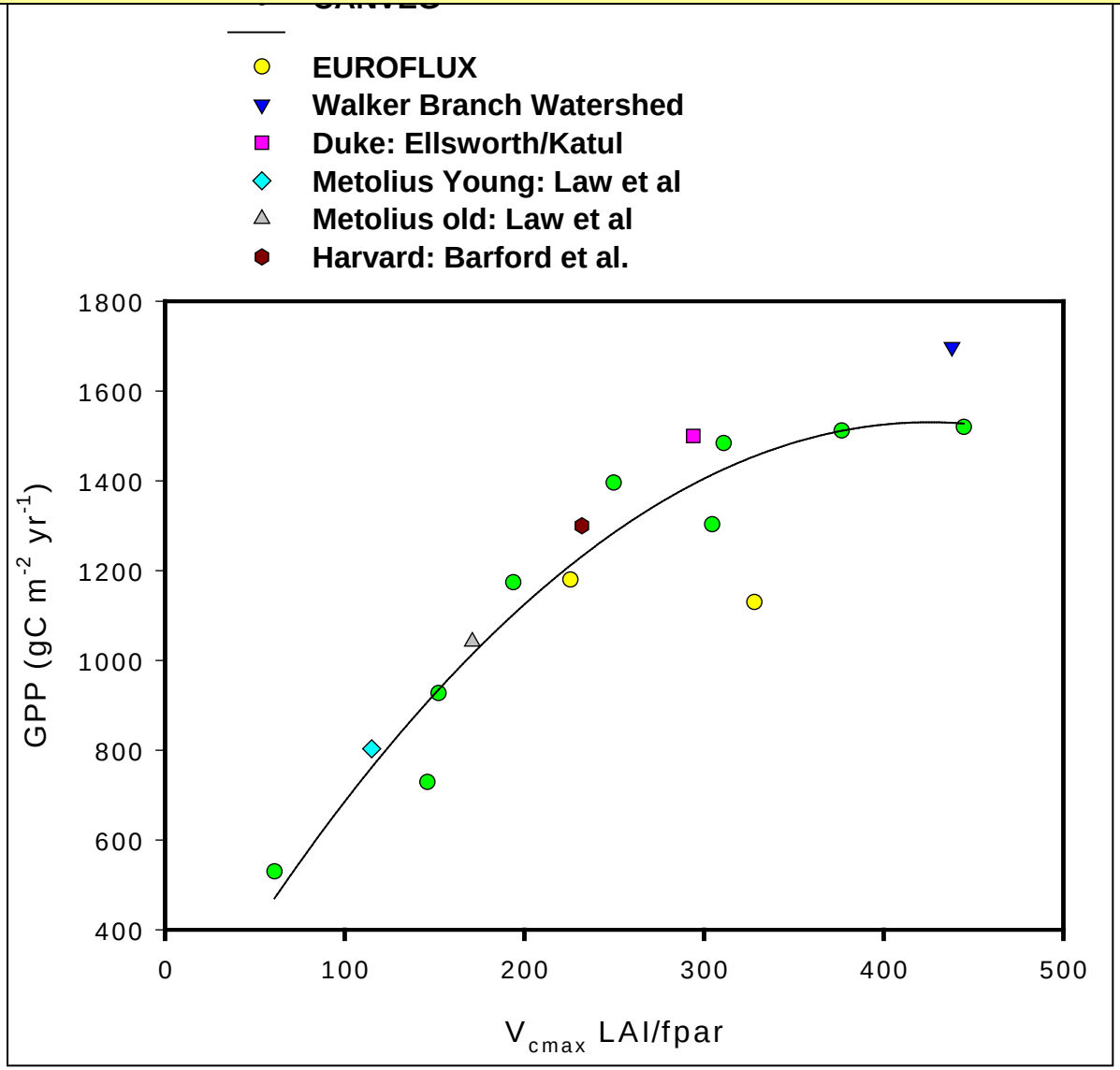
LUE and Leaf Area



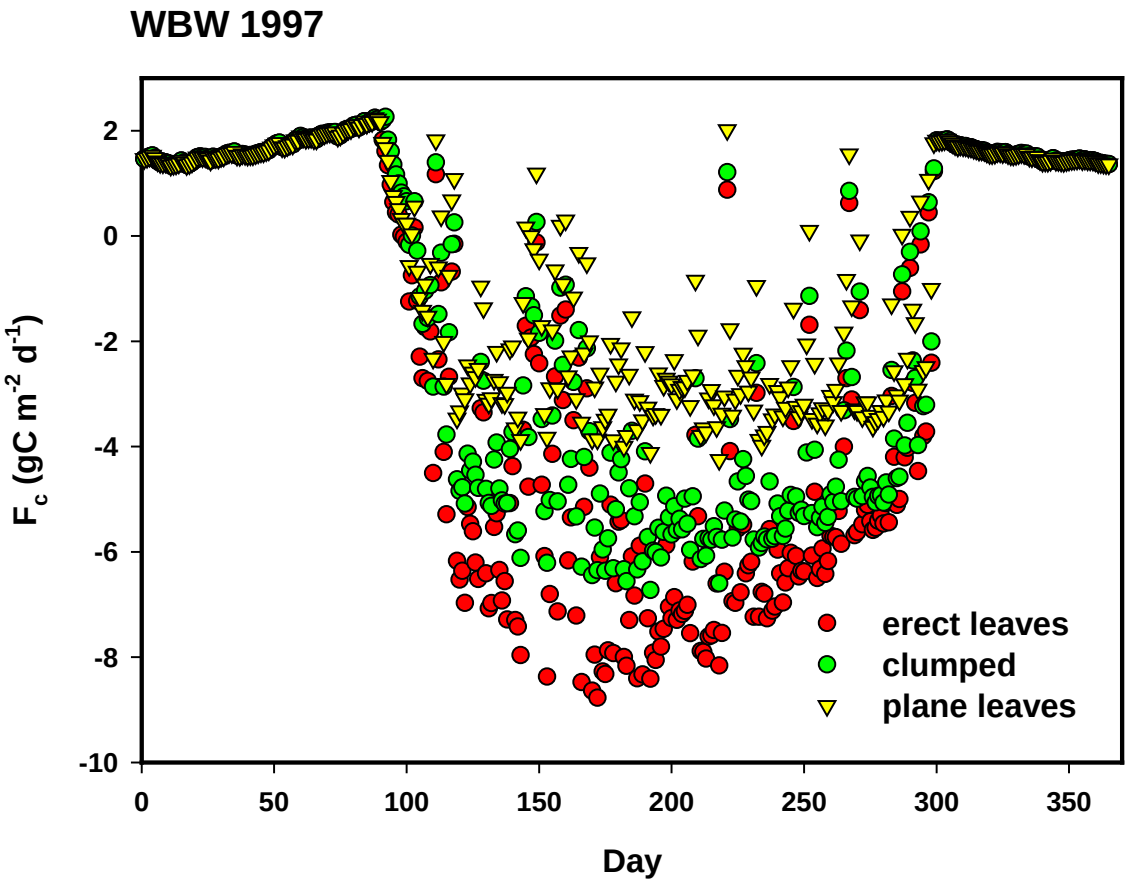
LUE and Ps Capacity



Developing Simple Model from Complex One

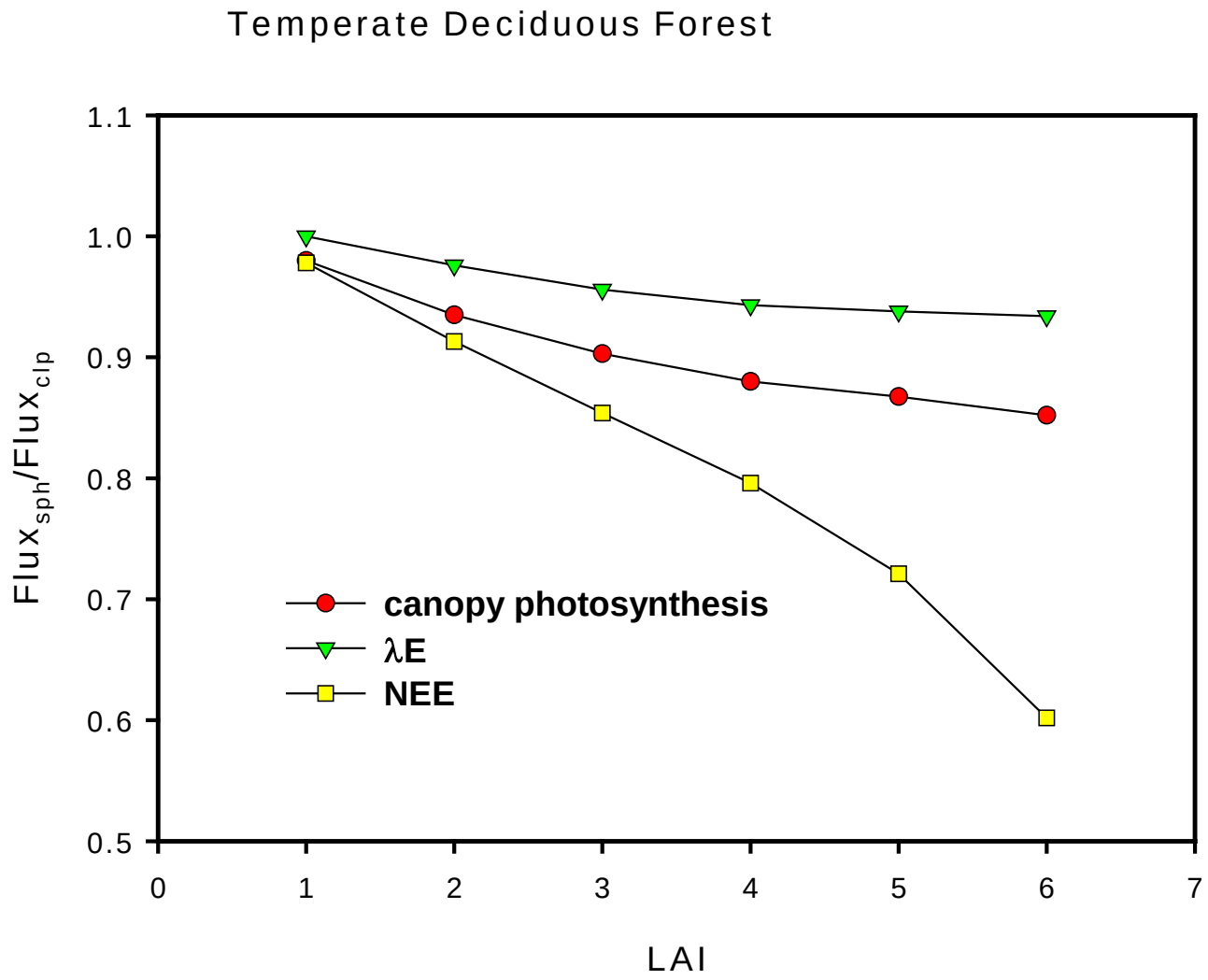


Role of Leaf Angle Inclination and Clumping on Fluxes

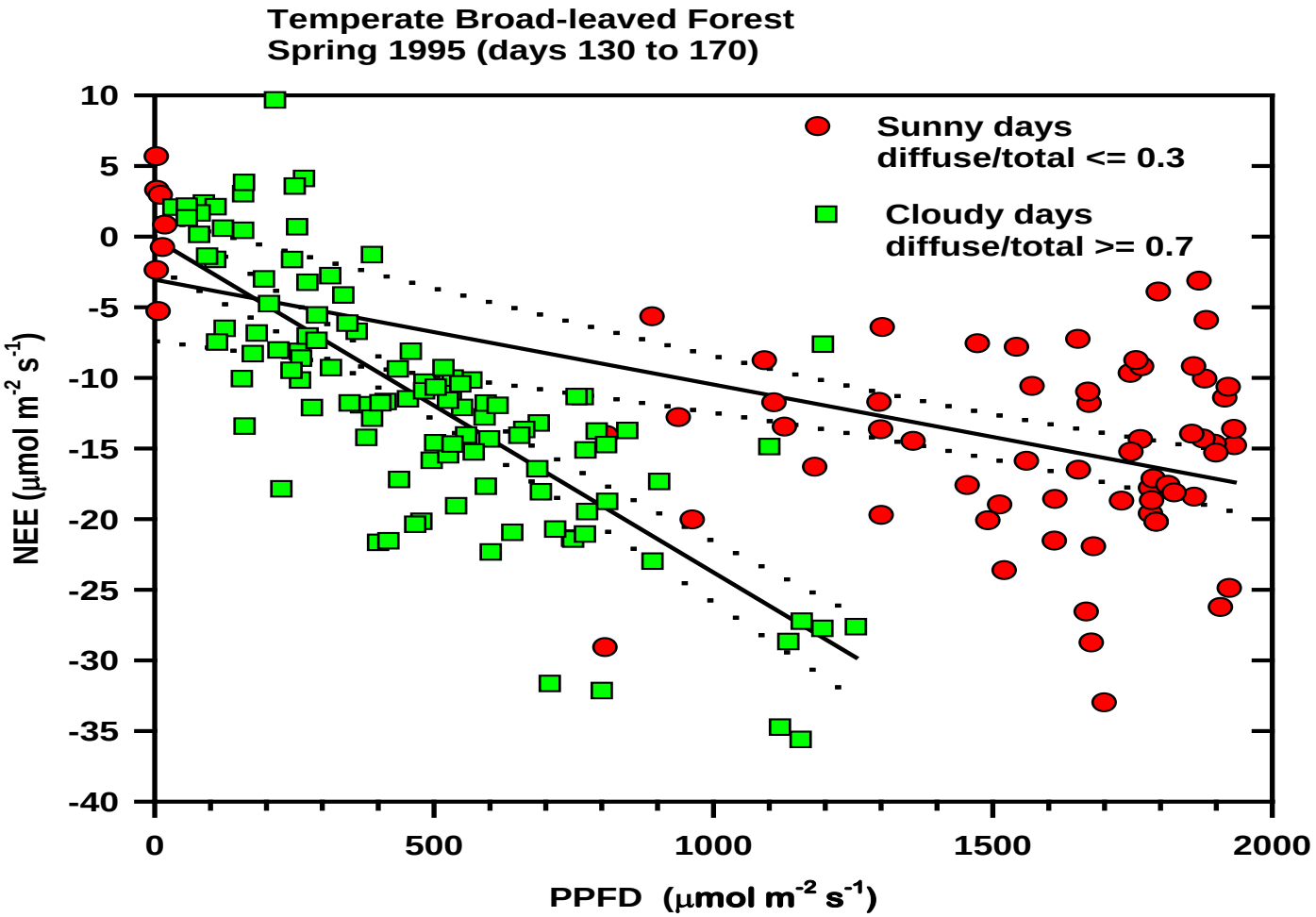


	clumped	random	spherical	erectophile	planophile
NEE (gC m^{-2} a^{-1})	-577	-354	-720	-1126	-224
λE (MJ m^{-2} a^{-1})	1690	1551	1774	2023	1473
H (MJ m^{-2} a^{-1})	1096	1032	1095	1171	1008

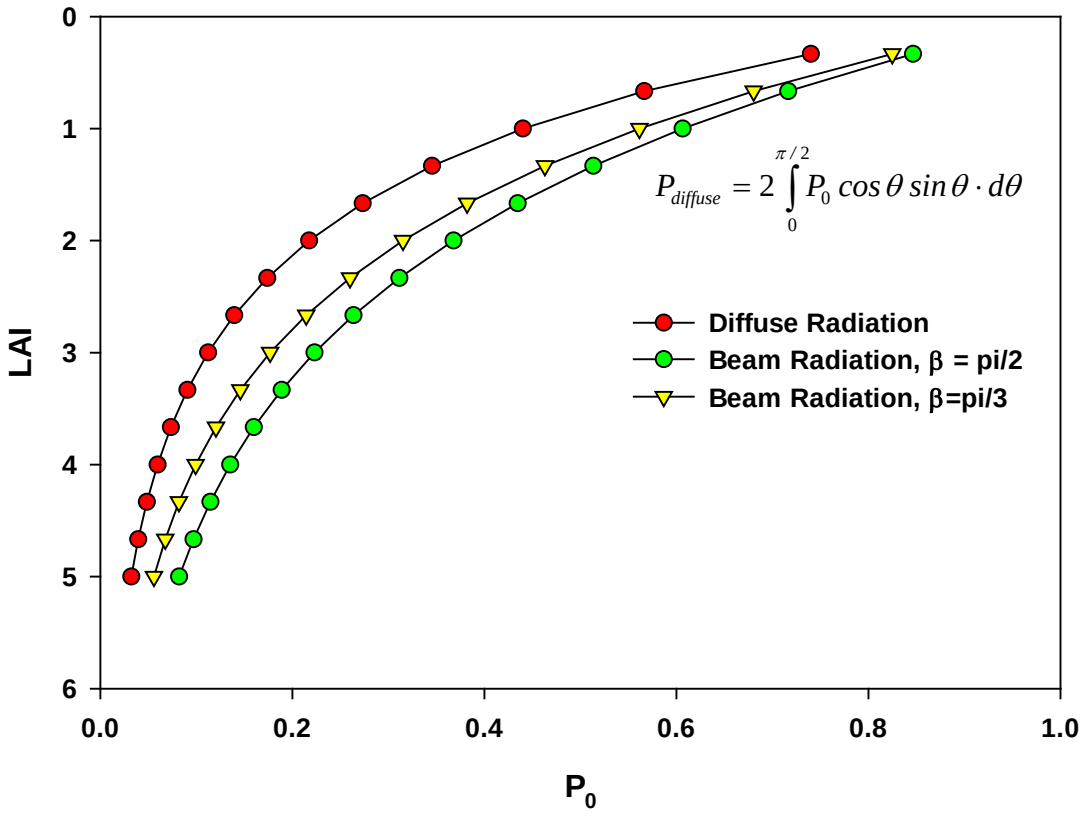
Interaction between Clumping and Leaf Area

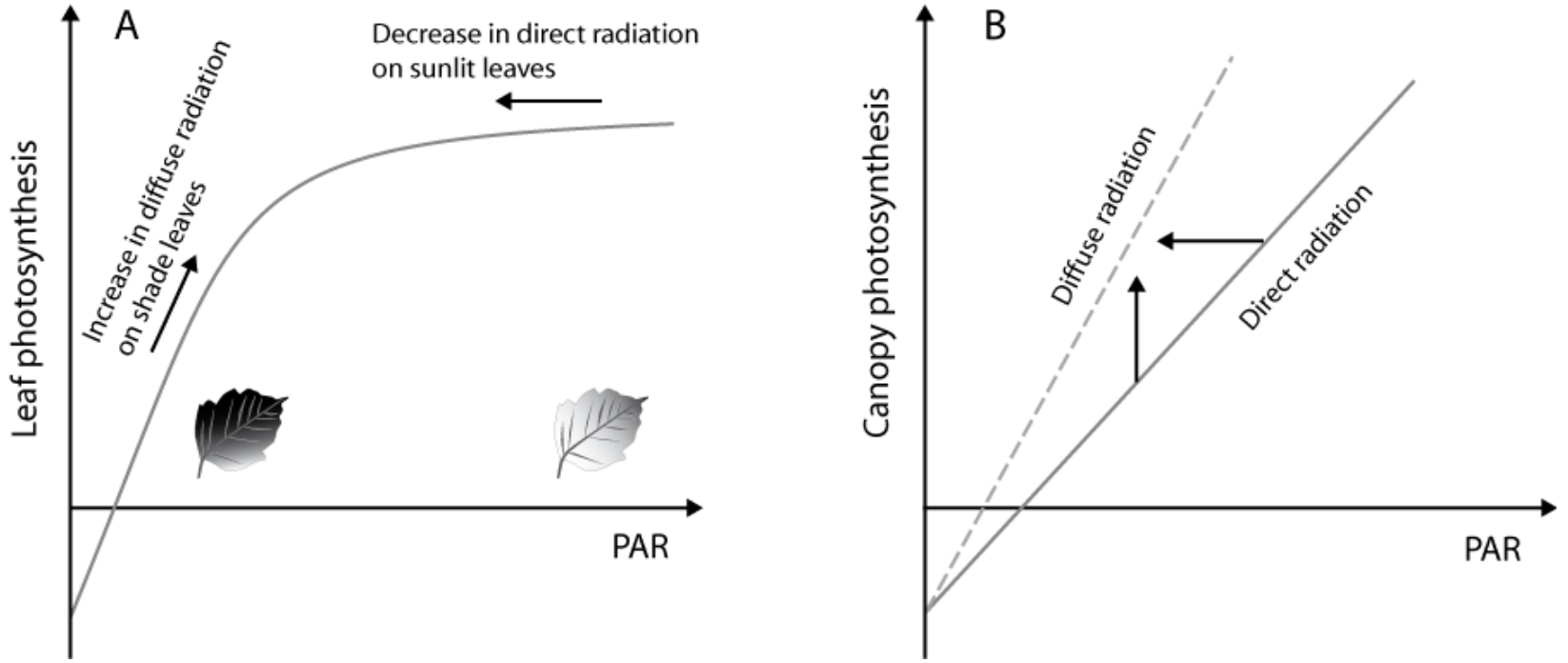


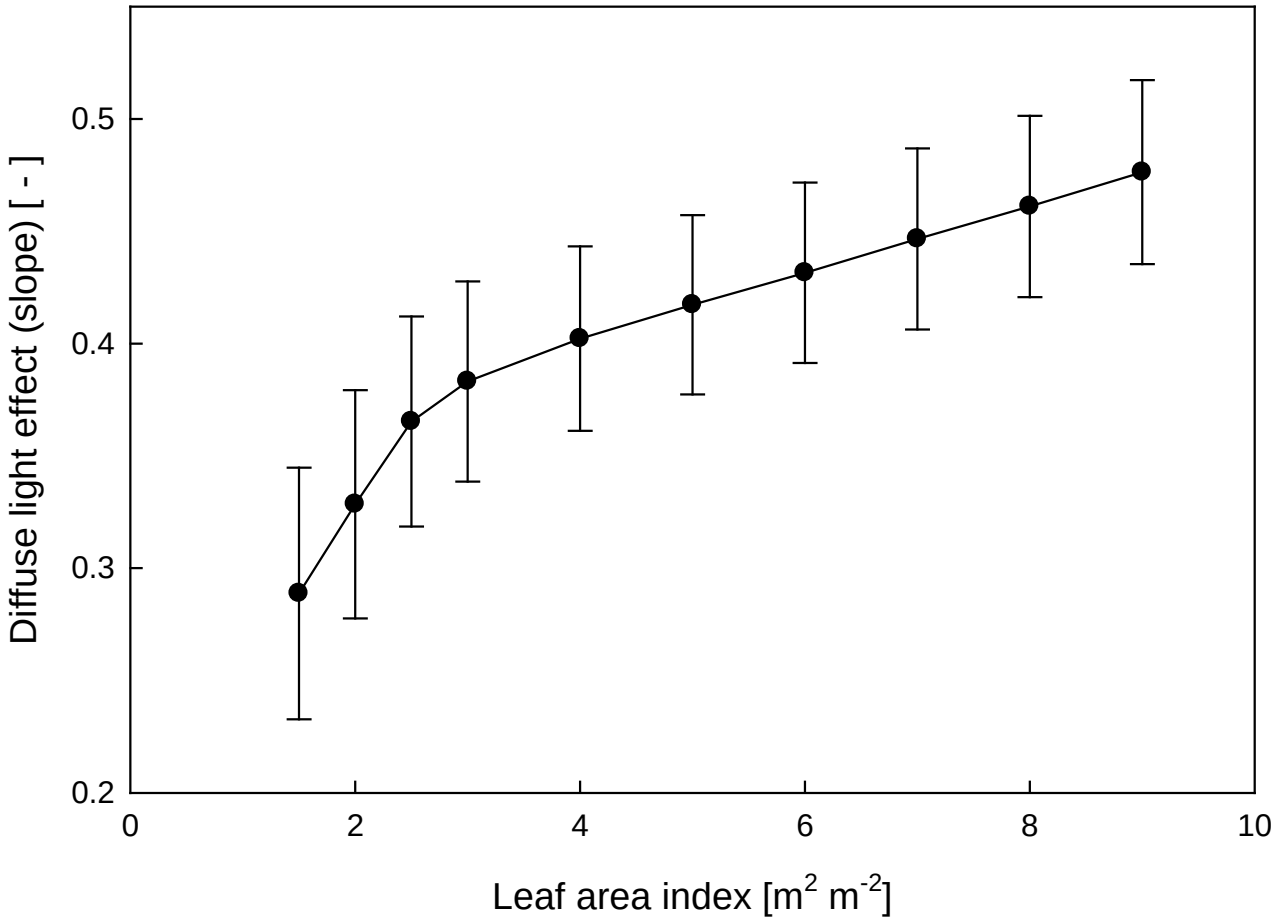
How Sky Conditions Affect NEE?



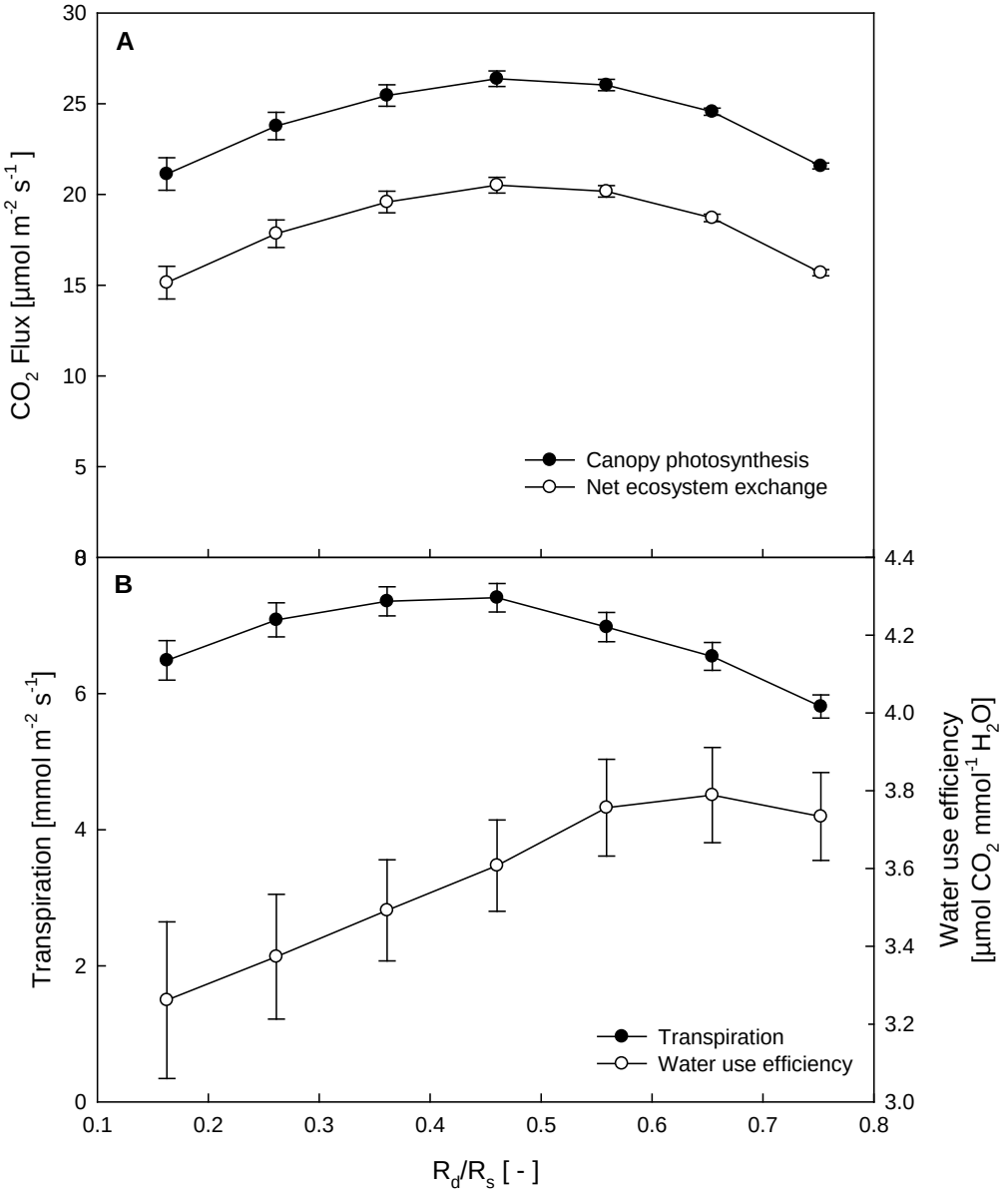
Conversion of direct to diffuse light increases light capture




A
Decrease in direct radiation
on sunlit leaves
Increase in diffuse radiation
on shade leaves
Leaf photosynthesis
PAR
B
Canopy photosynthesis
Diffuse radiation
Direct radiation
PAR

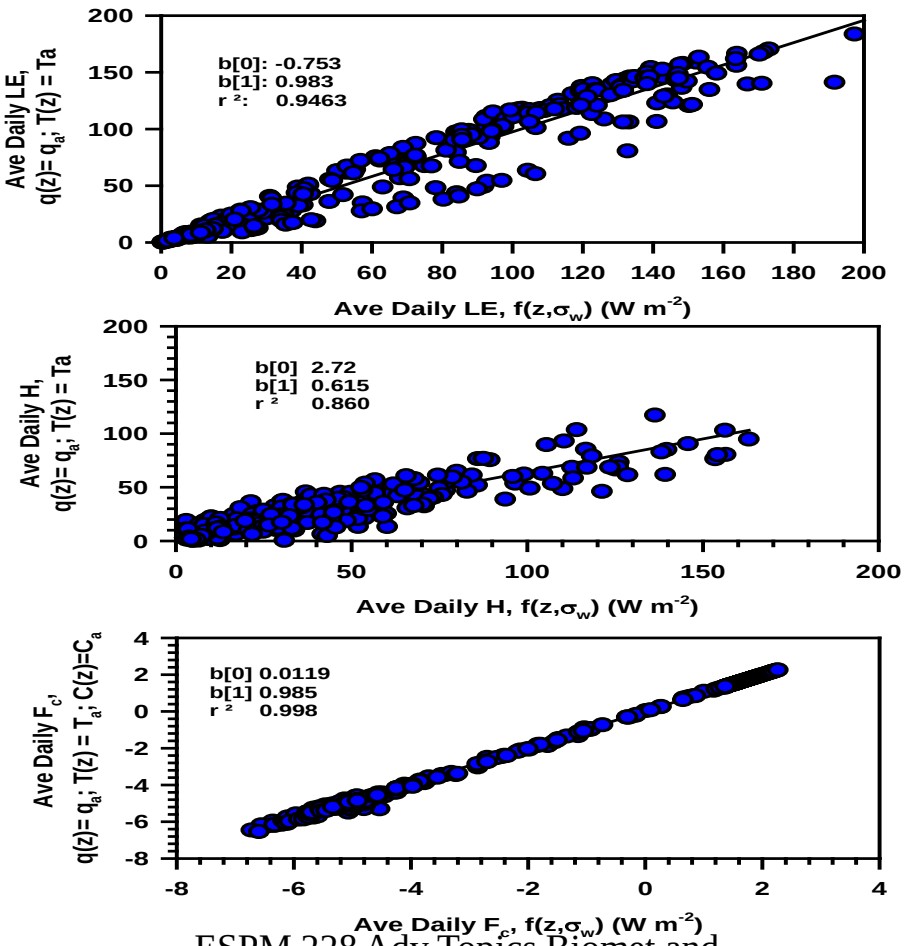


Knohl and Baldocchi, 2008 JGR Biogeosci

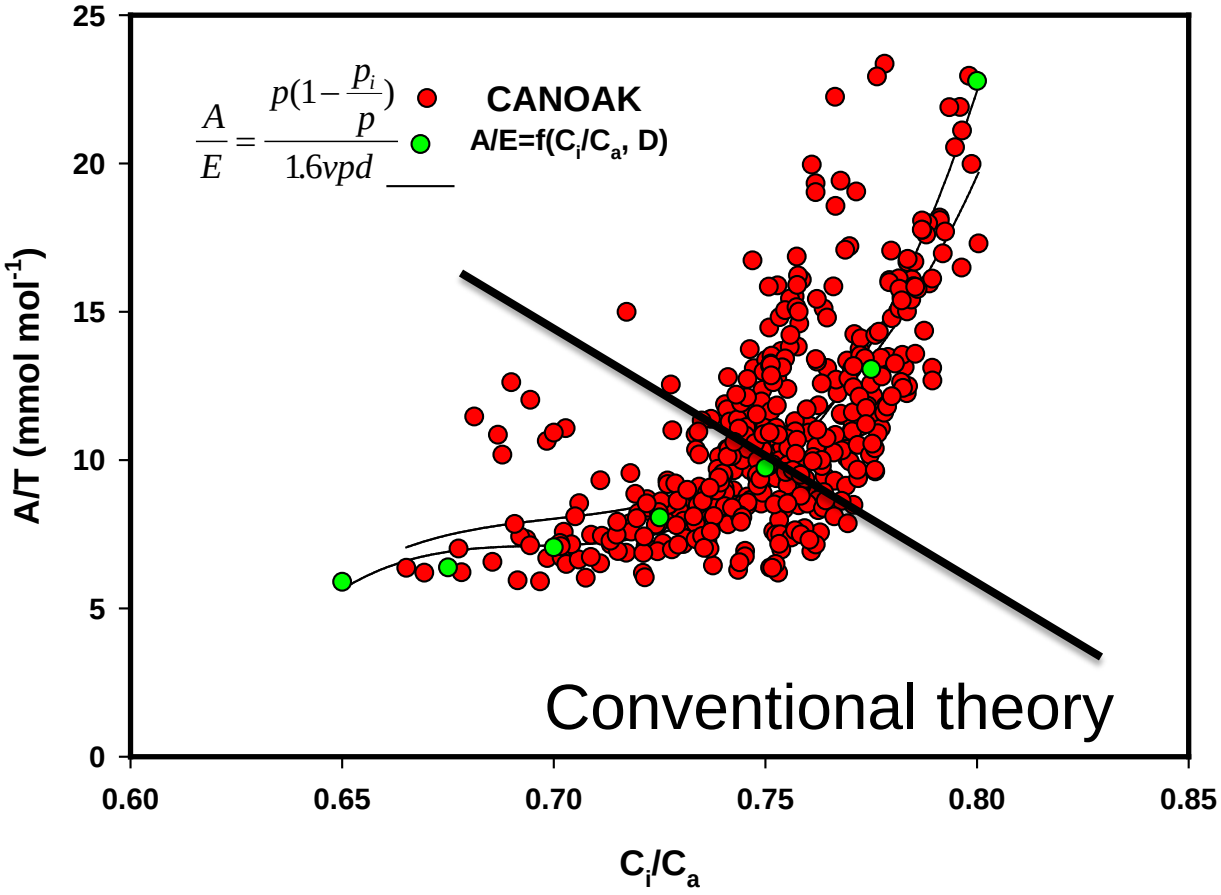


Knohl and Baldocchi, 2008 JGR Biogeosci

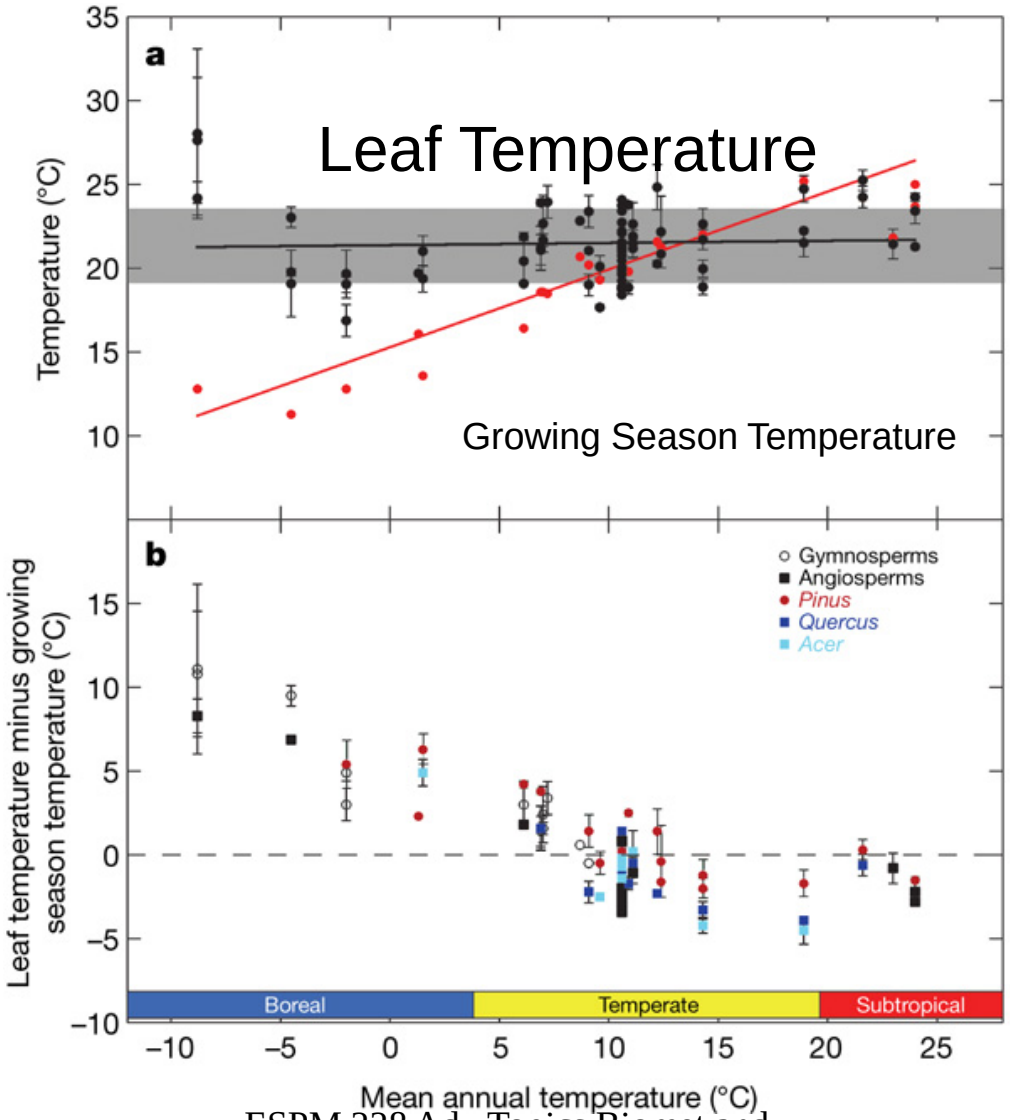
Do We Need to Consider Canopy Microclimate [C] Feedbacks on Fluxes?



Interpreting Stable Isotopes

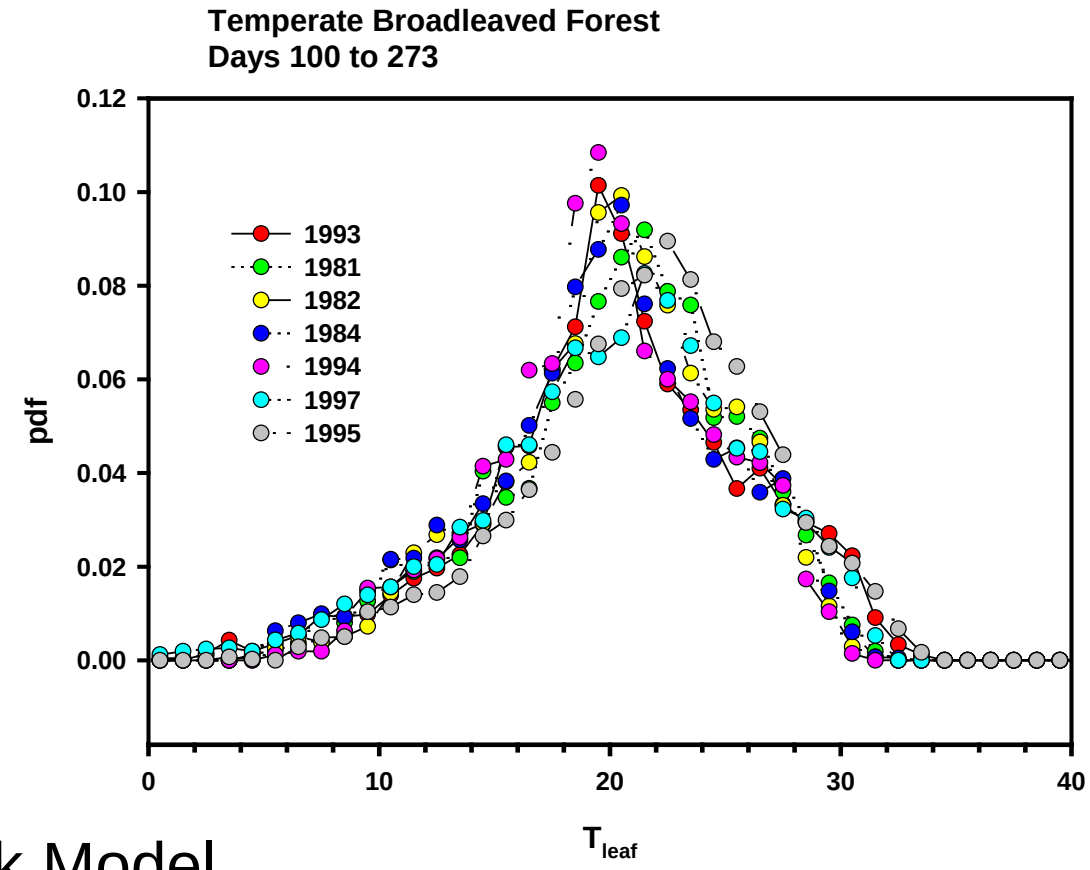


Isotopes Infer Leaf Temperatures of Tree Leaves are Constrained, ~ 21 C



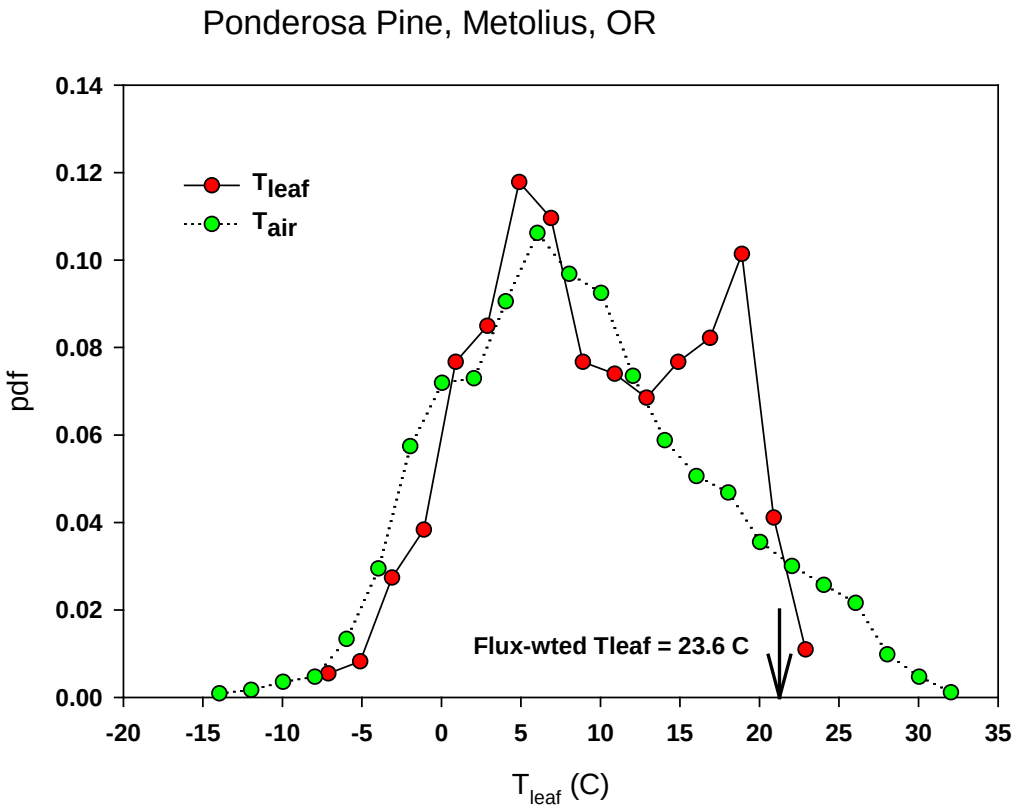
Helliker and Richter 2008 Nature

Leaf Temperature, Modeled with CANOAK, as a Central Tendency near 20 C



Canoak Model

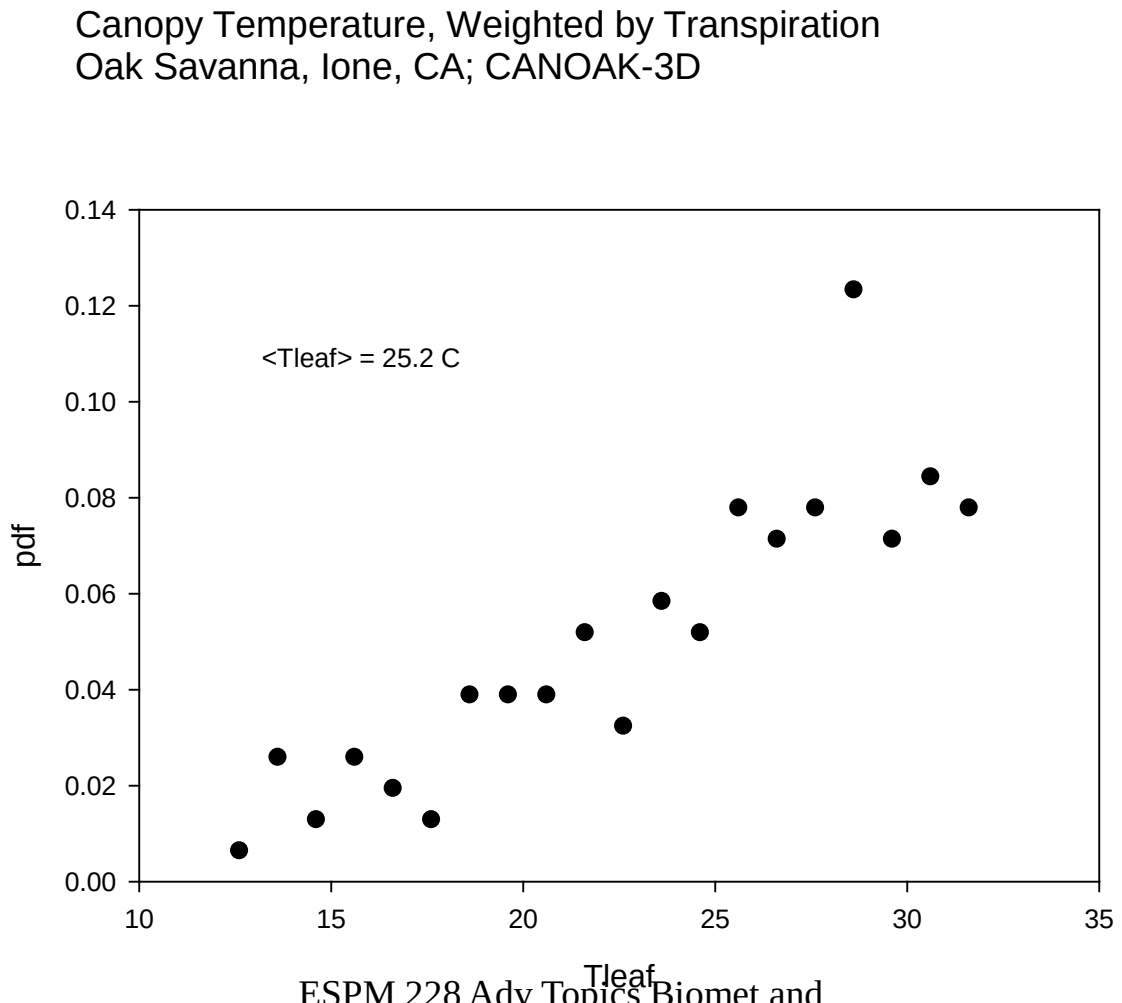
Isotopes Evaluate a Flux-Weighted Temperature



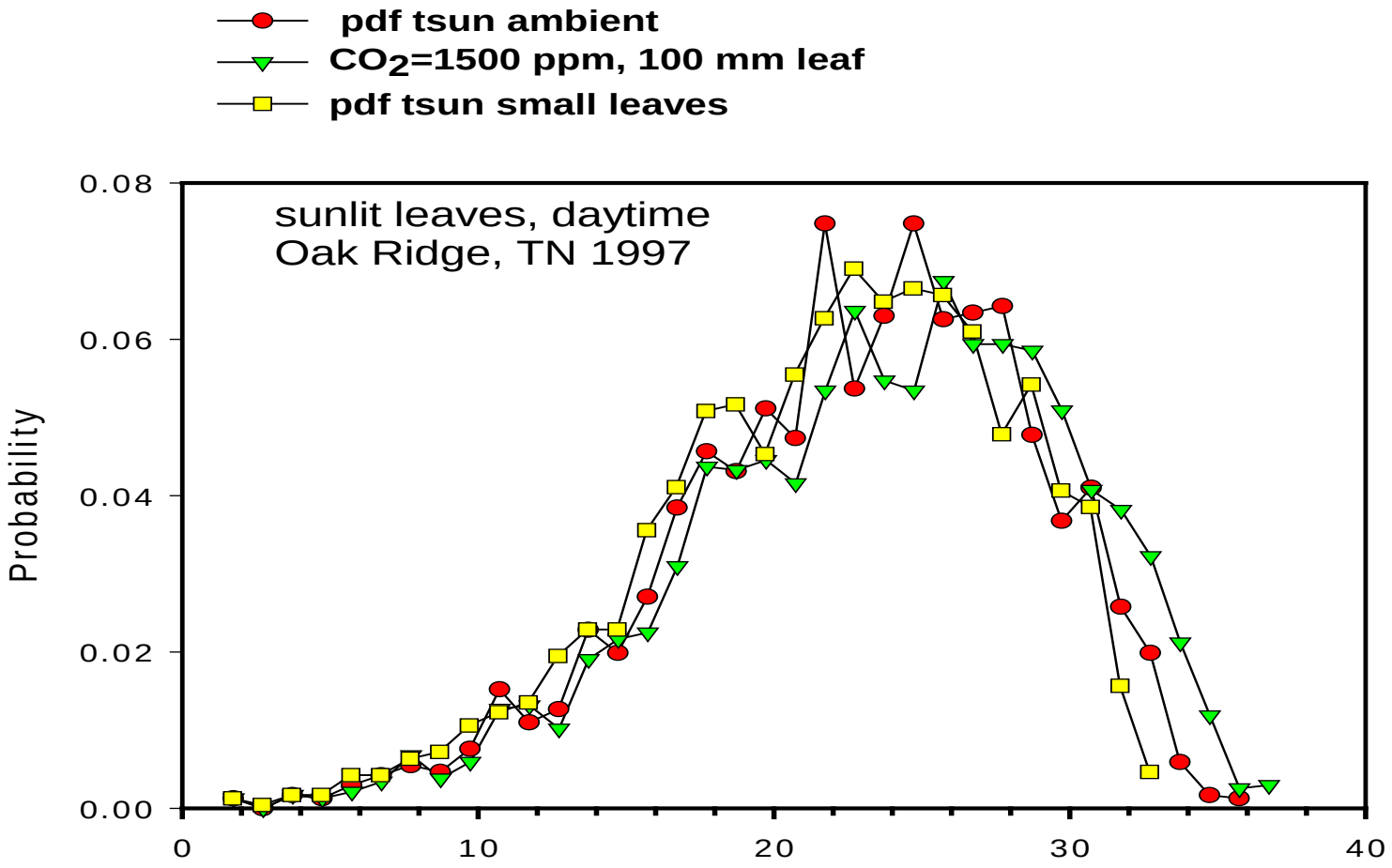
Transpiration (E) Weighted Leaf Temperature

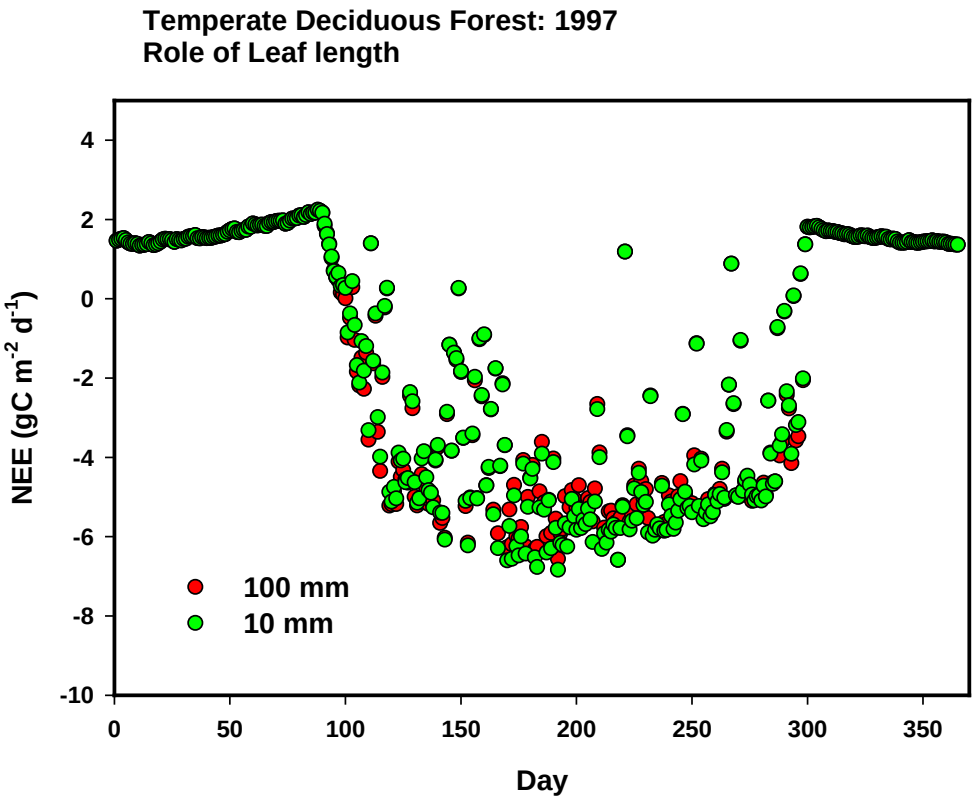
$$< T_{leaf} >= \frac{\int E\, T_{leaf}\, dt}{\int E\, dt}$$

Transpiration Weighted Leaf Temperature for Oak Savanna



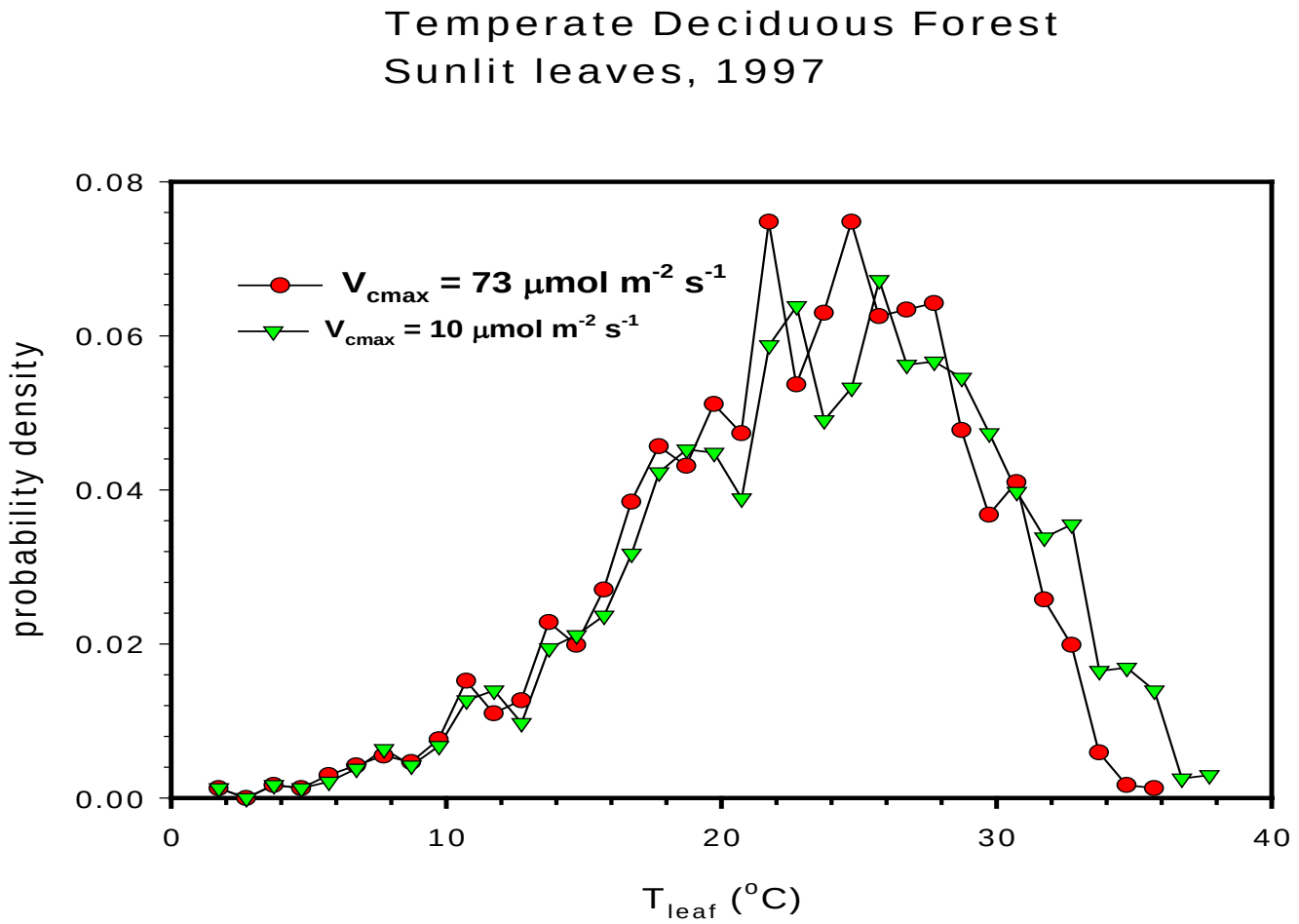
Leaf size, CO_2 and Temperature: why oak leaves are small in CA and large in TN



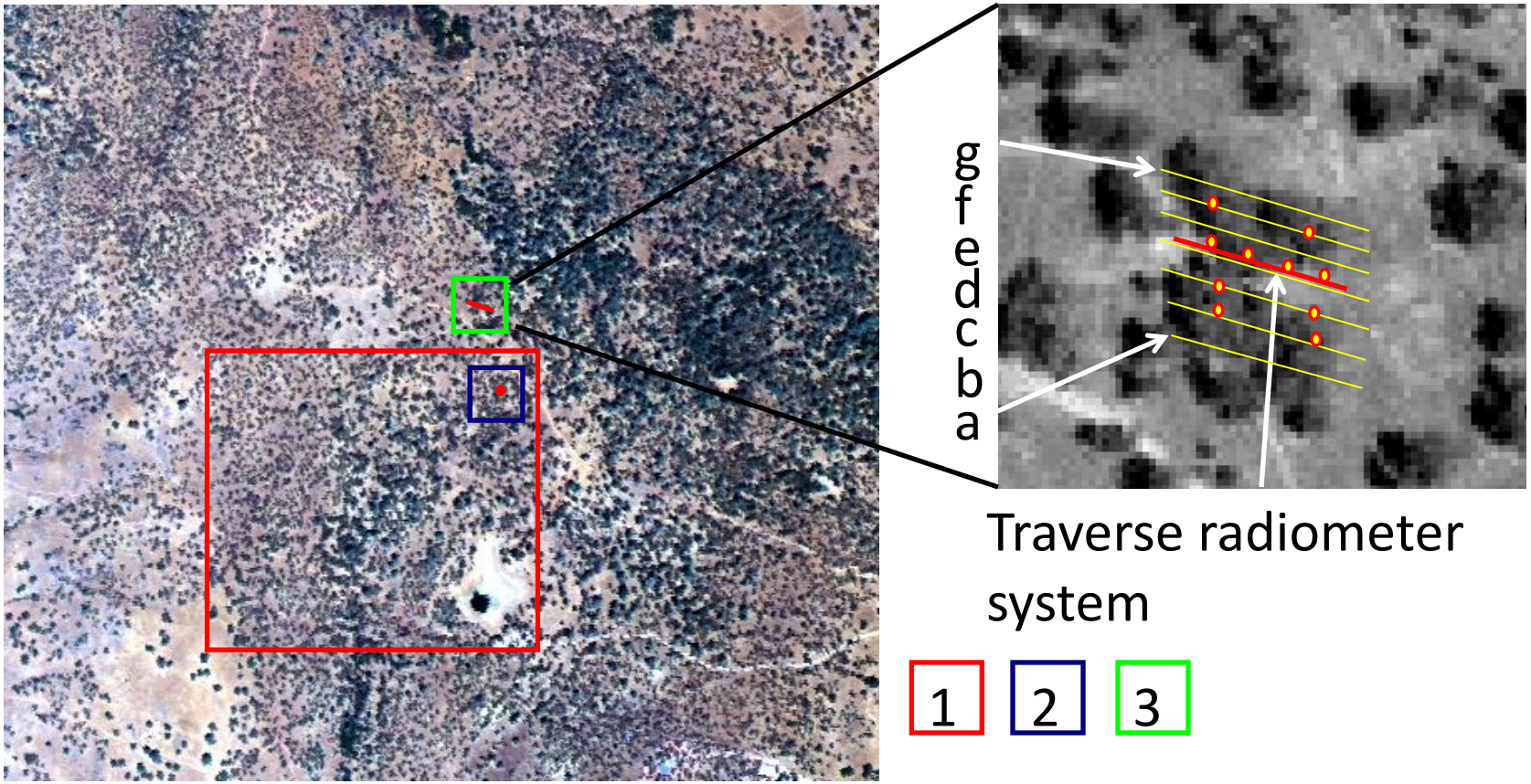


	0.1 m	0.01m	0.001 m
NEE (gC m-2 a^{-1})	-577	-588	-586
λE (MJ m^{-2} a^{-1})	1690	1652	1615
H (MJ m^{-2} a^{-1})	1096	1164	1202

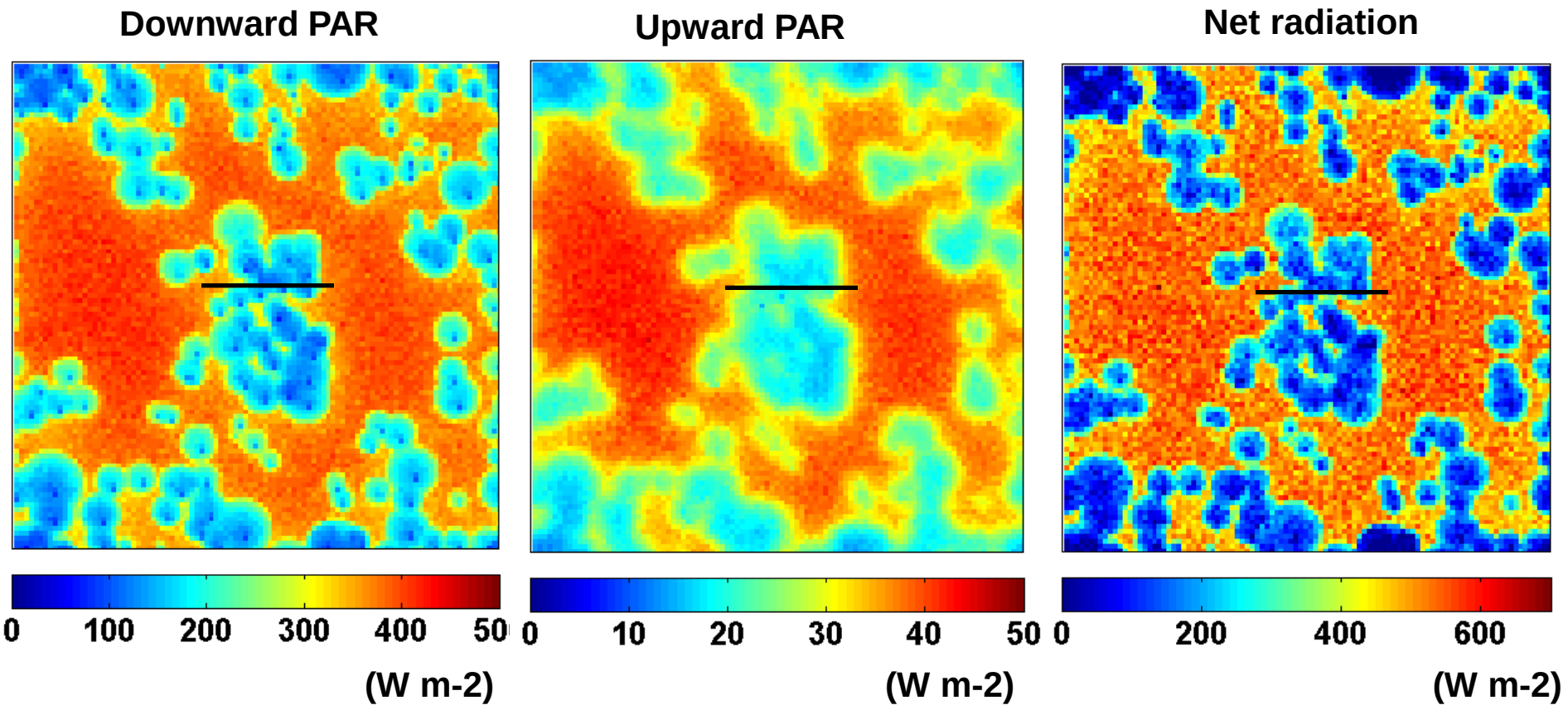
Physiological Capacity and Leaf Temperature: Why Low Capacity Leaves Can't Be Sunlit::or don't leave the potted Laurel Tree in the Sun



Study area for test of CANOAK-3d

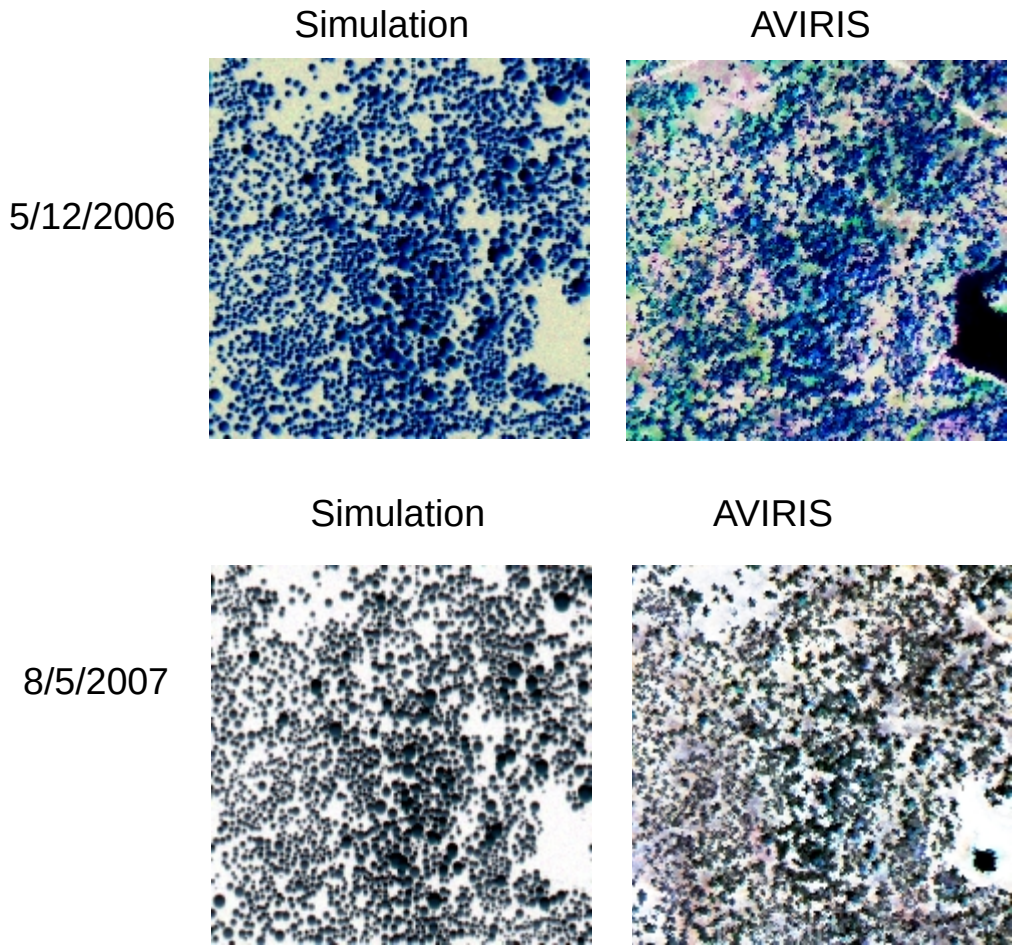


Simulated understory (1m above the ground) radiations near the tram site



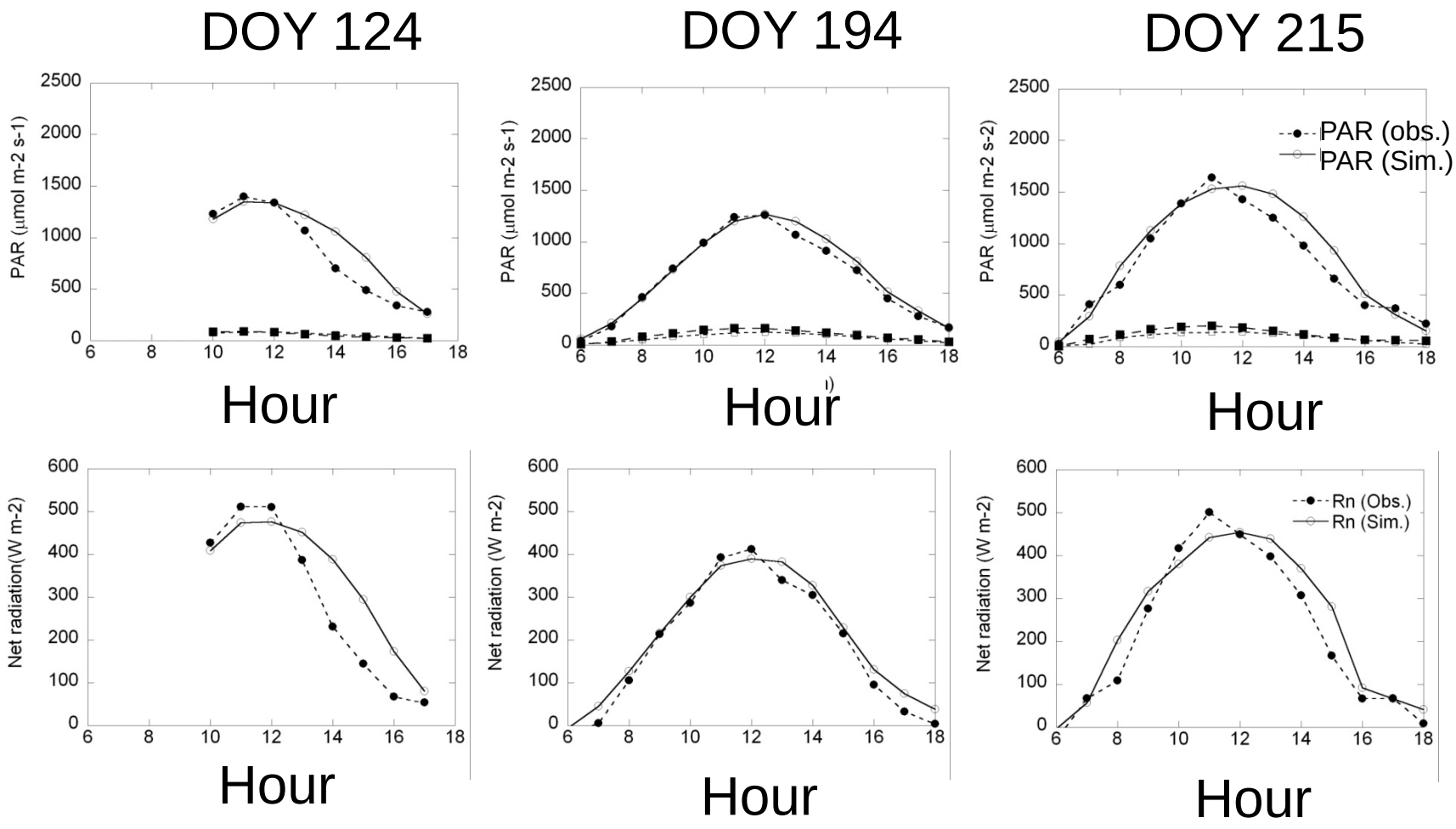
Kobayashi et al. 2011 AgForMet

Simulated images (RGB composite)



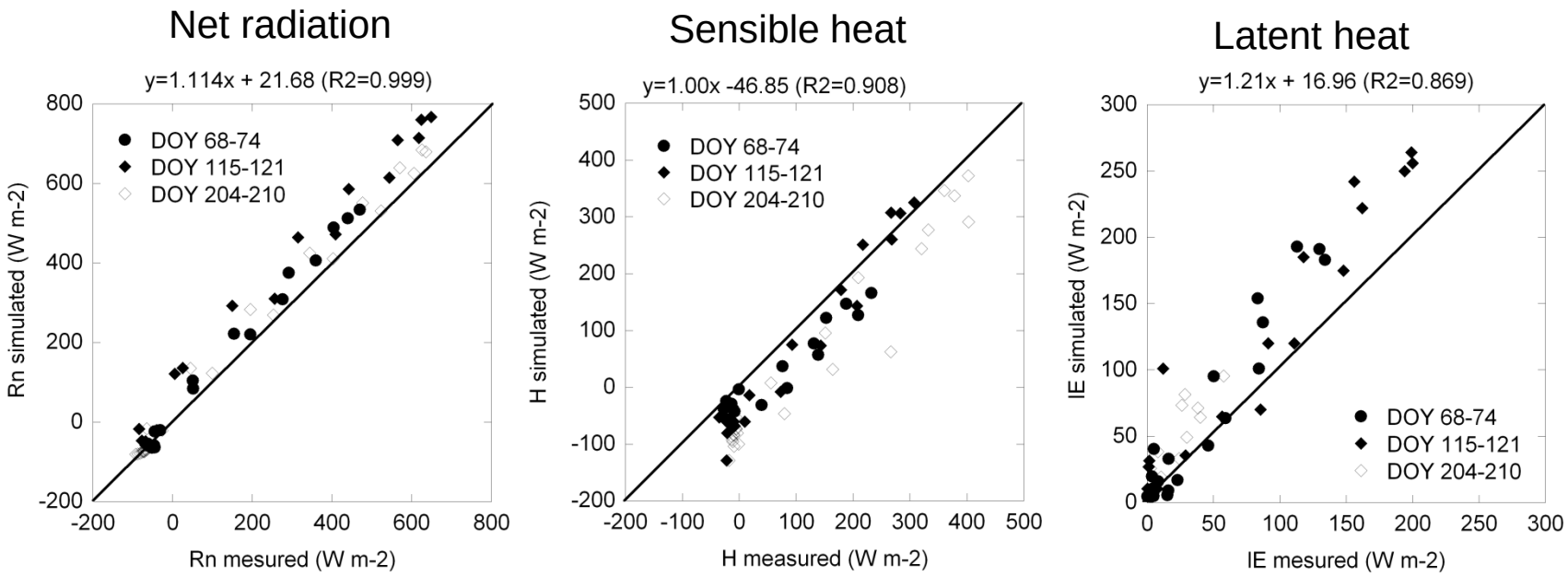
Kobayashi et al. 2011 AgForMet

Comparison of simulated and tram-measured PAR and net radiation



Kobayashi et al. 2011 AgForMet

Comparison of top of the tower net radiation, sensible heat and latent heat



Kobayashi et al. 2011 AgForMet

Below Canopy Fluxes

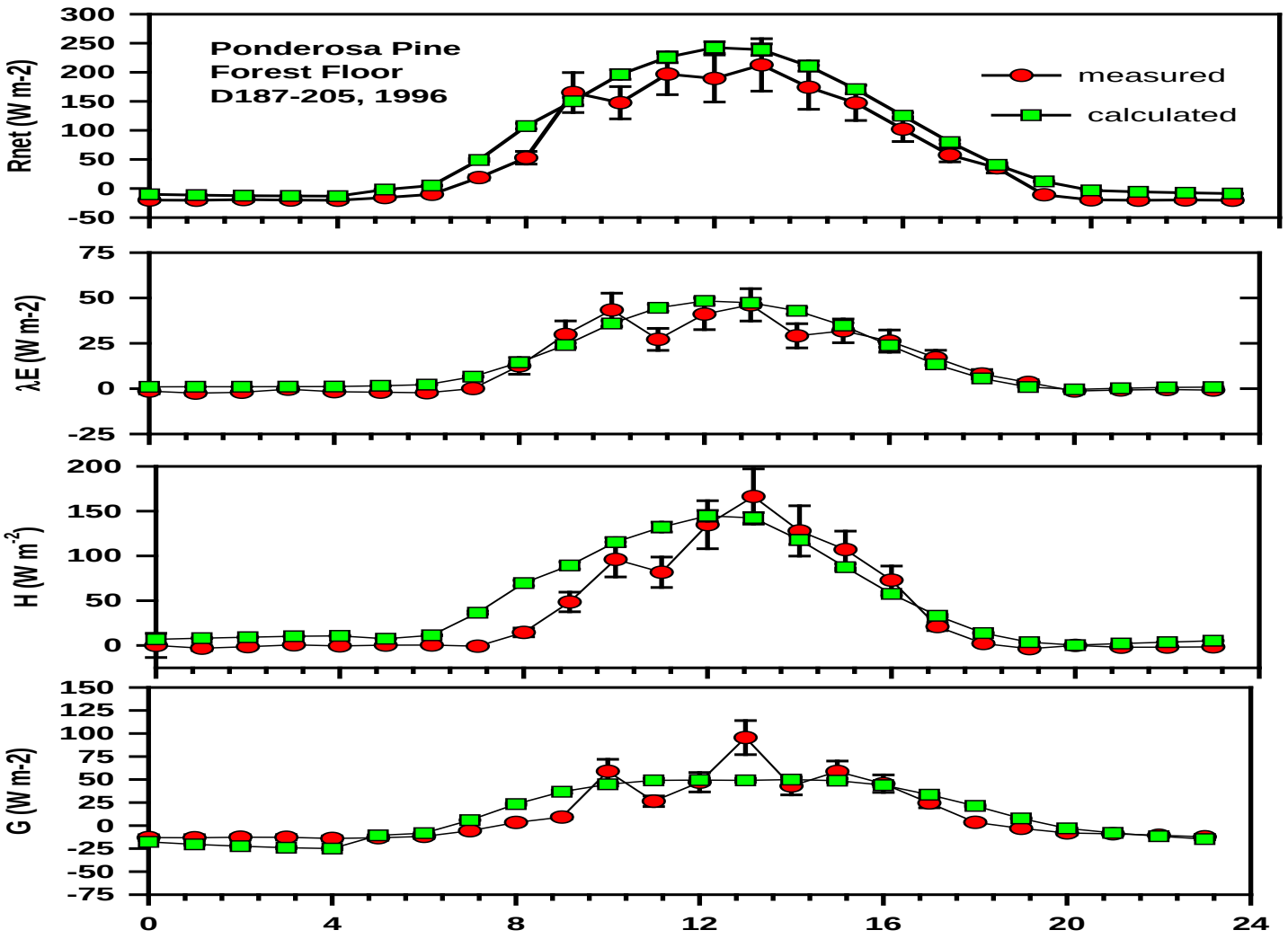
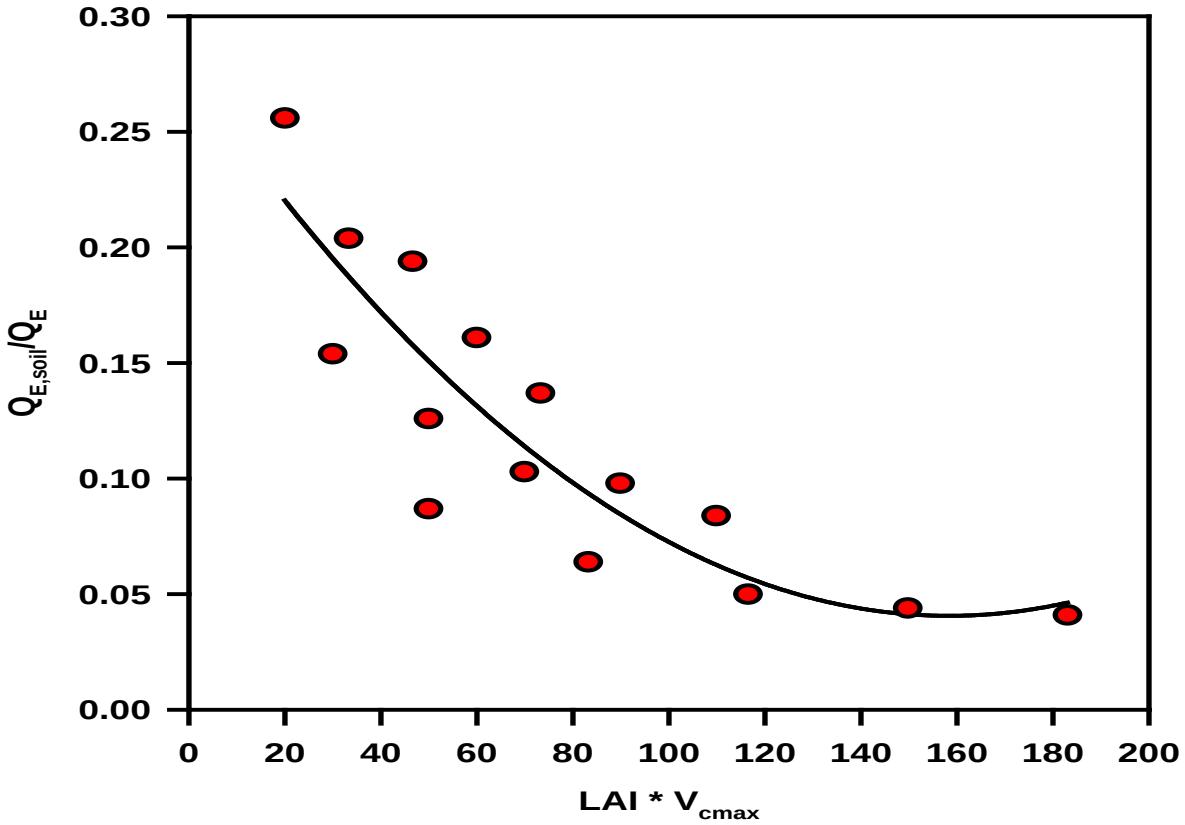


Figure 15
enbmod.spw
12/8/99: lai_{eff}=1.8, zlitter=0.08

Below Canopy Fluxes and Canopy Structure and Function



Impact of Thermal Stratification

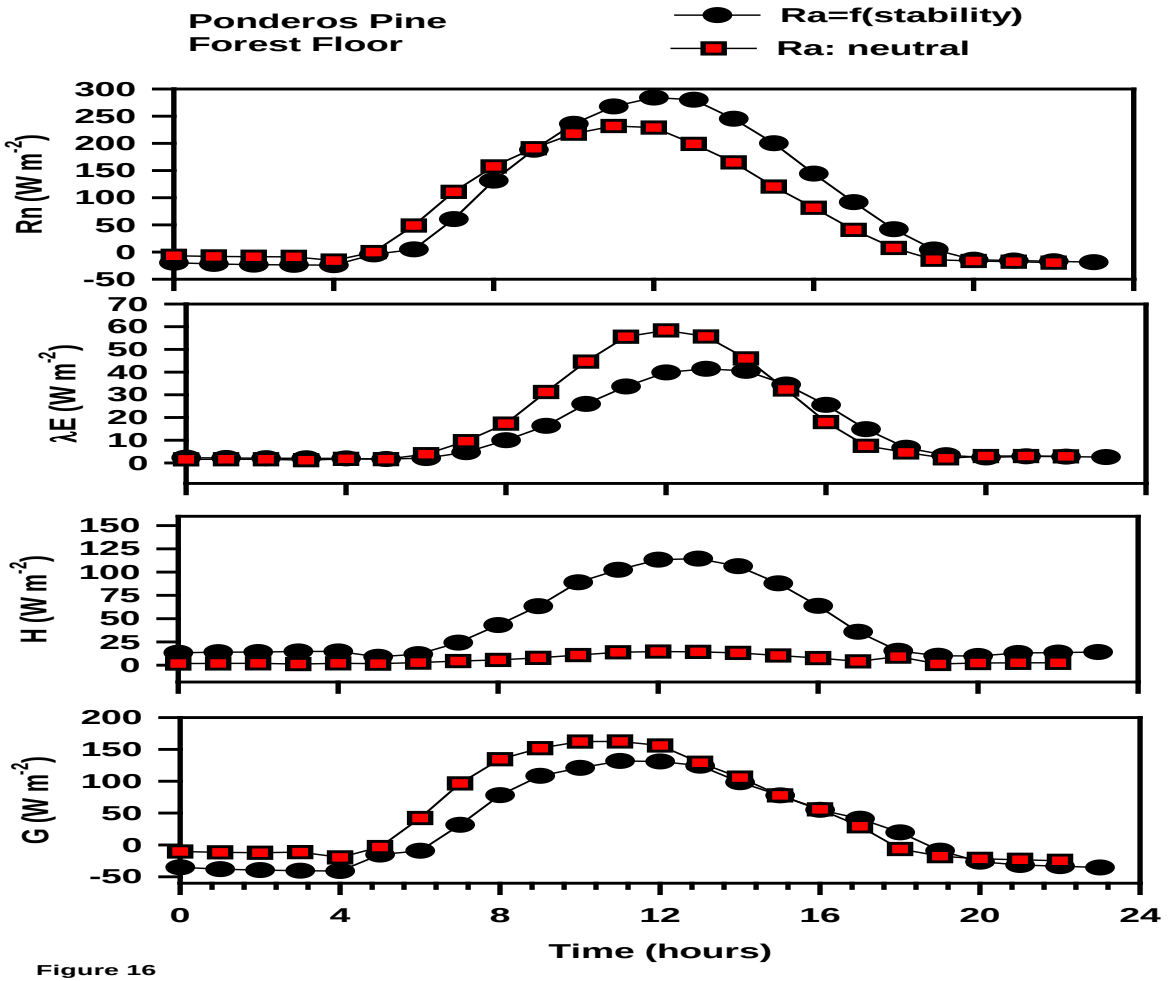


Figure 16
enmodstb.spw
12/8/99

Impact of Litter

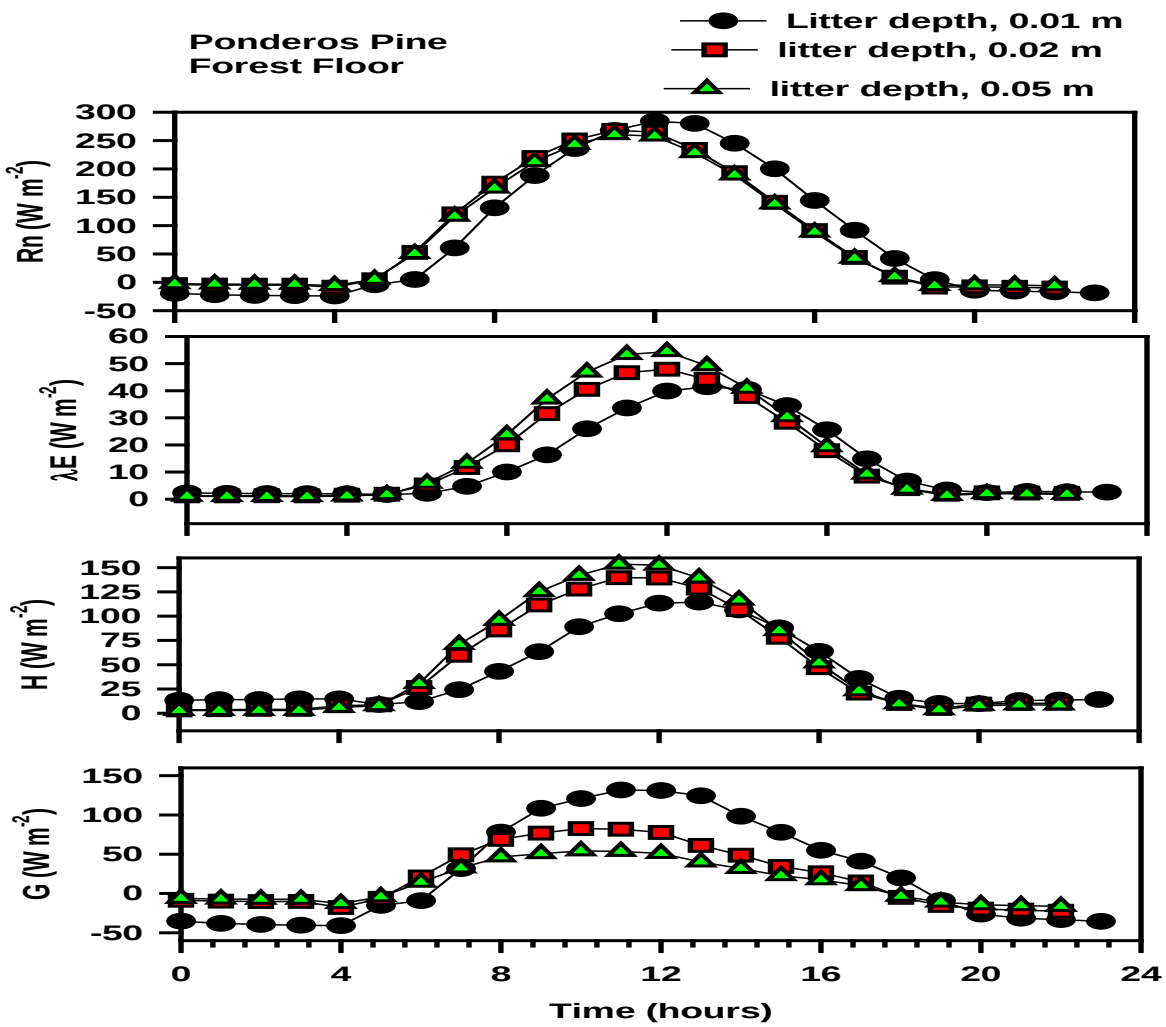


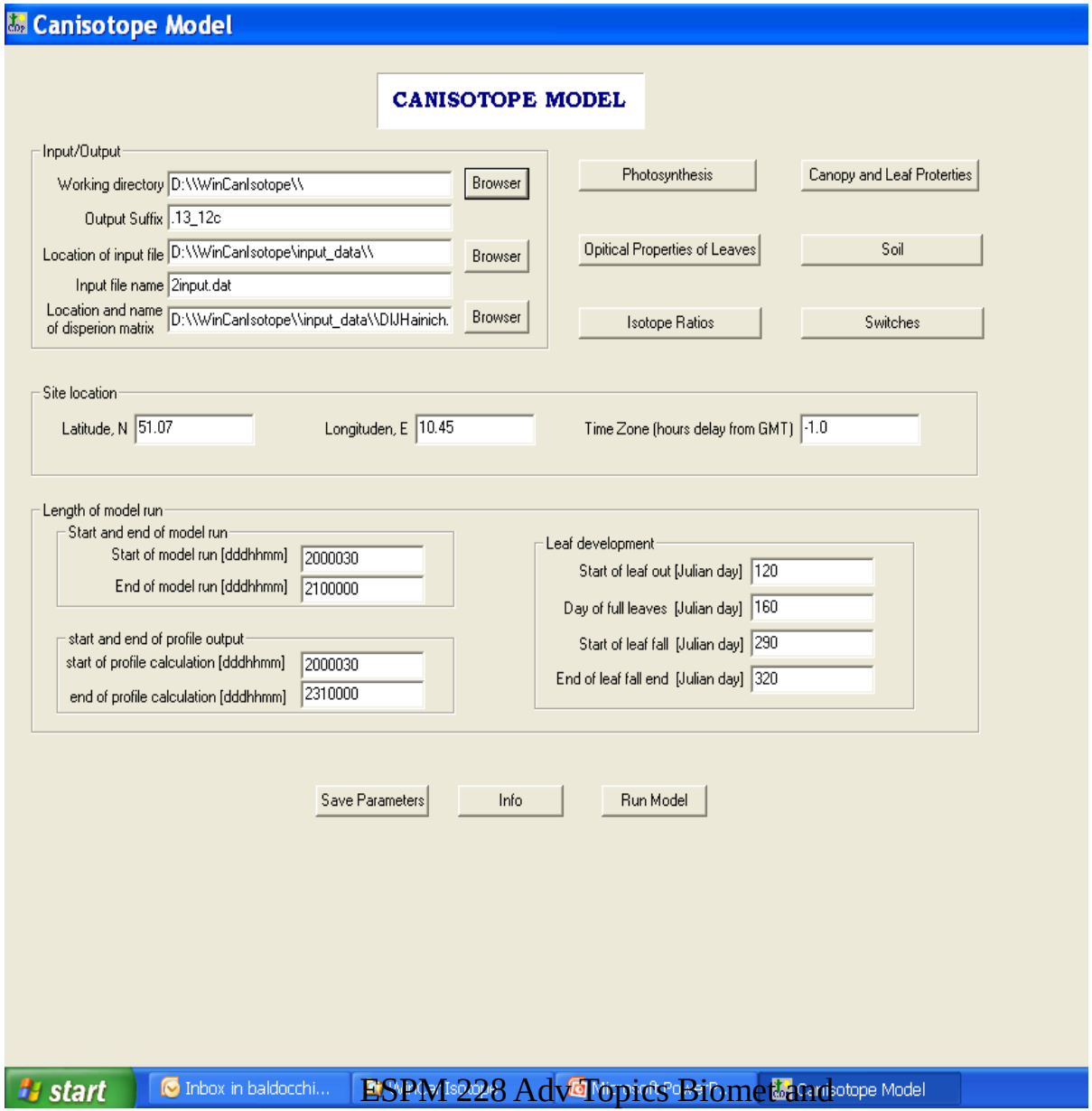
Figure 17
enmodlit.spw
12/8/99

Issues

- How Good is Good Enough?
- How Much Detail Is Enough?
  - Where and When can we Simplify?
- Assessing Errors and Variability in Model Parameters
- Constraining Model Parameters
- Assessing Errors in Driving Meteorological Conditions
- Biases in Test Data used to validate Models

Conclusions

- **Biophysical Models that Couple Aspects of Micrometeorology, Ecophysiology and Biogeochemistry Produce Accurate and Constrained Fluxes of C and Energy, across Multiple Time Scales**
- **Models can be used to Interpret Field Data**
  - **LUE is affected by LAI, Clumping, direct/diffuse radiation, Ps capacity**
  - **NEE is affected by length of growing season**
  - **Interactions between leaf size, Ps capacity and position help leaves avoid lethal temperatures**
  - **Below canopy fluxes are affected by T stratification and litter**


Canisotope Model
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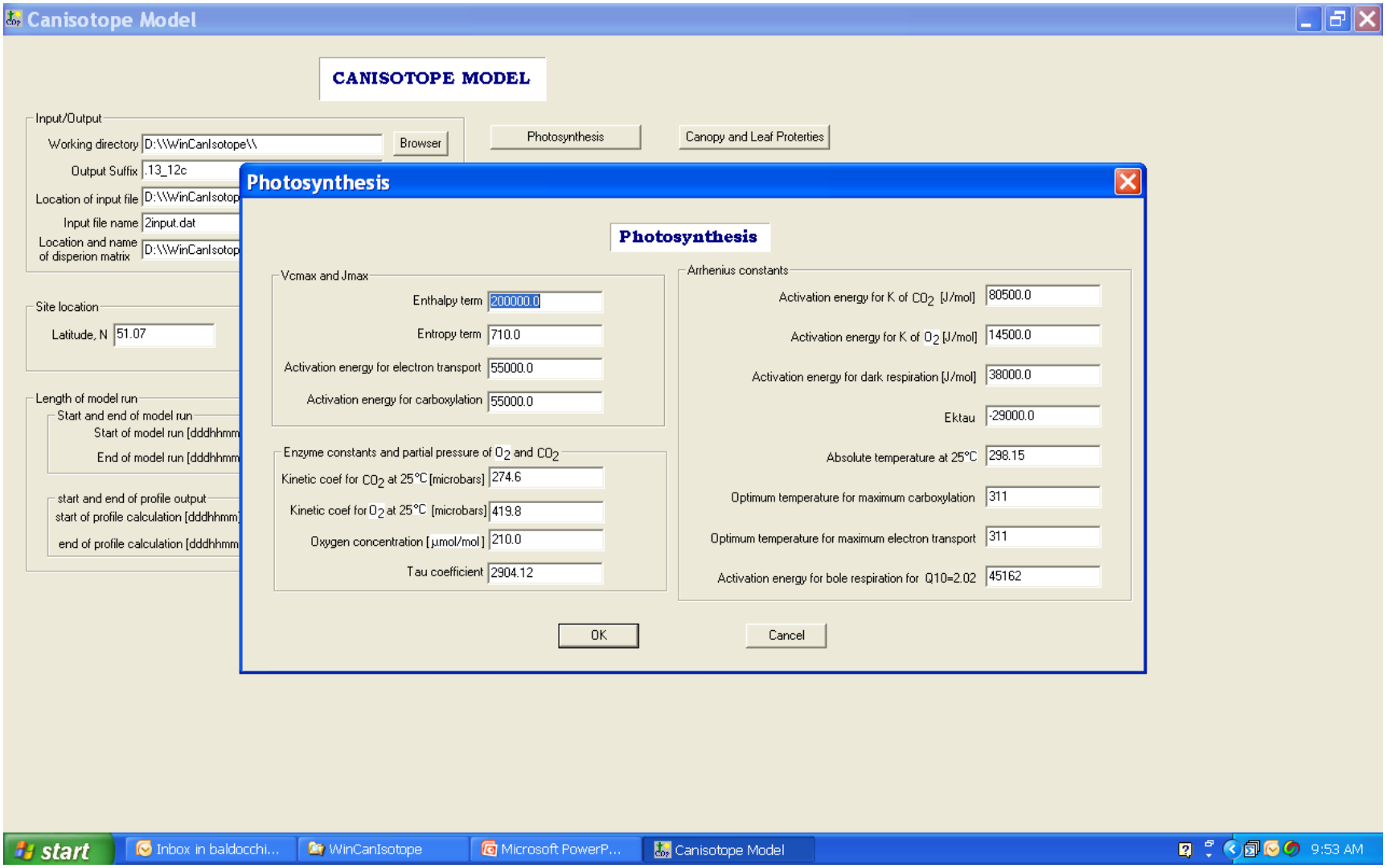
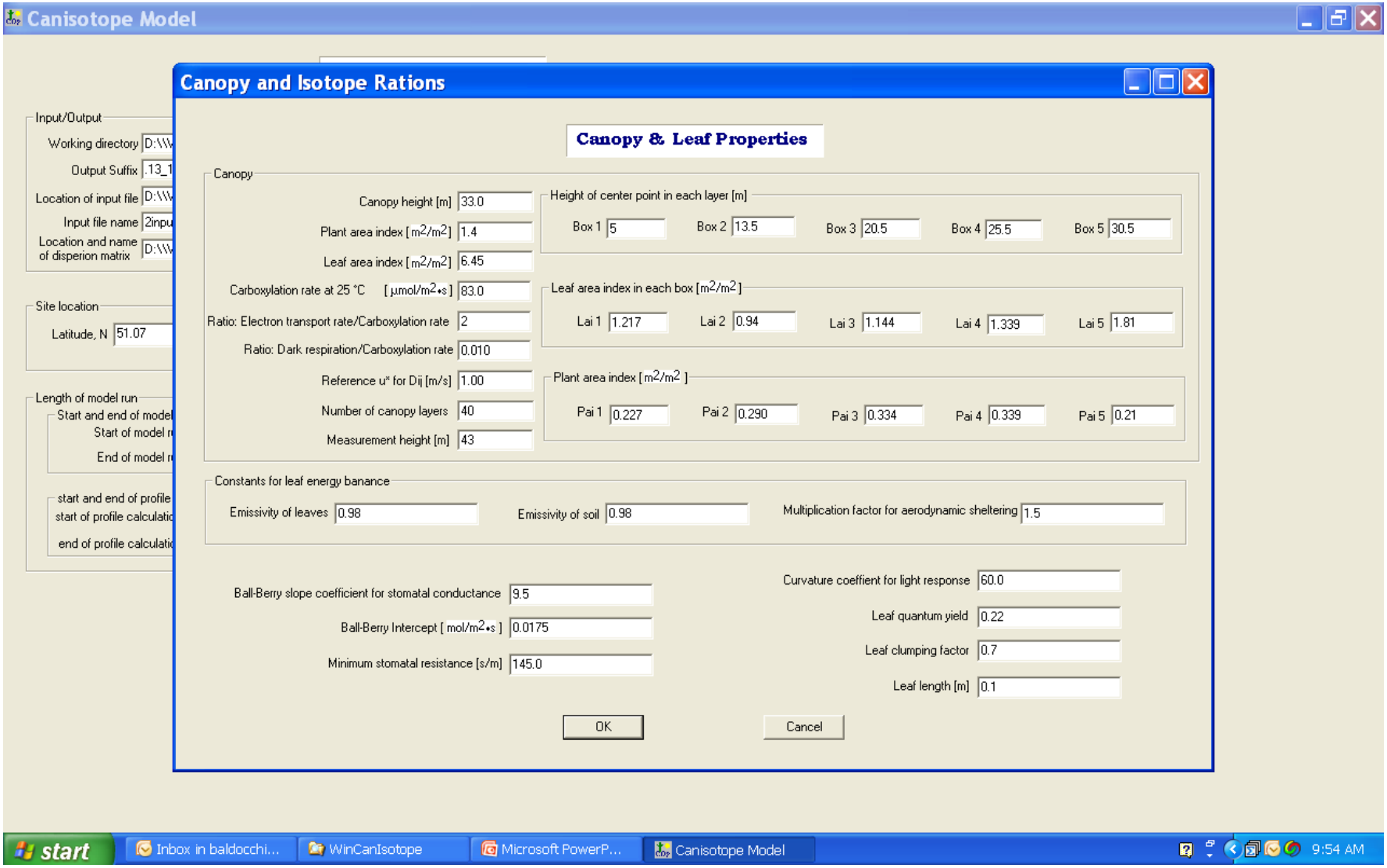
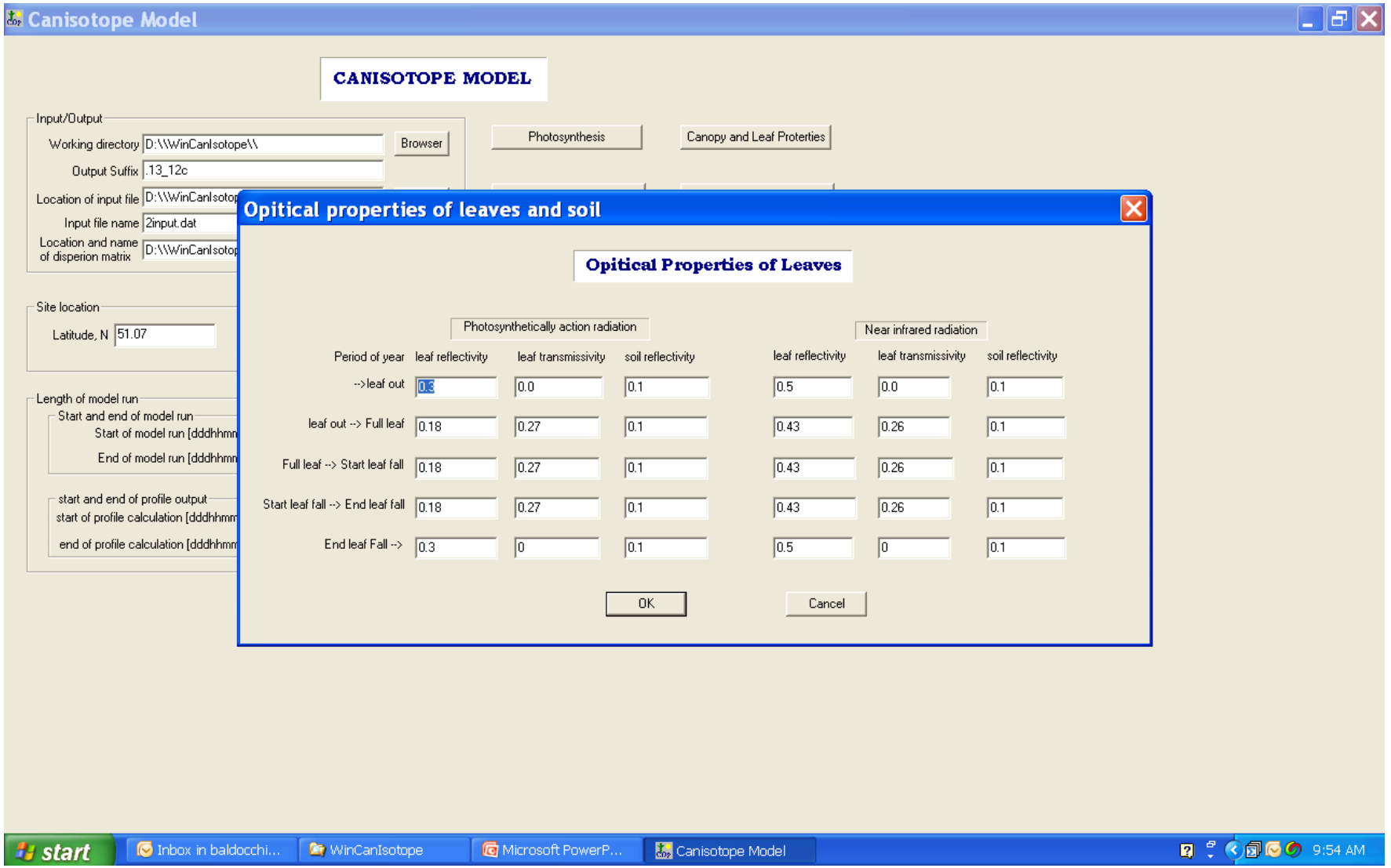
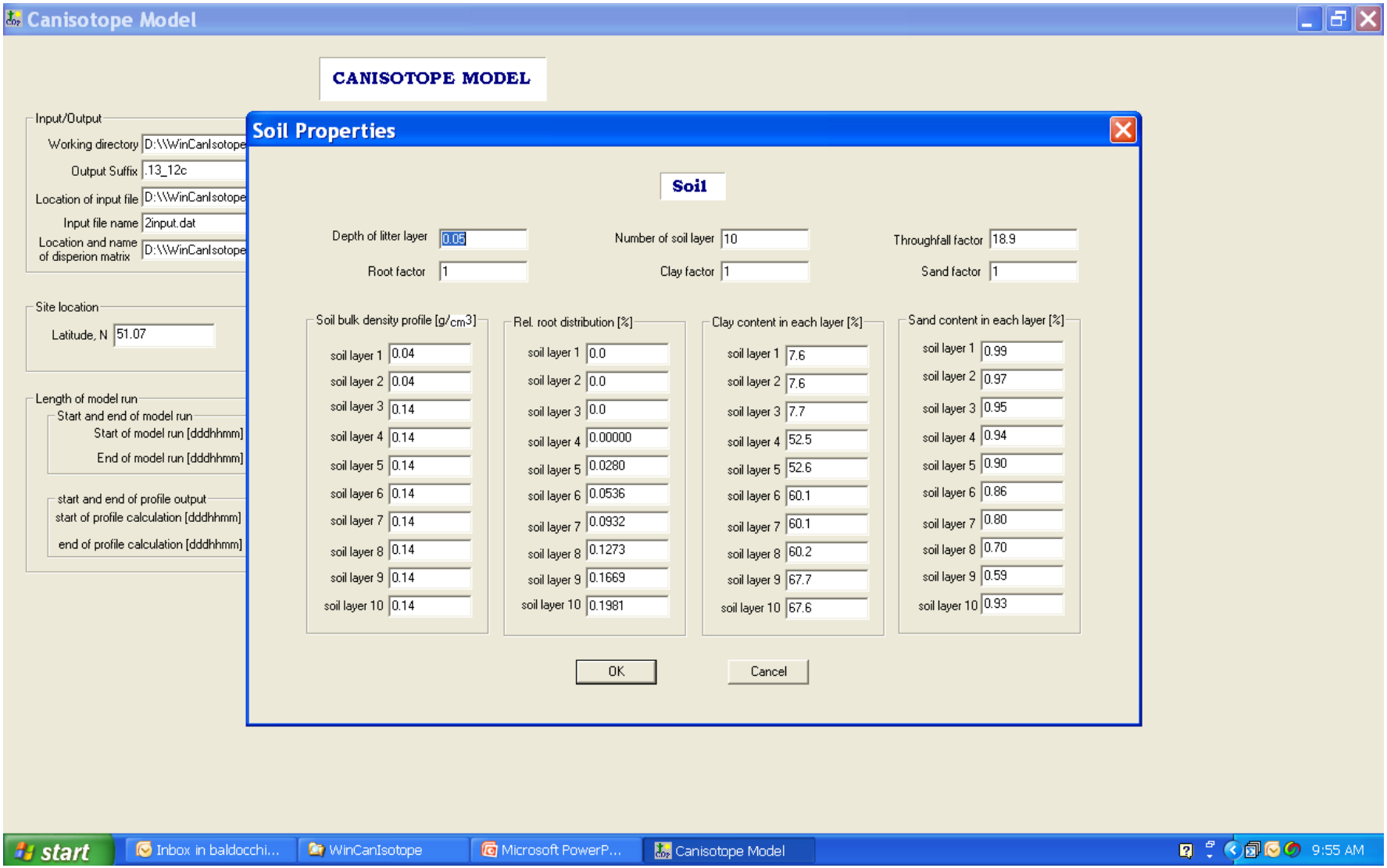
Input/Output
Working directory
D:\\WinCanIsotope\\
Browser
Output Suffix
.13_12c
Location of input file
D:\\WinCanIsotope\input_data\\
Browser
Input file name
2input.dat
Location and name of disperion matrix
D:\\WinCanIsotope\\input_data\\DIJHainich.
Browser
Photosynthesis
Canopy and Leaf Proterties
Optical Properties of Leaves
Soil
Isotope Ratios
Switches
Site location
Latitude, N
51.07
Longituden, E
10.45
Time Zone (hours delay from GMT)
-1.0
Length of model run
Start and end of model run
Start of model run [dddhhmm]
2000030
End of model run [dddhhmm]
2100000
start and end of profile output
start of profile calculation [dddhhmm]
2000030
end of profile calculation [dddhhmm]
2310000
Leaf development
Start of leaf out [Julian day]
120
Day of full leaves [Julian day]
160
Start of leaf fall [Julian day]
290
End of leaf fall end [Julian day]
320
Save Parameters
Info
Run Model
start
Inbox in baldocchi...
Canisotope Model


Canisotope Model
CANISOTOPE MODEL
Input/Output
Working directory D:\\WinCanIsotope\\
Browser
Output Suffix .13_12c
Location of input file D:\\WinCanIsotop
Input file name 2input.dat
Location and name of disperion matrix D:\\WinCanIsotop
Photosynthesis
Canopy and Leaf Proterties
Site location
Latitude, N 51.07
Length of model run
Start and end of model run
Start of model run [dddhhmm
End of model run [dddhhmm
start and end of profile output
start of profile calculation [dddhhmm
end of profile calculation [dddhhmm
Photosynthesis
Photosynthesis
Vcmax and Jmax
Enthalpy term 200000.0
Entropy term 710.0
Activation energy for electron transport 55000.0
Activation energy for carboxylation 55000.0
Enzyme constants and partial pressure of O2 and CO2
Kinetic coef for CO2 at 25°C [microbars] 274.6
Kinetic coef for O2 at 25°C [microbars] 419.8
Oxygen concentration [µmol/mol] 210.0
Tau coefficient 2904.12
Arrhenius constants
Activation energy for K of CO2 [J/mol] 80500.0
Activation energy for K of O2 [J/mol] 14500.0
Activation energy for dark respiration [J/mol] 38000.0
Ektau -29000.0
Absolute temperature at 25°C 298.15
Optimum temperature for maximum carboxylation 311
Optimum temperature for maximum electron transport 311
Activation energy for bole respiration for Q10=2.02 45162
OK
Cancel
start
Inbox in baldocchi...
WinCanIsotope
Microsoft PowerP...
Canisotope Model
9:53 AM

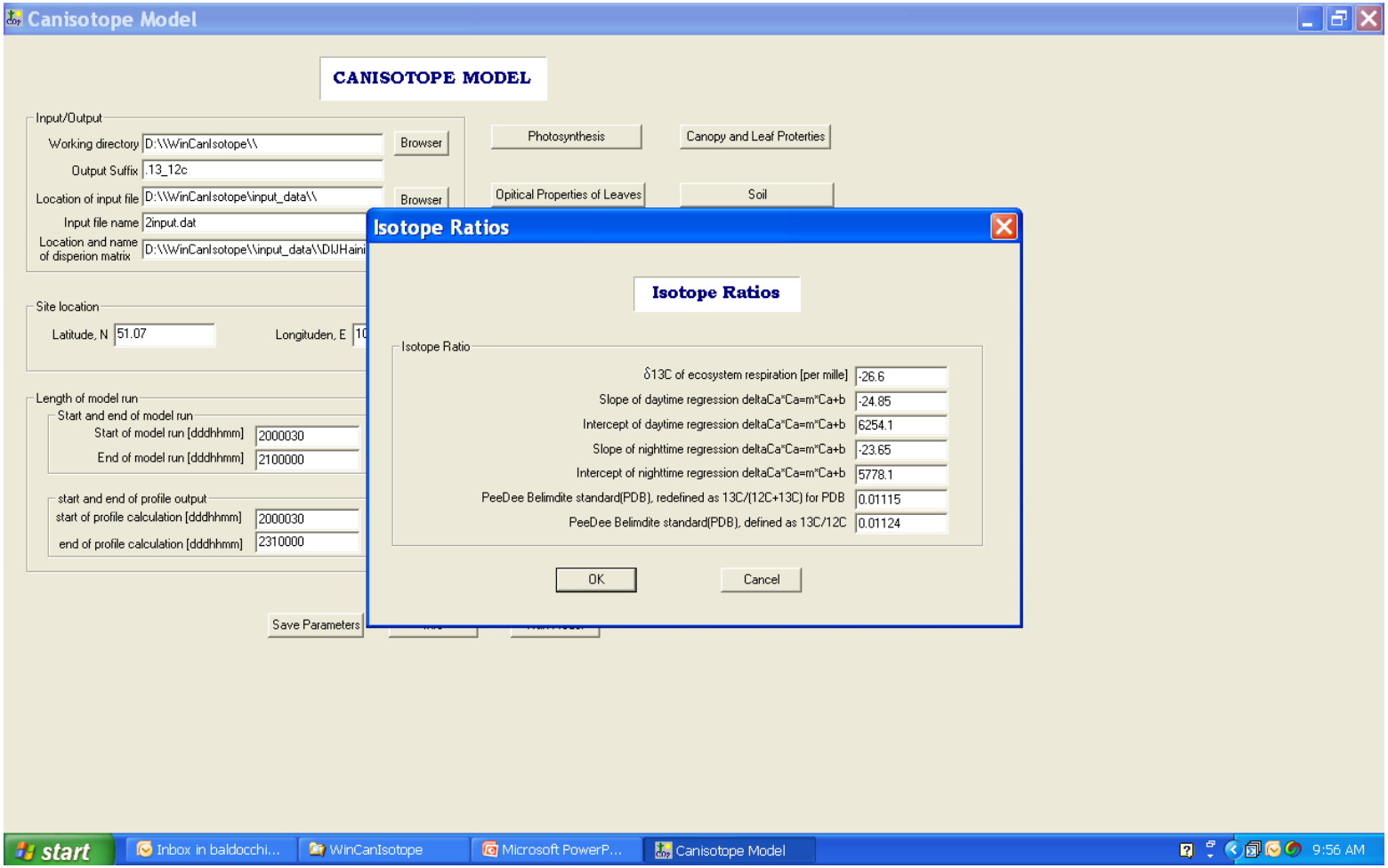


ESPM 228 Adv Topics Biomet and Micromet


Canisotope Model
CANISOTOPE MODEL
Input/Output
Working directory D:\\WinCanIsotope\\
Browser
Output Suffix .13_12c
Location of input file
Input file name 2input.dat
Location and name of disperion matrix
Photosynthesis
Canopy and Leaf Proterties
Site location
Latitude, N 51.07
Length of model run
Start and end of model run
Start of model run [dddhhmm
End of model run [dddhhmm
start and end of profile output
start of profile calculation [dddhhmm
end of profile calculation [dddhhmm
Opitical properties of leaves and soil
Opitical Properties of Leaves
Photosynthetically action radiation
Near infrared radiation
Period of year
leaf reflectivity
leaf transmissivity
soil reflectivity
leaf reflectivity
leaf transmissivity
soil reflectivity
-->leaf out 0.3 0.0 0.1 0.5 0.0 0.1
leaf out --> Full leaf 0.18 0.27 0.1 0.43 0.26 0.1
Full leaf --> Start leaf fall 0.18 0.27 0.1 0.43 0.26 0.1
Start leaf fall --> End leaf fall 0.18 0.27 0.1 0.43 0.26 0.1
End leaf Fall --> 0.3 0 0.1 0.5 0 0.1
OK
Cancel
start
Inbox in baldocchi...
WinCanIsotope
Microsoft PowerP...
Canisotope Model
9:54 AM



ESPM 228 Adv Topics Biomet and Micromet


Canisotope Model
CANISOTOPE MODEL
Input/Output
Working directory
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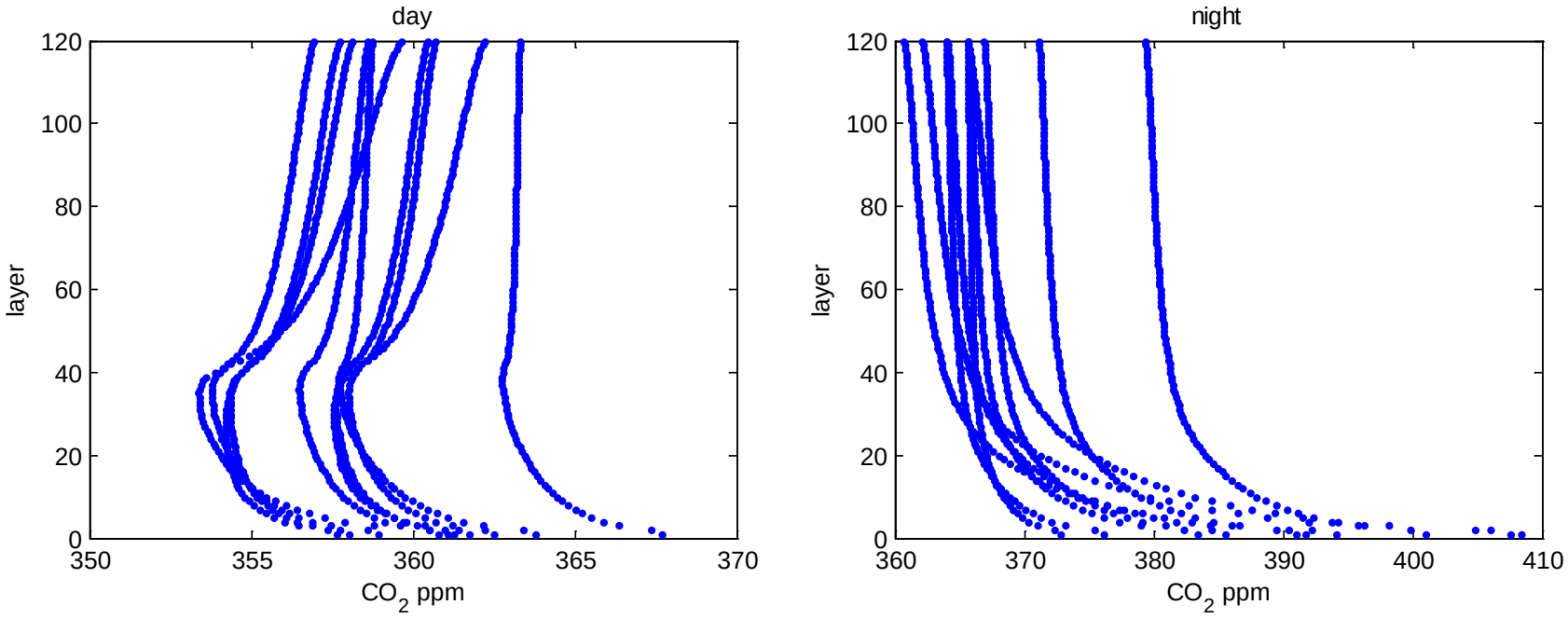
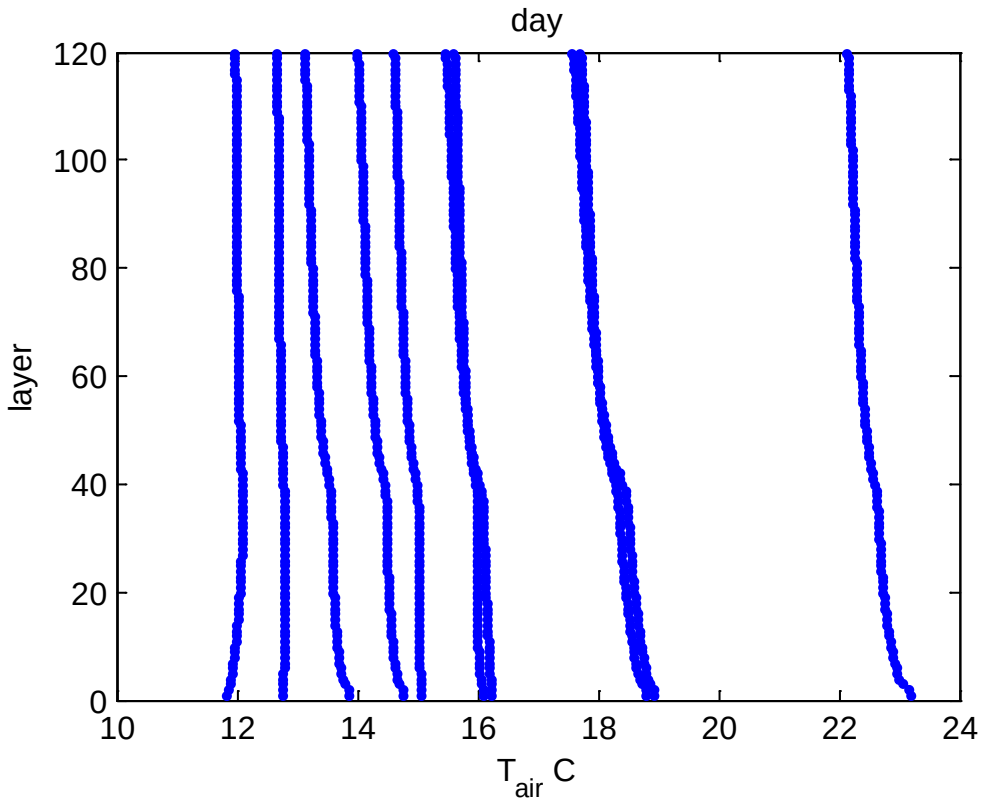
Browser
Output Suffix
.13_12c
Location of input file
D:\\WinCanIsotope\input_data\\
Browser
Input file name
2input.dat
Location and name of disperion matrix
D:\\WinCanIsotope\\input_data\\DIJHaini
Photosynthesis
Canopy and Leaf Proterties
Optical Properties of Leaves
Soil
Site location
Latitude, N
51.07
Longituden, E
Length of model run
Start and end of model run
Start of model run [dddhhmm]
2000030
End of model run [dddhhmm]
2100000
start and end of profile output
start of profile calculation [dddhhmm]
2000030
end of profile calculation [dddhhmm]
2310000
Save Parameters
Isotope Ratios
Isotope Ratios
Isotope Ratio
δ13C of ecosystem respiration [per mille]
-26.6
Slope of daytime regression deltaCa*Ca=m*Ca+b
-24.85
Intercept of daytime regression deltaCa*Ca=m*Ca+b
6254.1
Slope of nighttime regression deltaCa*Ca=m*Ca+b
-23.65
Intercept of nighttime regression deltaCa*Ca=m*Ca+b
5778.1
PeeDee Belimdite standard(PDB), redefined as 13C/(12C+13C) for PDB
0.01115
PeeDee Belimdite standard(PDB), defined as 13C/12C
0.01124
OK
Cancel
start
Inbox in baldocchi...
WinCanIsotope
Microsoft PowerP...
Canisotope Model
9:56 AM

CO_2 Microclimate



Temperature Microclimate



Lesson/Exercise

- Vary CO2 and compute fluxes, ambient, +100, +300, +500 ppm
- Vary LAI and compute Fluxes, 1,2,4,8