

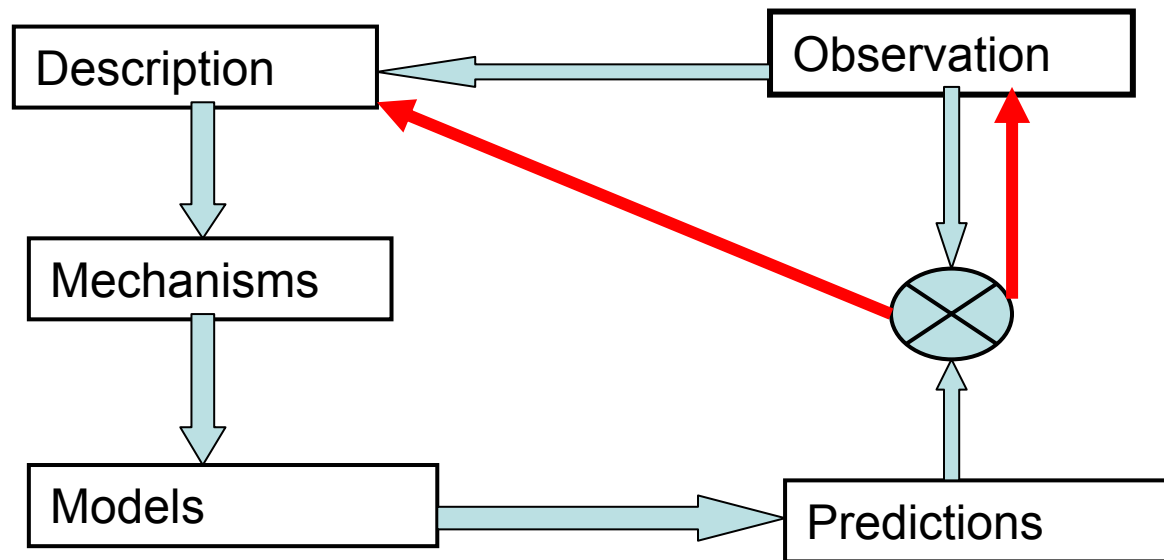
Introduction to CSIRO Biosphere Model (CBM)

Yingping Wang and Ray Leuning
CSIRO Marine and Atmospheric
Research, Australia

Modelling

- Why modelling?
- Models as a set of hypothesis
- Models as a synthesis tool
- Interactions between modelling and measurements

Model as a set of hypothesis



Use of surface flux models for interpreting eddy flux measurements

- Absorbed radiation drives surface processes
- Conservation of mass and energy
- Energy partitioning: demand and supply

Energy partitioning: the demand and supply

- Energy partitioning: $R_n = \lambda E + H + G$

$$\text{Bowen ratio} : \beta = \frac{H}{\lambda E}$$



$\beta = 0.3$



$\beta = 10$

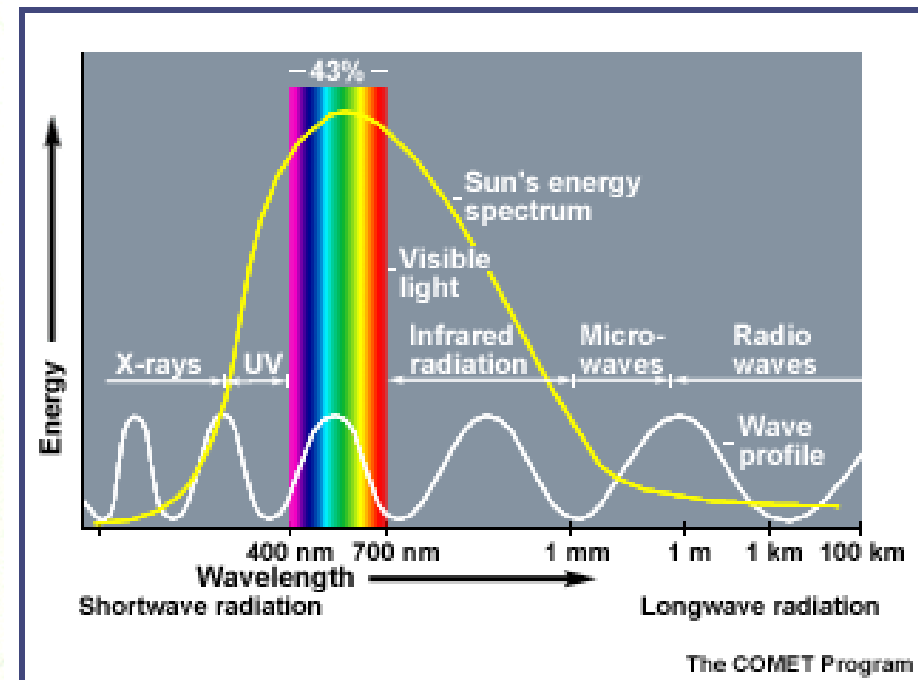
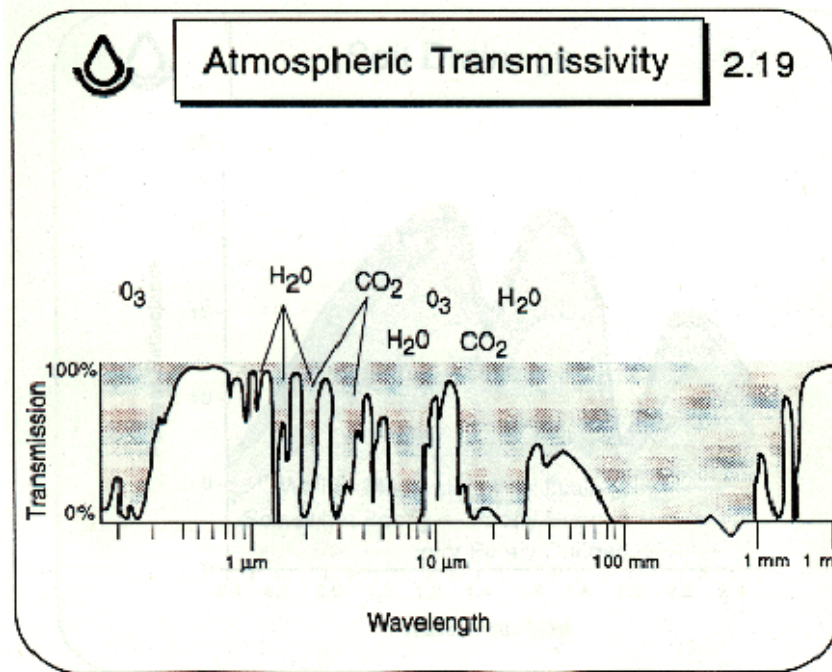
Overview of CBM

- CBM (CSIRO Biosphere Model) simulates exchange of heat, water and CO₂ between land surface and atmosphere
- Key processes
 - Radiative transfer
 - Leaf energy balance
 - Stomatal conductance: coupling transpiration and photosynthesis
 - Leaf photosynthesis model
 - Plant and soil respiration
 - Soil heat, water

The two-leaf canopy

- Why two-leaf approach?
 - Multi-layered canopy requires more computing
 - One-leaf approach is inaccurate
- Essence of two-leaf canopy
 - Bulk parameter formulation for sunlit and shaded leaves separately
 - Same equations for single leaf is used for big leaf

Solar radiation and its spectra



Radiation flux

- The energy unit for radiation is Joule $\text{m}^{-2} \text{s}^{-1}$, or Watt m^{-2} ;
- For photosynthesis, it is not the energy, but number of photos important for the photosystems in a leaf
- The amount of energy per photo decreases with an increase in wavelength. On average

$$1 \text{ W m}^{-2} = 4.6 \mu\text{mol m}^{-2} \text{ s}^{-1} \text{ for visible}$$

Four radiation wavebands

Three radiation wavebands of solar radiation
(or shortwave radiation):

Solar radiation (short-wave radiation)

- Ultraviolet (0.2 to 0.4 μm); 5-8%
- Visible (0.4 to 0.7 μm), 46-50%
- Near infrared (0.7 to 1.5 μm) 44-46%

Long-wave radiation >10 (μm)

Leaf optical properties

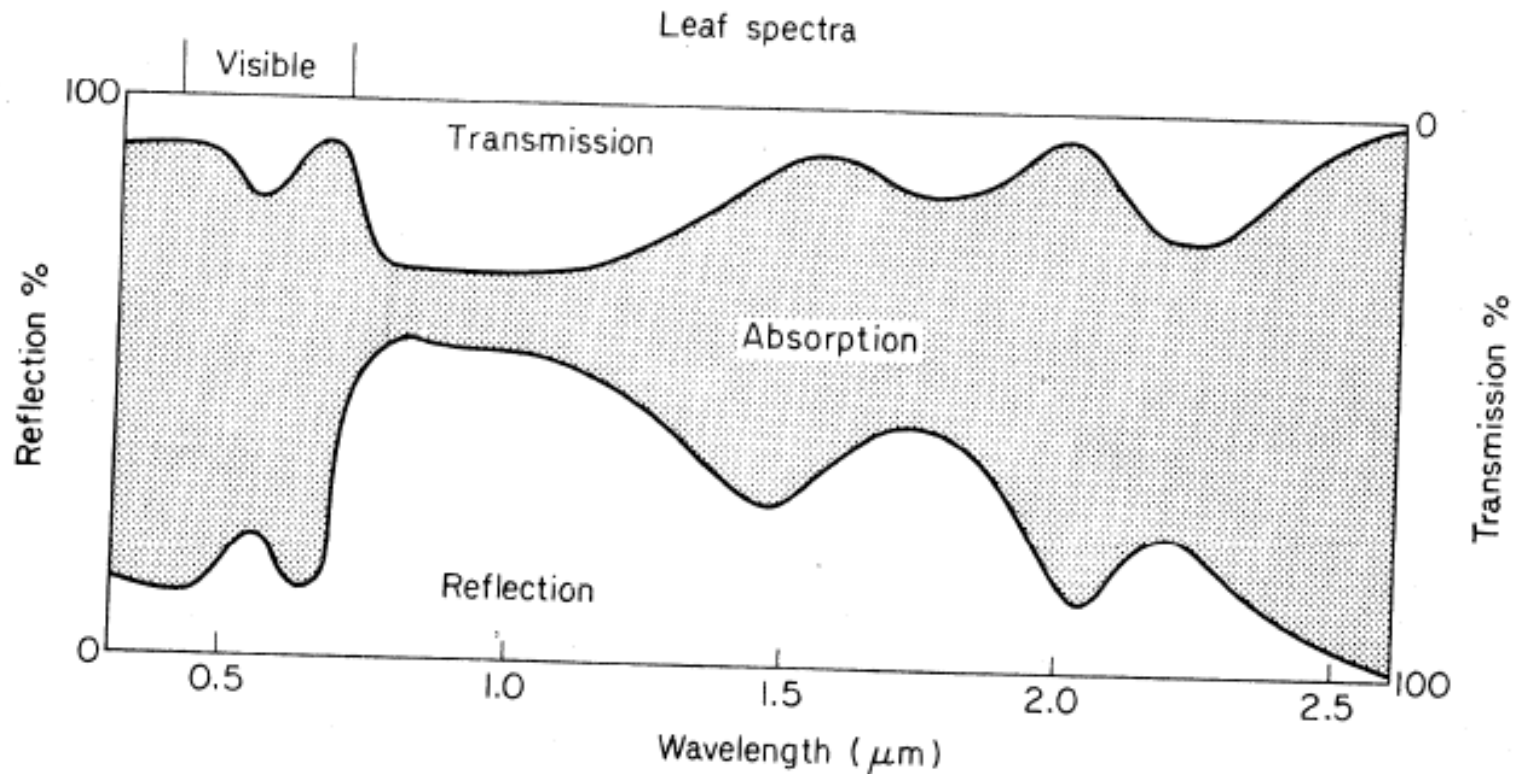


Fig. 6.5 Idealized relation between the reflectivity, transmissivity and absorptivity of a green leaf.

Surface radiation balance

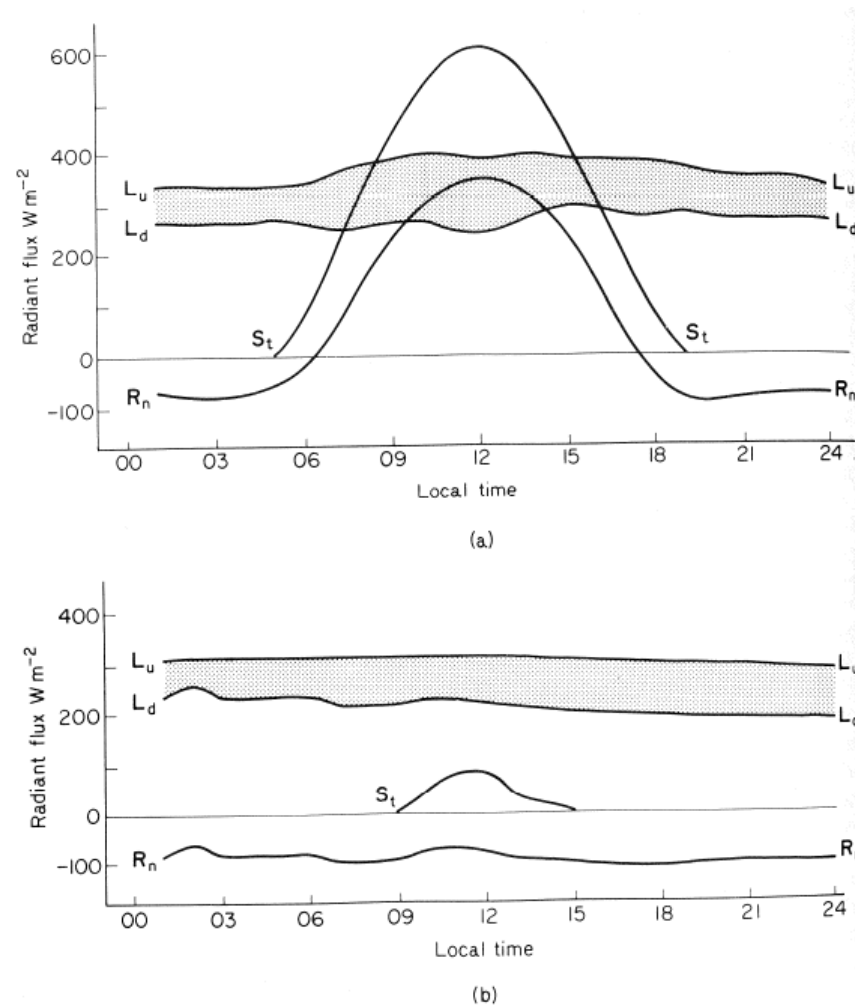
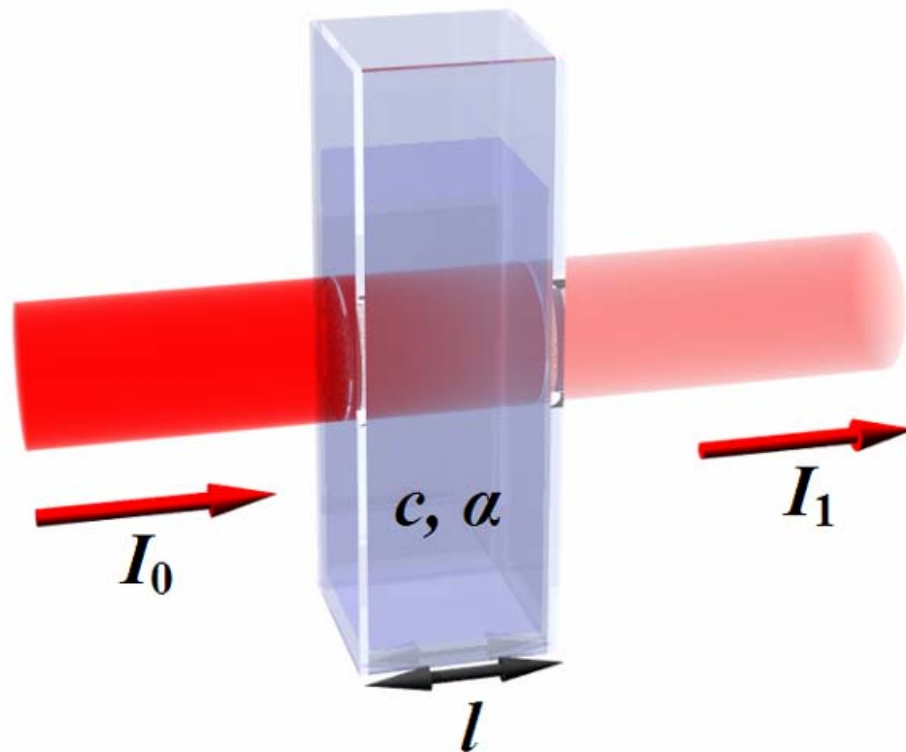


Fig. 4.12 Radiation balance at Bergen, Norway (60°N , 5°E): (a) on 13 April 1968, (b) on 11 January 1968. The grey area shows the net long wave loss and the line R_n is net radiation. Note that net radiation was calculated from measured fluxes of incoming short and long wave radiation, assuming that the reflectivity of the surface was 0.20 in April (e.g. vegetation) and 0.70 in January (e.g. snow). The radiative temperature of the surface was assumed equal to the measured air temperature.

The Beer's law

- Beer's law was independently discovered (in various forms) by [Pierre Bouguer](#) in 1729, [Johann Heinrich Lambert](#) in 1760 and [August Beer](#) in 1852.



$$\frac{I_1}{I_0} = \exp(-alc) = \exp(-kL)$$

Where

a : is absorption coefficient;

l : path length;

c : concentration of absorbant;

k : extinction coefficient;

L : canopy leaf area index.

Extinction coefficient (k)

- Canopy extinction coefficient, k , is defined as $k=G/\sin\beta$, where G is the ratio of mean projected area of a leaf on a plane normal to the sun's ray and the actual leaf area.

- $G=A_p/A$

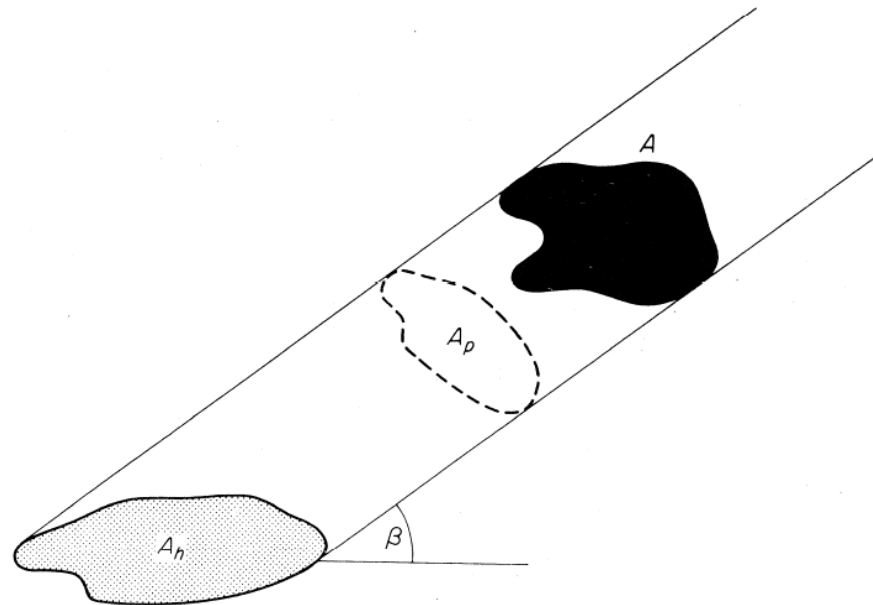
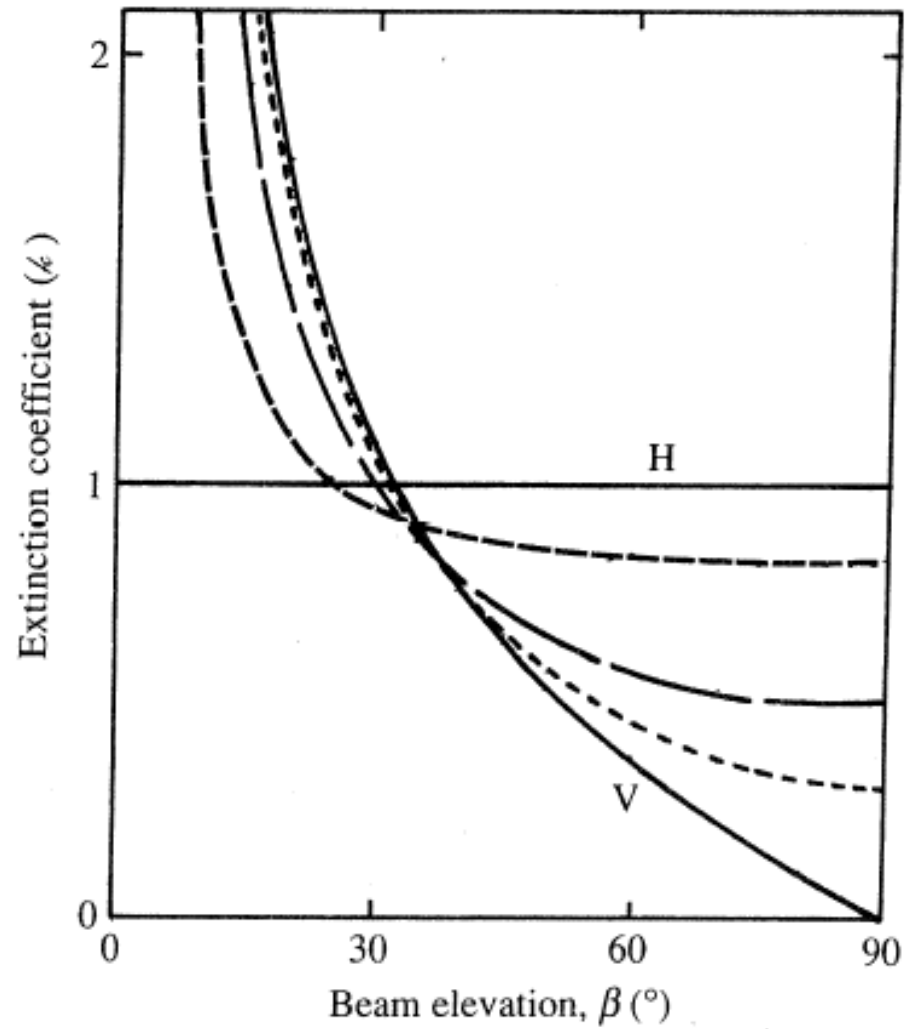


Fig. 5.1 Area A projected on surface at right angles to solar beam (A_p) and on horizontal surface (A_h).

Leaf angle distribution and k_b

Leaf angle distribution	k_b
Horizontal leaves	$k_b=1$
Vertical leaves	$k_b=2\cot\beta/\pi$
Spherical leaves	$k_b=1/(2\sin\beta)$
Ellipsoidal leaves	$k_b=(x^2+\cot^2\beta)^{0.5}/(A(x)x)$

Extinction coefficient for direct beam radiation (k_b)



Extinction coefficient for diffuse radiation (k_d)

$$k_d = \frac{1}{L} \ln \left(\frac{\iint i_d \exp(-k_b L) \sin \theta \cos \theta d\theta d\phi}{\iint i_d \sin \theta \cos \theta d\theta d\phi} \right)$$

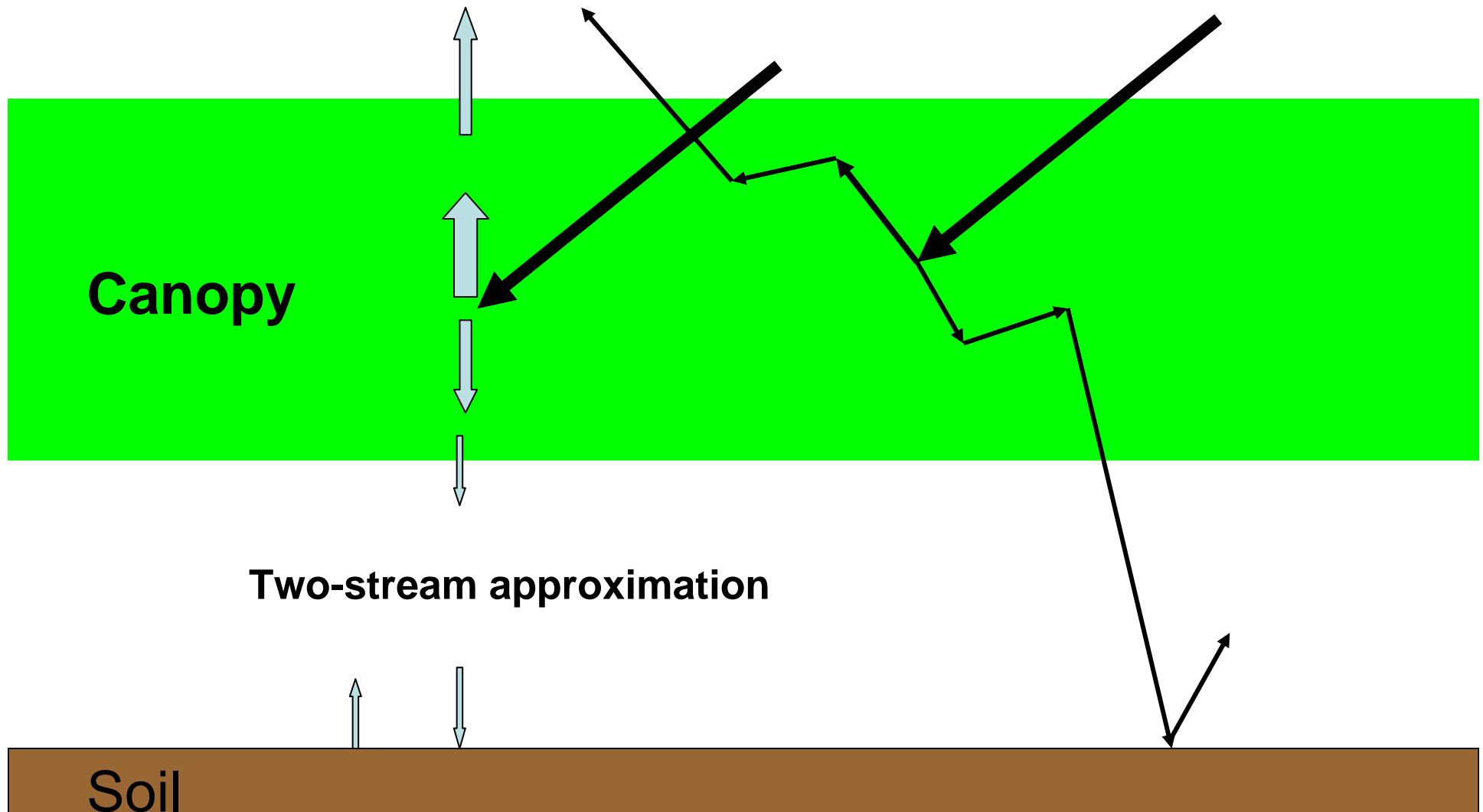
$$k_d \in [0.5, 0.8]$$

Sunlit leaf area fraction

- Fraction of sunlit leaf area, f_{sun} is equal to gap fraction, $\exp(-k_b L)$.
- For a canopy, total sunlit leaf area index, L_{sun} , is given by

$$L_{\text{sun}} = \int_0^L \exp(-k_b \xi) d\xi = (1 - \exp(-k_b L)) / L$$

The two-stream approximation (The Goudriaan's model)



Two-stream approximation

Analytic solution to two-stream approximation suggests:

- the flux density of un-intercepted diffuse radiation and scattered diffuse radiation decreases exponentially with the exponent being $k_d^* \xi$, where x is cumulative canopy LAI from the canopy top, and $k_d^* = k_d \sqrt{1 - \omega}$.

Radiation absorption within a plant canopy

Radiation absorbed by the shaded leaves, q_{shade}

$$q_{shade} = \underbrace{I_d k_d^* (1 - \rho_d) \exp(-k_d^* \xi)}_{\text{Absorbed diffuse radiation}} + \underbrace{I_b \left[k_b^* (1 - \rho_b) \exp(-k_b^* \xi) - k_b (1 - \omega) \exp(-k_b \xi) \right]}_{\text{absorbed scattered direct beam radiation}}$$

Radiation absorbed by the sunlit leaves, q_{sun} :

$$q_{sun} = q_{shade} + I_b k_b (1 - \omega)$$

Total amount of radiation absorbed

All sunlit leaves, Q_{sun}

$$Q_{sun} = \int_0^L \exp(-k_b \xi) q_{sun}(\xi) d\xi .$$

All shaded leaves, Q_{shade}

$$Q_{shade} = \int_0^L (1 - \exp(-k_b \xi)) q_{shade}(\xi) d\xi .$$

Leaf energy balance

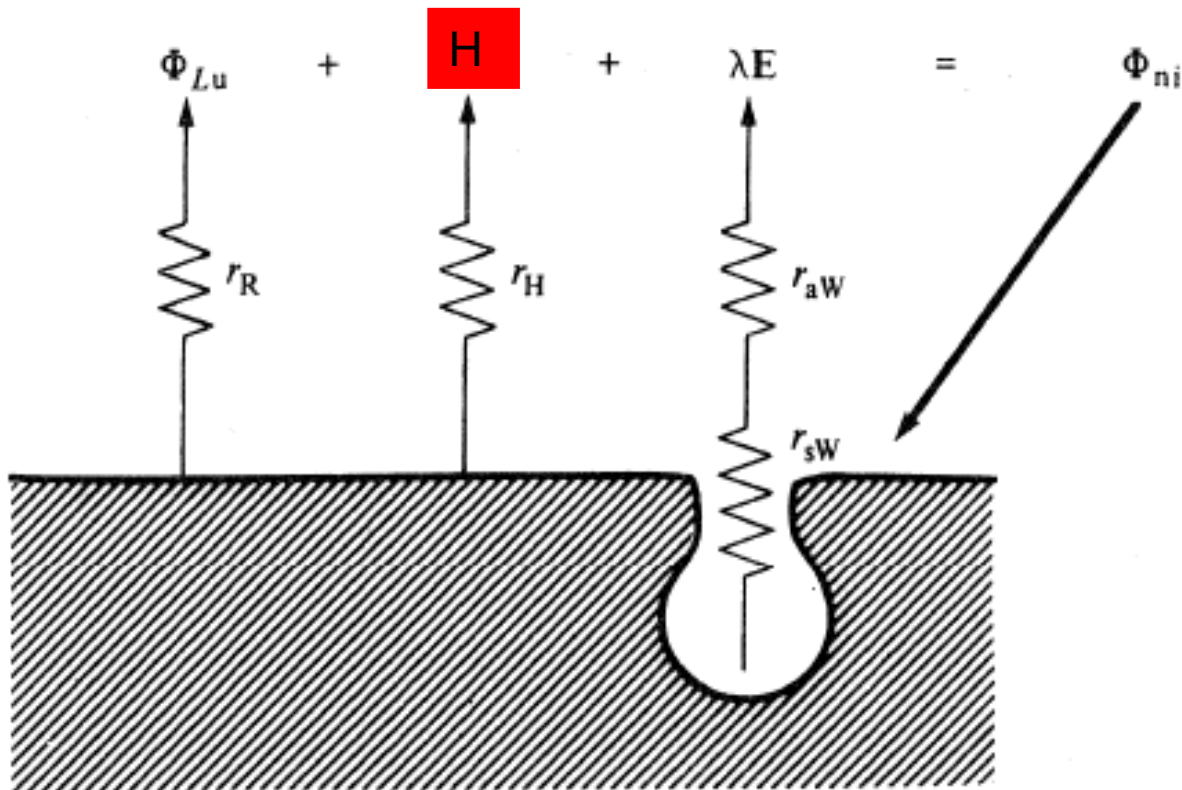


Fig. 5.1. Energy exchanges for a leaf, where the radiative heat loss Φ_{Lu} is the difference between actual net radiation and isothermal net radiation.

Leaf energy balance

- The governing equation:

$$R_{nf} = \lambda E_f + H_f$$

- Sensible heat:

$$H_f = c_p \rho_a (T_f - T_a) g_h$$

- Latent heat (Penman-monteith equation):

$$\lambda E_f = \frac{s R_{nf,i} + D_a c_p \rho_a g_h}{s + \gamma \frac{g_h}{g_w}}$$

Net energy available to a leaf

Net available energy R_{nf} can be calculated as

$$\begin{aligned}R_{nf} &= Q + 2(\varepsilon_a \sigma T_a^4 - \varepsilon_f \sigma T_f^4) \\ \varepsilon_a \sigma T_a^4 - \varepsilon_f \sigma T_f^4 &= \varepsilon_a \sigma T_a^4 - \varepsilon_f \sigma T_a^4 + \varepsilon_f \sigma T_a^4 - \varepsilon_f \sigma T_f^4 \\ &= (\varepsilon_a - \varepsilon_f) \sigma T_a^4 + \varepsilon_f \sigma (T_a^4 - T_f^4) \\ &\approx (\varepsilon_a - \varepsilon_f) \sigma T_a^4 - 4\varepsilon_f \sigma T_a^3 (T_f - T_a)\end{aligned}$$

If we define the radiative conductance (g_r) as

$$g_r = \left(\frac{8\varepsilon_f \sigma T_a^3}{\rho_a C_p} \right)$$

isothermal net radiation available to the leaf, $R_{nf,i}$ as

$$R_{nf} = R_{nf,i} - \rho_a c_p (T_f - T_a) g_r$$

$$R_{nf,i} = Q + 2(\varepsilon_a - \varepsilon_f) \sigma T_a^4$$

Conductance for heat, water and CO₂

$$g_h^{-1} = g_a^{-1} + (0.5 / g_b)^{-1}$$

$$g_w^{-1} = g_s^{-1} + (1.075 g_b)^{-1} + g_a^{-1}$$

$$g_c^{-1} = (1.57 g_s)^{-1} + (1.27 g_b)^{-1} + g_a^{-1}$$

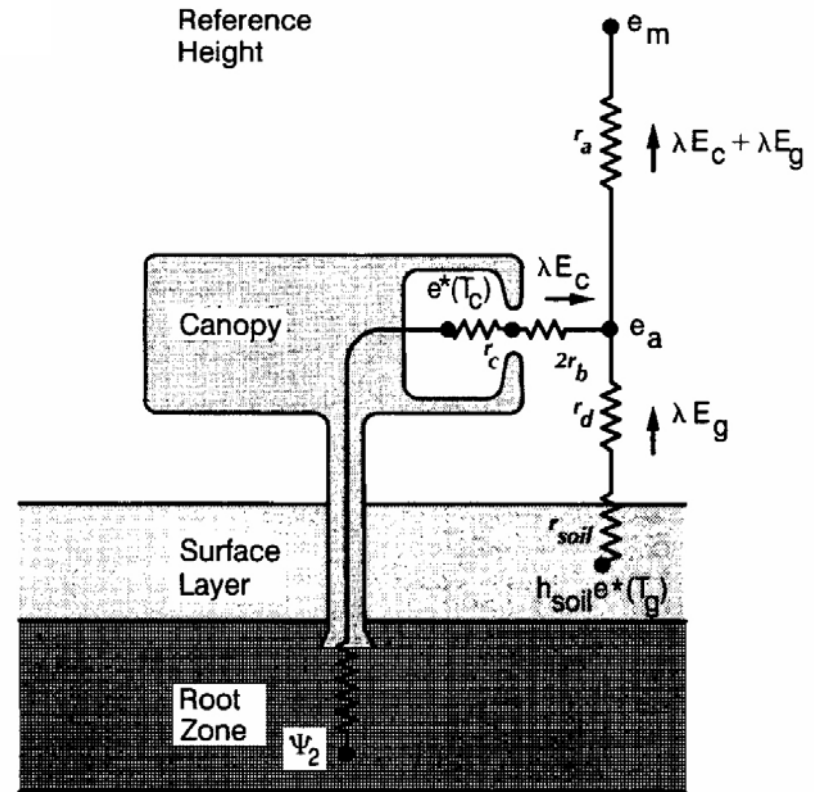


Table 5.1. *Temperature dependence of the ‘radiative’ conductance g_R , and some typical values of the total thermal conductance (g_{HR}) for a range of values of g_H . The value in brackets is g_H as a percentage of g_{HR}*

Temperature (°C)	g_R (mm s ⁻¹)	g_{HR} (mm s ⁻¹)		
		$g_H = 2$	20	200 (mm s ⁻¹)
0	3.54	5.5 (36)	23.5 (85)	204 (98)
10	4.10	6.1 (33)	24.1 (83)	204 (98)
20	4.69	6.7 (30)	24.7 (81)	205 (98)
30	5.37	7.4 (27)	25.4 (79)	205 (97)
40	6.10	8.1 (25)	26.1 (77)	206 (97)

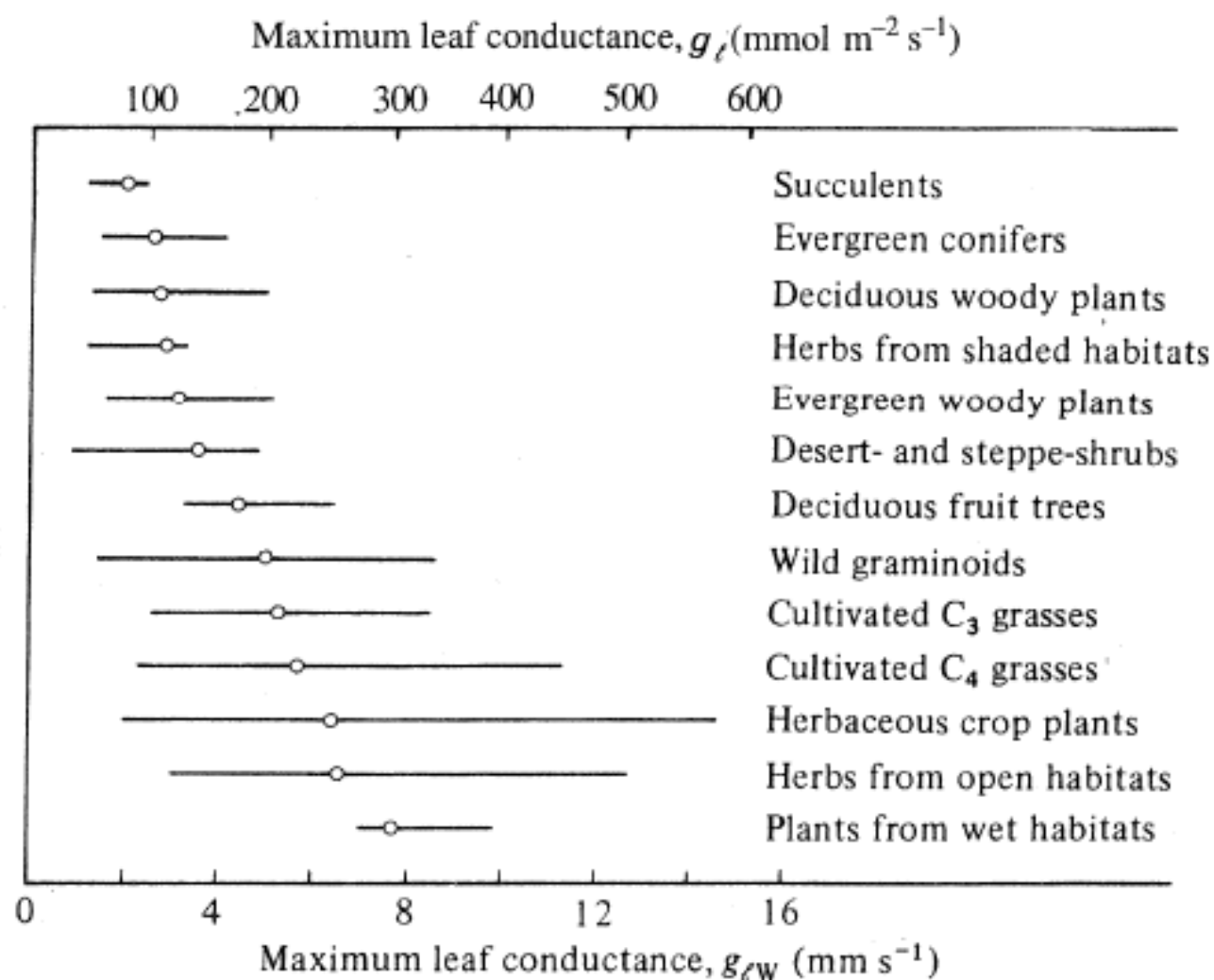


Fig. 6.6. Maximum leaf conductance (g_{lw}) in different groups of plants. The lines cover about 90% of individual values reported. The open circles represent group average conductances. (Adapted from Körner *et al.* 1979).

Stomatal conductance: coupling water use and CO₂ uptake

- Through stomata, CO₂ enters and H₂O exits the leaf;
 - When [CO₂] in intercellular space and guard cell ↓, K⁺ moves into guard cell, stomata opens, vice versa;
 - Too much water loss, stomata closing;
 - Soil dries, ABA produced at root tips transported to leaf, and induce stomata closure.

The Ball - Berry - Leuning model

$$g_s = g_0 + \frac{af_w A_n}{(C_s - \Gamma)(1 + D_s / D_0)}$$

The combined model of stomatal conductance, photosynthesis and transpiration for a leaf

$$H_f = c_p \rho_a (T_f - T_a) g_h; \quad \text{unknowns : } T_f, H_f$$

$$\lambda E_f = (s R_{n,i} + D_a c_p \rho_a g_h) / (s + \gamma g_h / g_w); \quad \text{unknowns : } E_f, g_s$$

$$R_n = H_f + \lambda E_f + c_p \rho_a (T_f - T_a) g_r; \quad \text{unknowns : } H_f, E_f, T_f$$

$$g_s = g_0 + \frac{af_w A_n}{(C_s - \Gamma)(1 + D_s / D_0)}; \quad \text{unknowns : } g_s, A_n, C_s, D_s$$

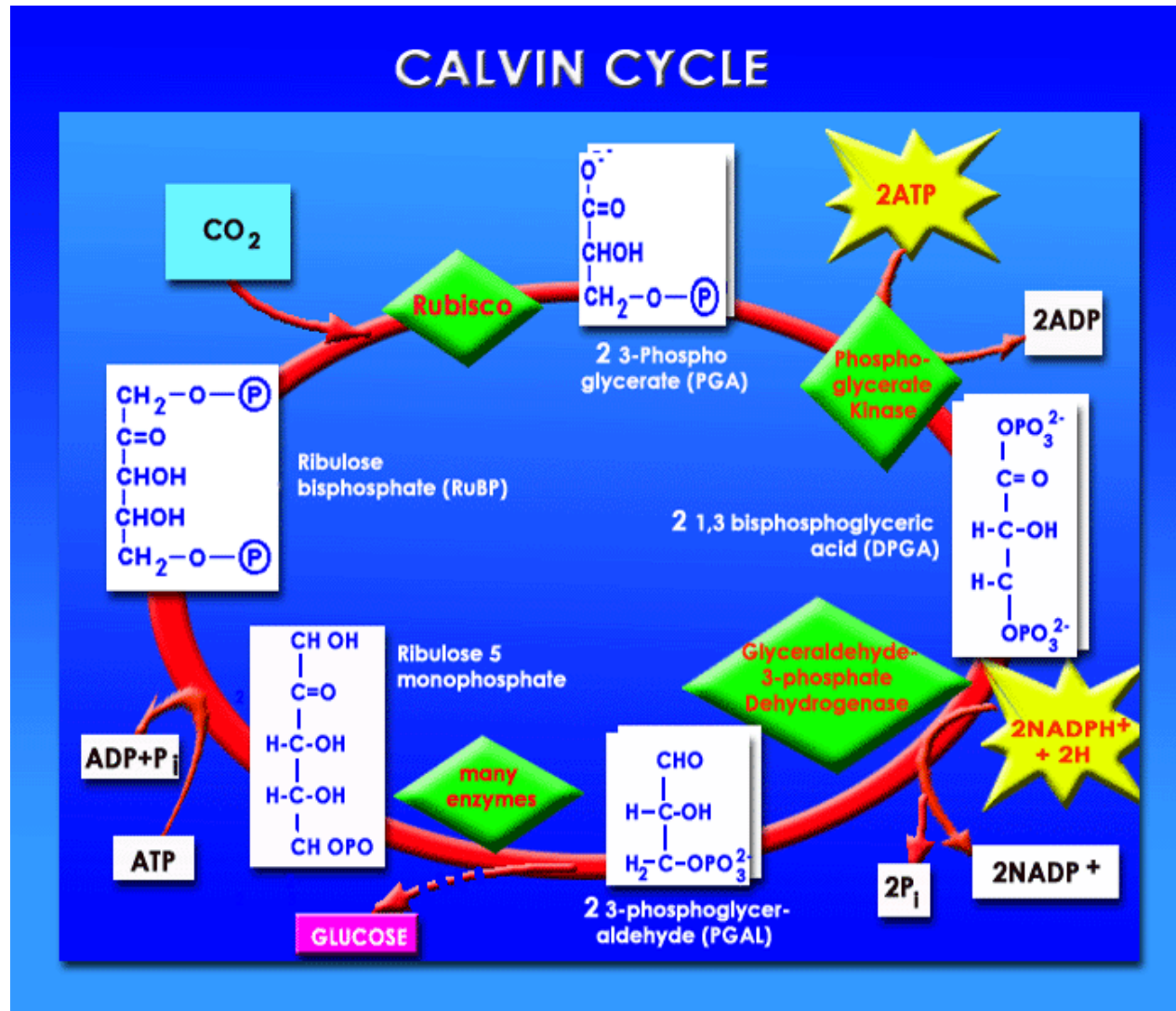
$$D_s = D_a + s(T_f - T_a); \quad \text{unknowns : } D_s, T_f$$

$$A_n = (C_a - C_s) g_{bc}; \quad \text{unknowns : } A_n, C_s$$

$$A_n = (C_s - C_i) g_{sc}; \quad \text{unknowns : } A_n, C_s, C_i, g_s$$

$$A_n = V_c (C_i, Q_{PAR}, T_f) - r_d; \quad \text{unknowns, } A_n, V_c$$

Leaf photosynthesis: the Calvin cycle



C3 photosynthesis model

$$A_n = \min \left(\underbrace{V_{c,c}}_{\text{Rubisco limited}}, \underbrace{V_{c,j}}_{\text{RuBP-limited}}, \underbrace{V_{c,p}}_{\text{sink-limited}} \right) \left(1 - \underbrace{\frac{\Gamma^*}{C_i}}_{\text{Photorespiration loss}} \right) - \underbrace{R_d}_{\text{day respiration}}$$

Rubisco-limited

Light-limited

Sink-limited

$$V_{c,c} = \frac{V_{c \max} C_i}{C_i + K_c \left(1 + \frac{O_i}{K_o} \right)}$$

$$V_{c,j} = \frac{J}{4} \frac{C_i - \Gamma^*}{C_i + 2\Gamma^*}$$

$$V_{c,p} = \frac{V_{c \max}}{2}$$

Respiration: plants

Plant respiration includes growth and maintenance respiration ($R_p = R_g + R_m$)

- Growth respiration (R_g): about 30% of the total carbon for growth is respired;
- Maintenance respiration (R_m): a function of substrate concentration and temperature.

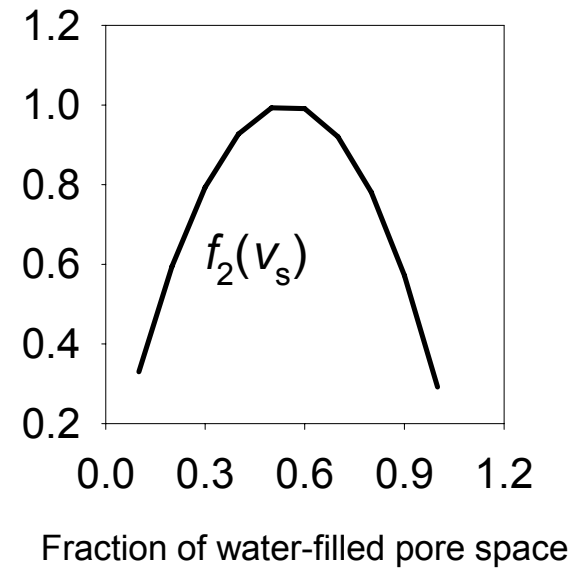
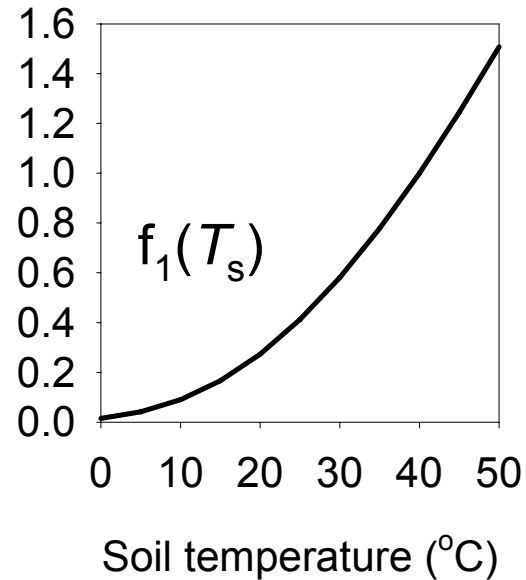
- $R_m = R_0 \exp(kT)$

- $k = a - bT$

Respiration: soil

- Soil respiration, R_s , can be modelled as

$$R_s = R_0 f_1(T_s) f_2(v_s)$$



Soil temperature and moisture

Darcy equation :

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left(\kappa \frac{\partial T}{\partial z} \right) \quad \text{for temperature}$$

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(K \frac{\partial \theta}{\partial z} \right) \quad \text{for moisture}$$

Soil temperature

When thermal conductivity, κ , is constant, and

$$T(0, t) = \bar{T} + A(0) \sin \omega t$$

Solution to the Darcy equation

for soil temperature

$$T(z, t) = \bar{T} + A(0) \exp(-z/D) \sin(\omega t - z/D)$$

and

$$D = \sqrt{\frac{2\kappa}{\omega}}$$

Soil temperature profile

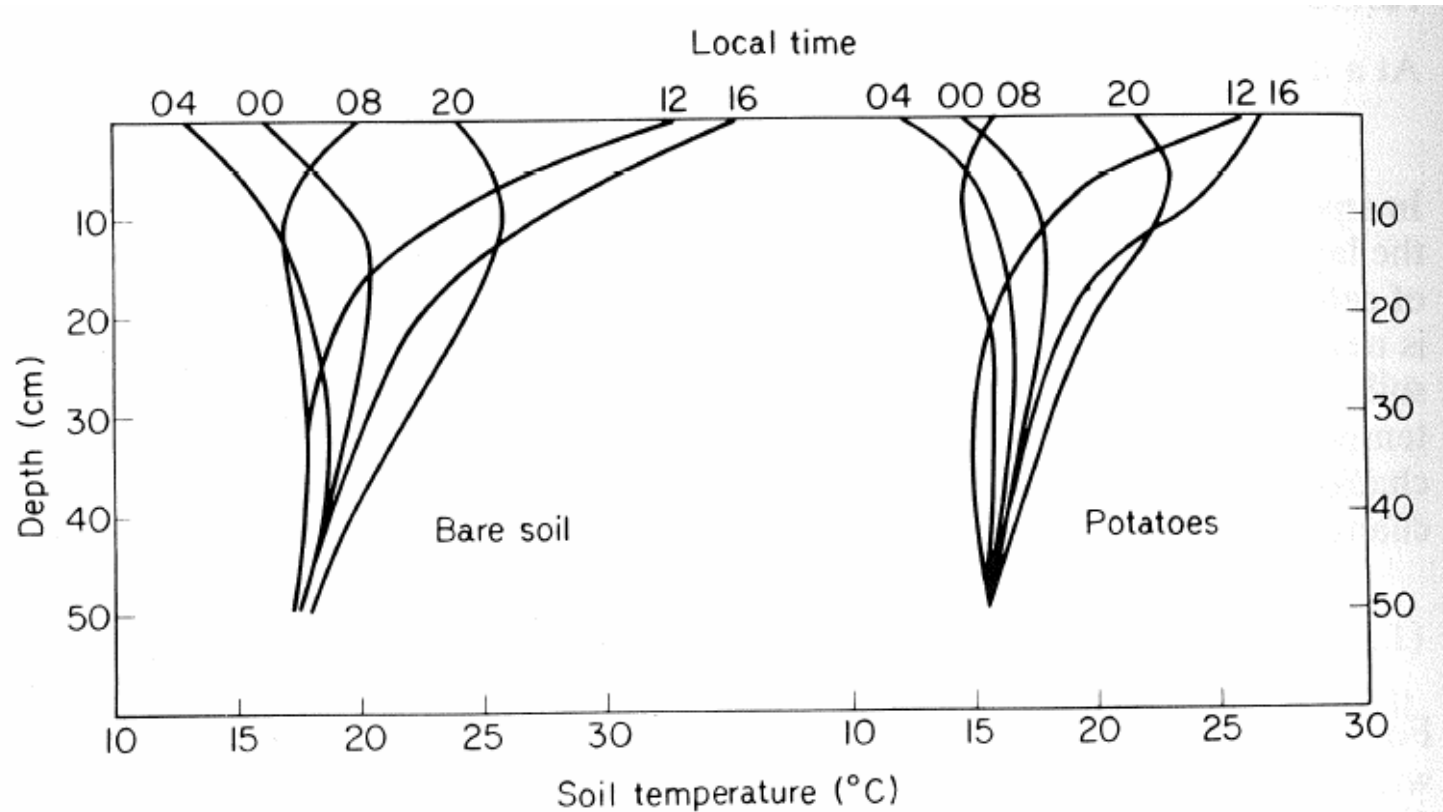
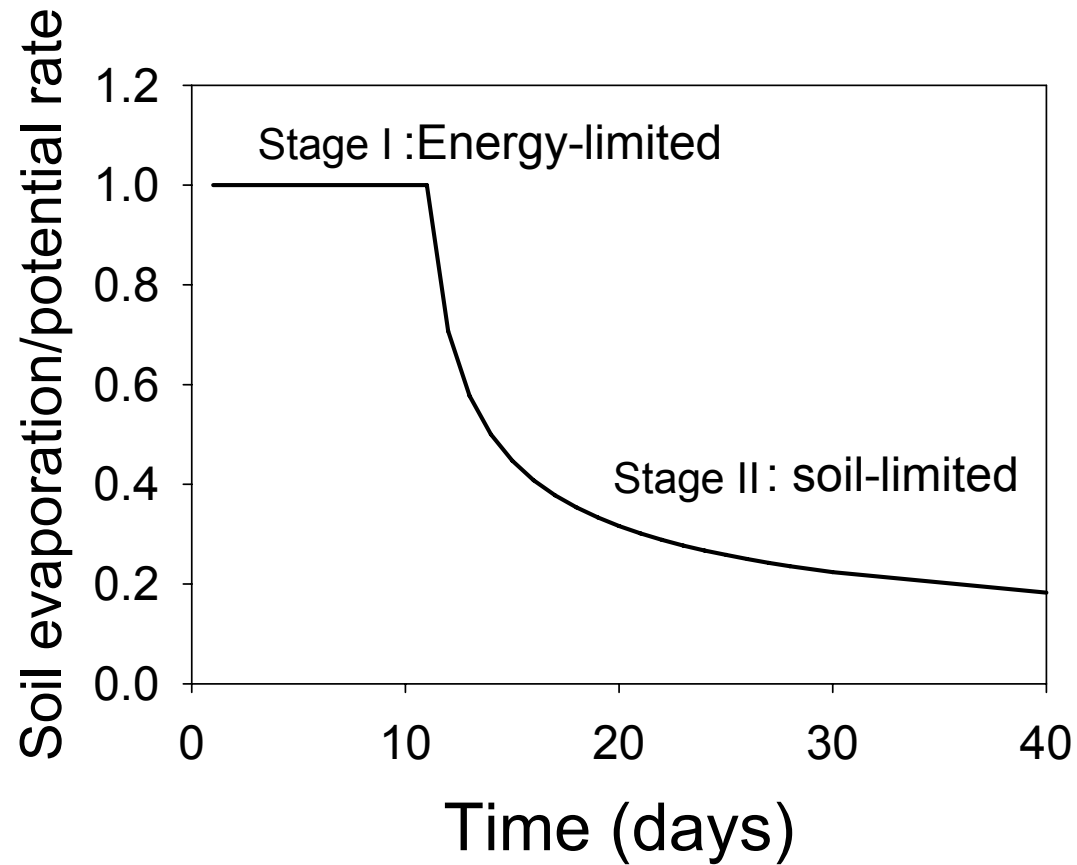


Fig. 13.5 Diurnal change of soil temperature measured below a bare soil surface and below potatoes (from van Eimern, 1964).

Soil evaporation

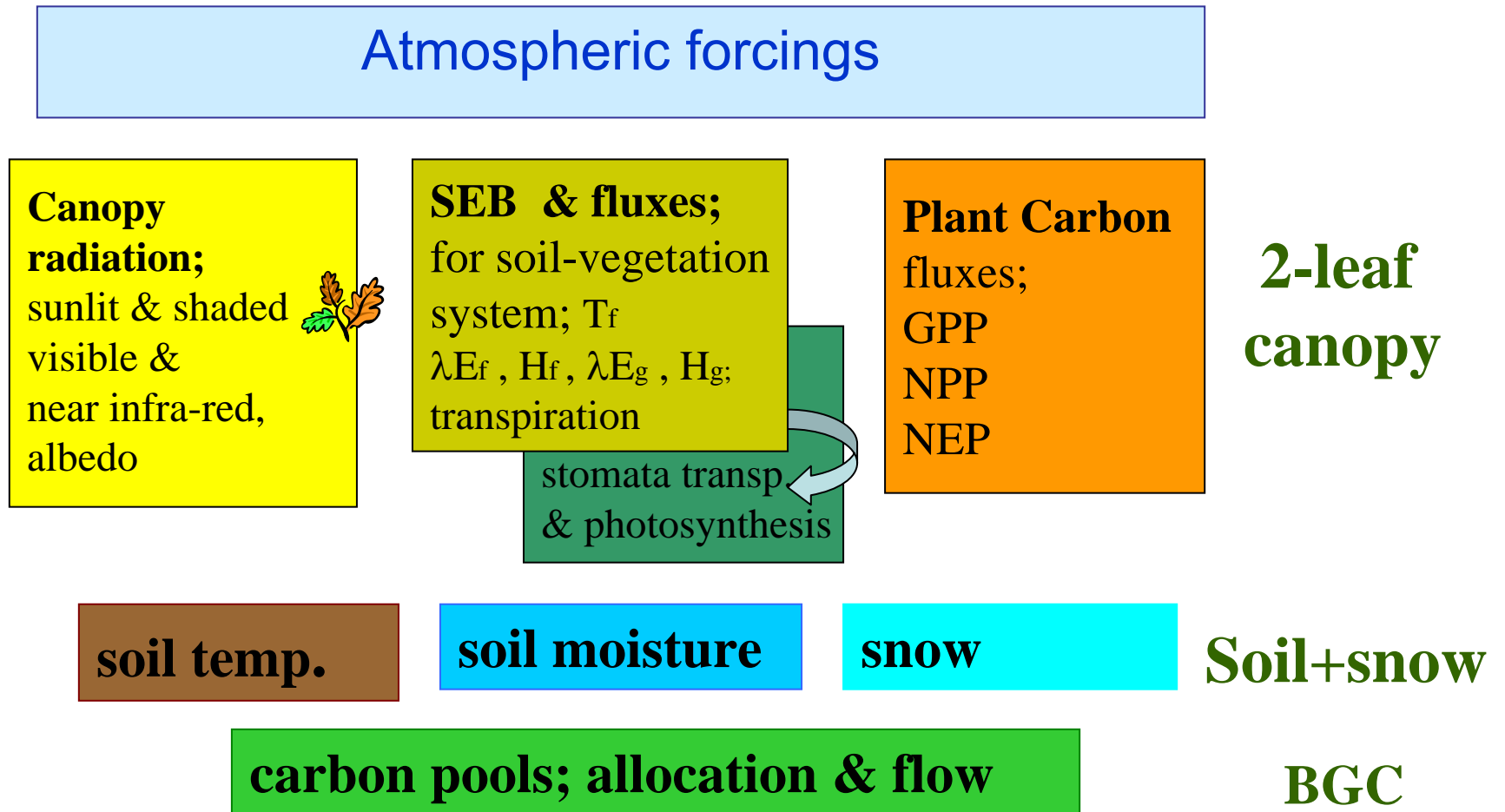
Two-staged processes



Modelling soil evaporation

$$E_s = \min \left(\underbrace{\rho_a \Delta q g_a}_{\text{atmospheric demand}}, \underbrace{\frac{R_{ns} s}{(s + \gamma) \lambda}}_{\text{energy-limited}}, \underbrace{\frac{\theta_s \Delta h}{\Delta t}}_{\text{soil supply}} \right)$$

The general structure of CABLE



Estimating parameters in a surface flux model

- Parameters and variables
- Models
- Errors: systematic errors and random errors

Inversion

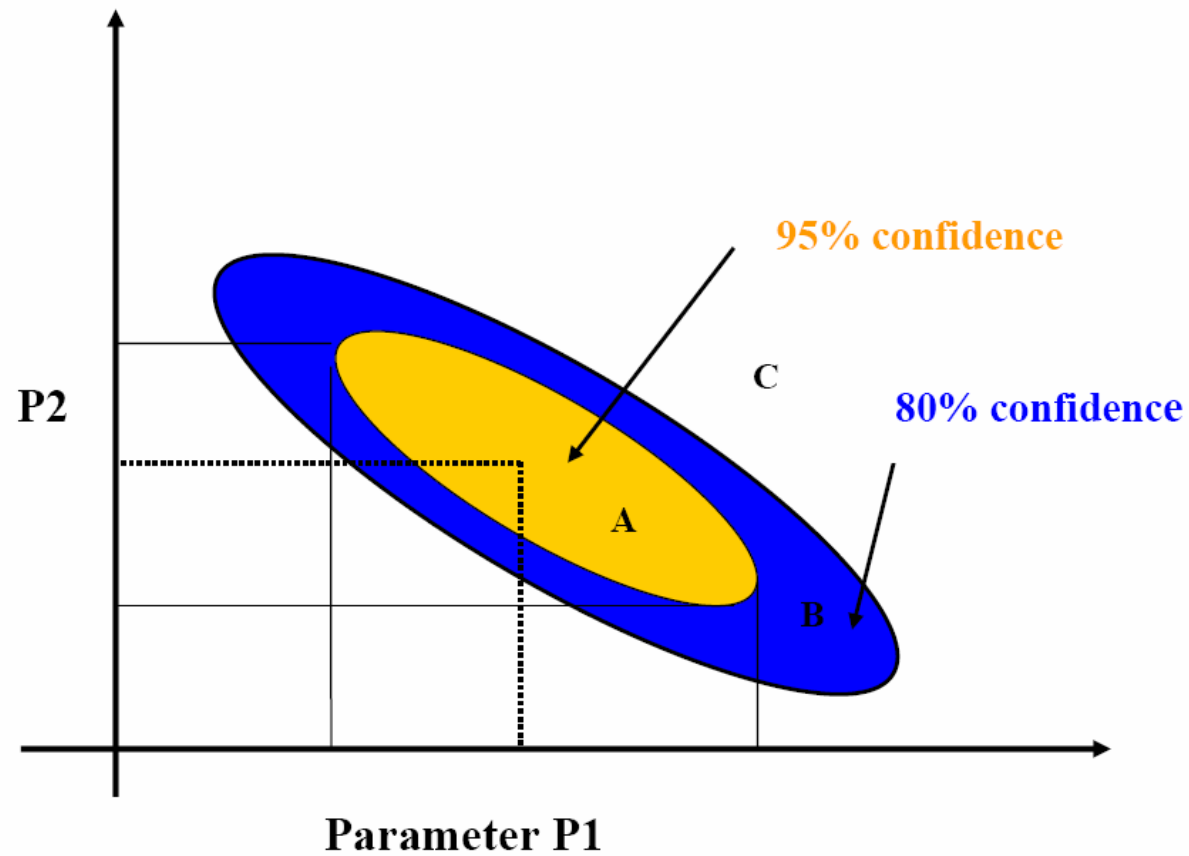
- You often do it without knowing it.
- Many commercial packages available
- Knowing your measurements well before inversion
- Often requires a few trials and errors to get the right answer

Basic concepts

- Maximum likelihood
- Least squares
- Sensitivity (derivatives)

Some basic concepts

- Estimate and probability distribution



Variance and covariance

$$\text{var}(P_1) = \sigma_1^2; \quad \text{var}(P_2) = \sigma_2^2$$

$$\text{var}(P_1 + P_2) = \sigma_1^2 + \sigma_2^2 + 2\rho_{12}\sigma_1\sigma_2$$

Therefore

$$\rho_{12} = 0 \quad \text{var}(P_1 + P_2) = \text{var}(P_1) + \text{var}(P_2)$$

$$\rho_{12} < 0 \quad \text{var}(P_1 + P_2) < \text{var}(P_1) + \text{var}(P_2)$$

General linear regression

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{\substack{\text{dependent variable} \\ n \text{ by } 1}} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{pmatrix} \underbrace{\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}}_{\substack{\text{parameter} \\ m \text{ by } 1}} + \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix} \underbrace{\hspace{1cm}}_{\substack{\text{error} \\ n \text{ by } 1}}$$

independent variables
n by m

In matrix form

$$Y = \hat{Y} + e = Xb + e$$

Linear inversion theory

- For a given set of measurements of $(\mathbf{X}_0, \mathbf{Y}_0)$, the maximum likelihood estimate of coefficient \mathbf{b} is given by

$$\mathbf{b} = \left(\mathbf{X}_0^T \mathbf{X}_0 \right)^{-1} \mathbf{X}_0^T \mathbf{Y}_0$$

- The covariance of \mathbf{b} ($\text{cov}(\mathbf{b})$) is given by

$$\text{cov}(\mathbf{b}) = \sigma^2 \left(\mathbf{X}_0^T \mathbf{X}_0 \right)^{-1}$$

An example

Y: dependent variable; x_1 and x_2 are two independent variables. The five set of observations are: (x_{1i}, x_{2i}, y_i)

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ 1 & x_{13} & x_{23} \\ 1 & x_{14} & x_{24} \\ 1 & x_{15} & x_{25} \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} + \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \end{pmatrix}$$

$$y = \hat{y} + b_0 + b_1 x_1 + b_2 x_2 + \varepsilon$$

The covariance matrix : $\text{cov}(\mathbf{b}) = \sigma^2 (\mathbf{X}_0^T \mathbf{X}_0)^{-1}$

$$\text{cov}(\mathbf{b}) = \begin{pmatrix} \sigma_0^2 & \sigma_0\sigma_1 & \sigma_0\sigma_2 \\ \sigma_0\sigma_1 & \sigma_1^2 & \sigma_1\sigma_2 \\ \sigma_0\sigma_2 & \sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

$$= \sigma^2 \begin{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ x_{11} & x_{12} & x_{13} & x_{14} & x_{15} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} \end{pmatrix} \begin{pmatrix} 1 & x_{11} & x_{21} \\ 1 & x_{12} & x_{22} \\ 1 & x_{13} & x_{23} \\ 1 & x_{14} & x_{24} \\ 1 & x_{15} & x_{25} \end{pmatrix} \end{pmatrix}^{-1}$$

Nonlinear inverse theory

- Let's assume a general nonlinear relationship between Y and X with parameter p , and we wish to estimate parameter p from a set of observations of (X_0, Y_0) .
- The regression model can be written as

$$Y = \hat{Y} + e = F(X, p) + e$$

Nonlinear inverse theory

- The least square cost, Φ , is given

$$\phi = \sum_m (Y_{obs} - F(X, p)) Q (Y_{obs} - F(X, p))^T$$

- The optimal is found when

$$\frac{\partial \phi}{\partial p} = 0$$

Nonlinear inverse theory

Using the least square theory, the estimate of parameter \mathbf{p} , \mathbf{p}_{es} , can be calculated as

$$\mathbf{p}_{es} = (\mathbf{J}^T \mathbf{J})^{-1} \mathbf{J}^T (\mathbf{Y}_{obs} - \hat{\mathbf{Y}})$$

and the covariance of \mathbf{p} is given by

$$\text{cov}(\mathbf{p}) = \sigma^2 (\mathbf{J}^T \mathbf{J})^{-1}$$

What does it mean?

- Linear:

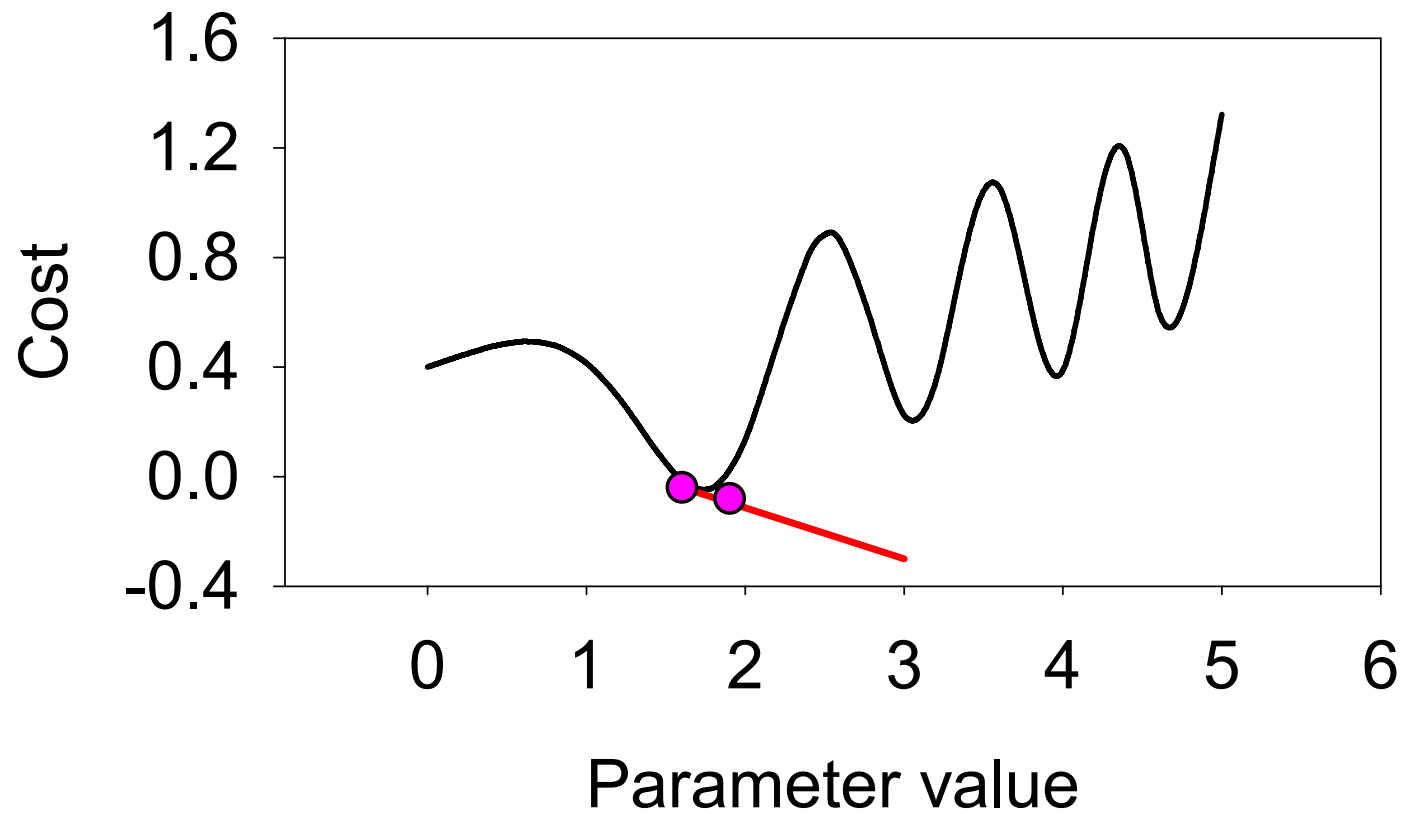
$$\text{cov}(\mathbf{b}) = \sigma^2 (\mathbf{X}_0^T \mathbf{Q} \mathbf{X}_0)^{-1}$$

- Nonlinear:

$$\text{cov}(\mathbf{p}) = \sigma^2 (\mathbf{J}^T \mathbf{Q} \mathbf{J})^{-1}$$

- Solution to nonlinear problem is an tangent linear approximation

Nonlinear parameter estimation



Case study: Penman-Monteith equation

- The equation:
$$\lambda E_f = \frac{sR_{n,i} + D_a c_p \rho_a g_h}{s + \gamma \frac{g_h}{g_w}}$$

- Independent variables: T_a , D_a , R_{ni}

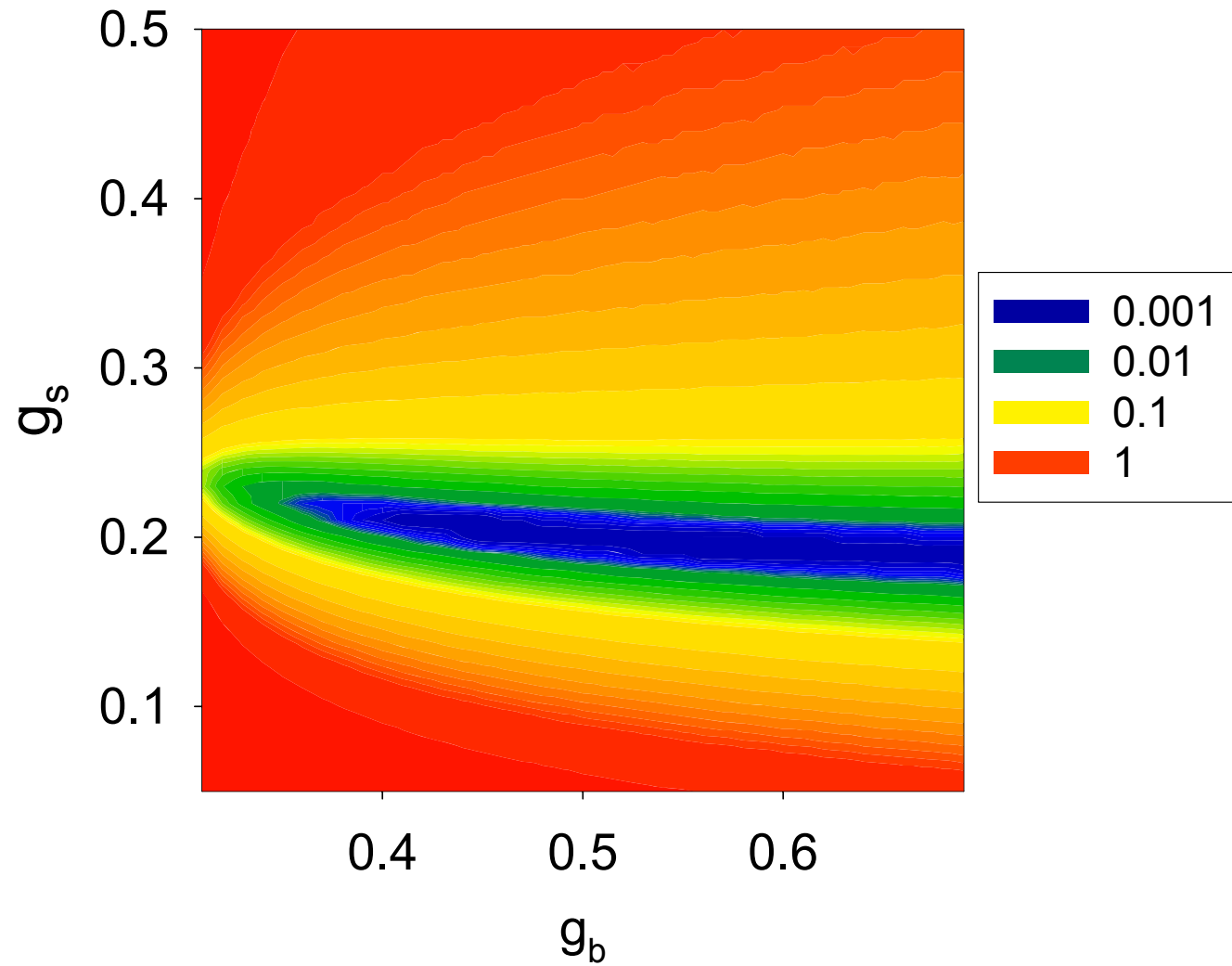
- Dependent variable: E_f

- Parameters, g_a , g_b , g_s

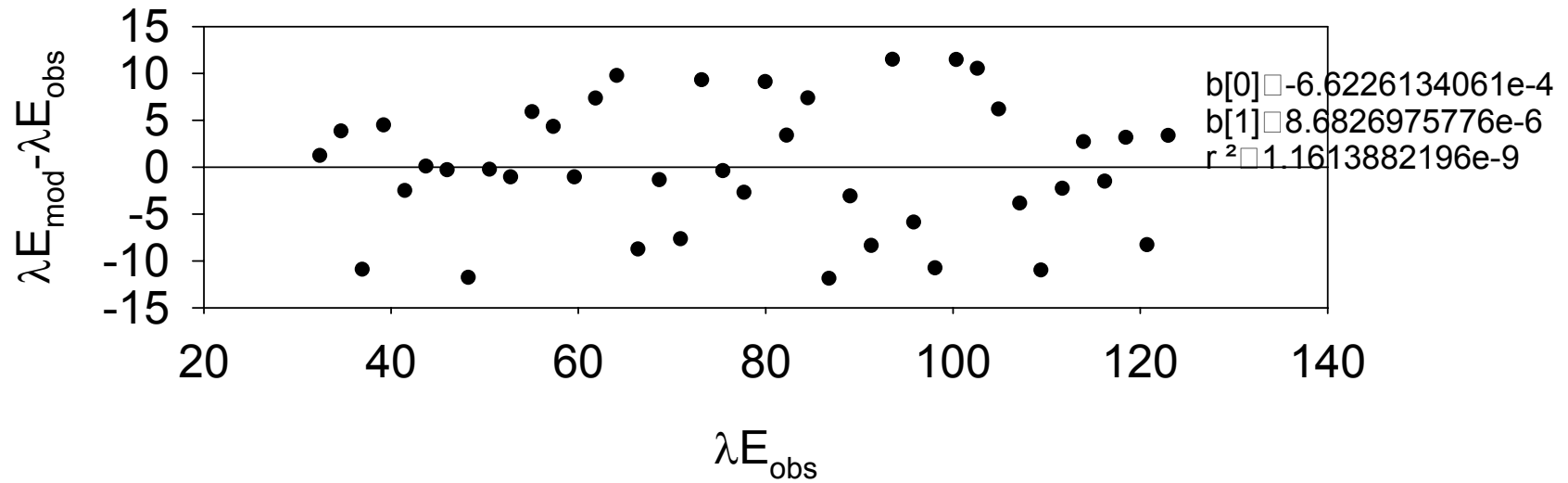
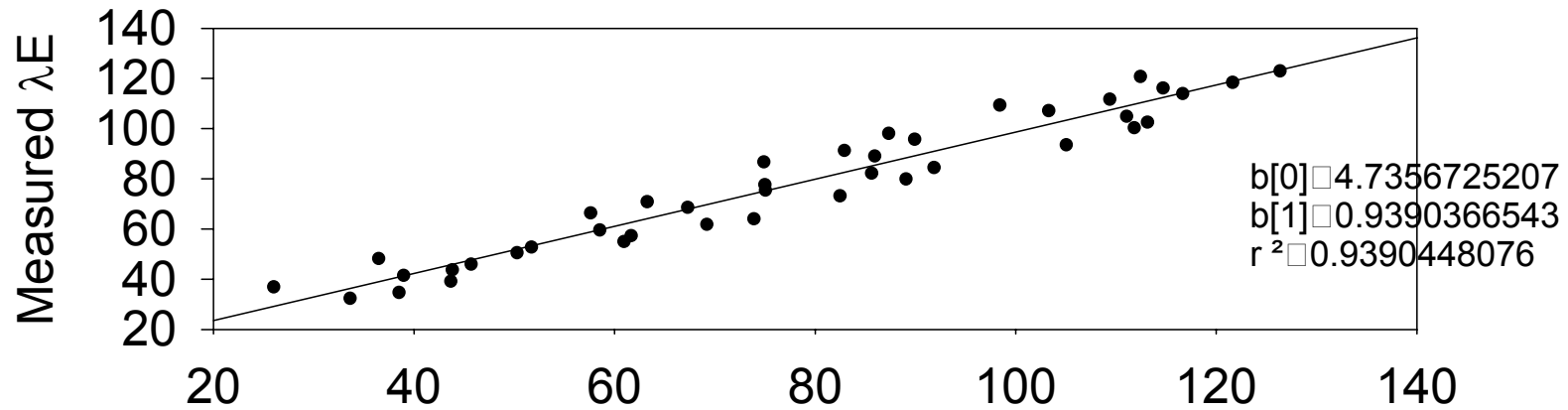
$$g_h^{-1} = g_a^{-1} + (0.5 / g_b)$$

$$g_w^{-1} = g_s^{-1} + (1.075 g_b)^{-1} + g_a^{-1}$$

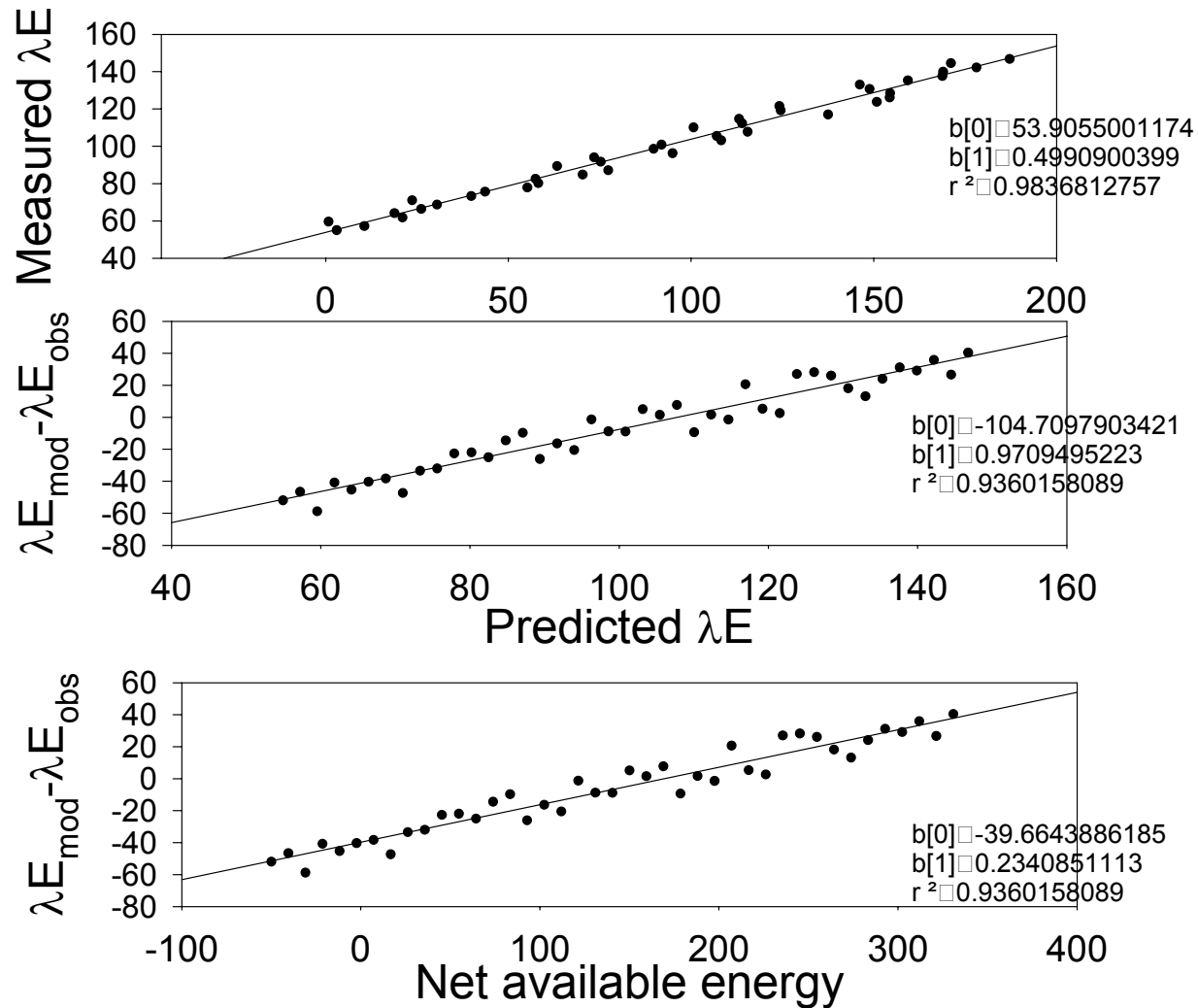
$$\text{Cost} = \frac{1}{n} \sum (\lambda E_{\text{mod}} - \lambda E_{\text{obs}})^2$$



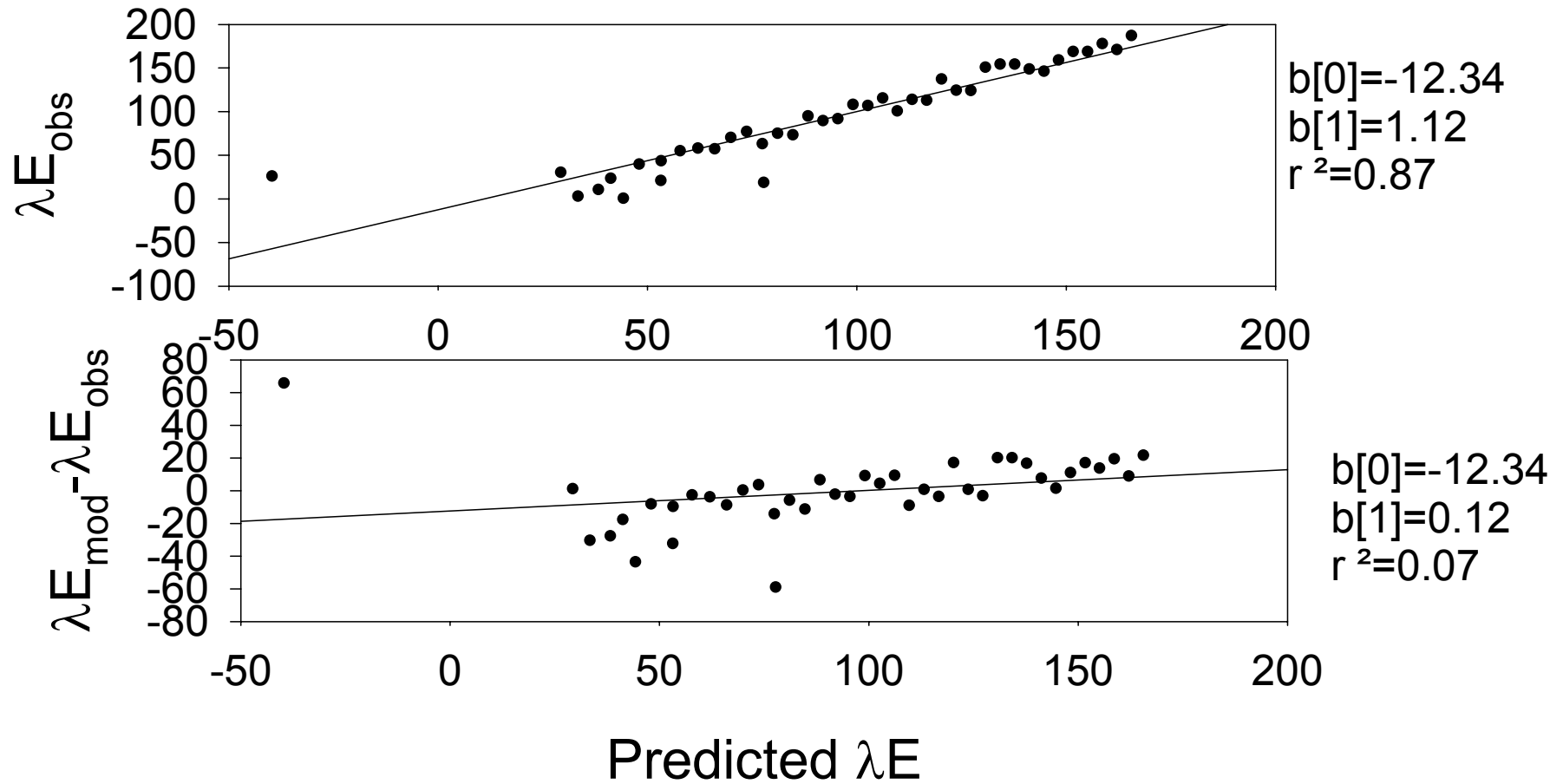
Examining the results



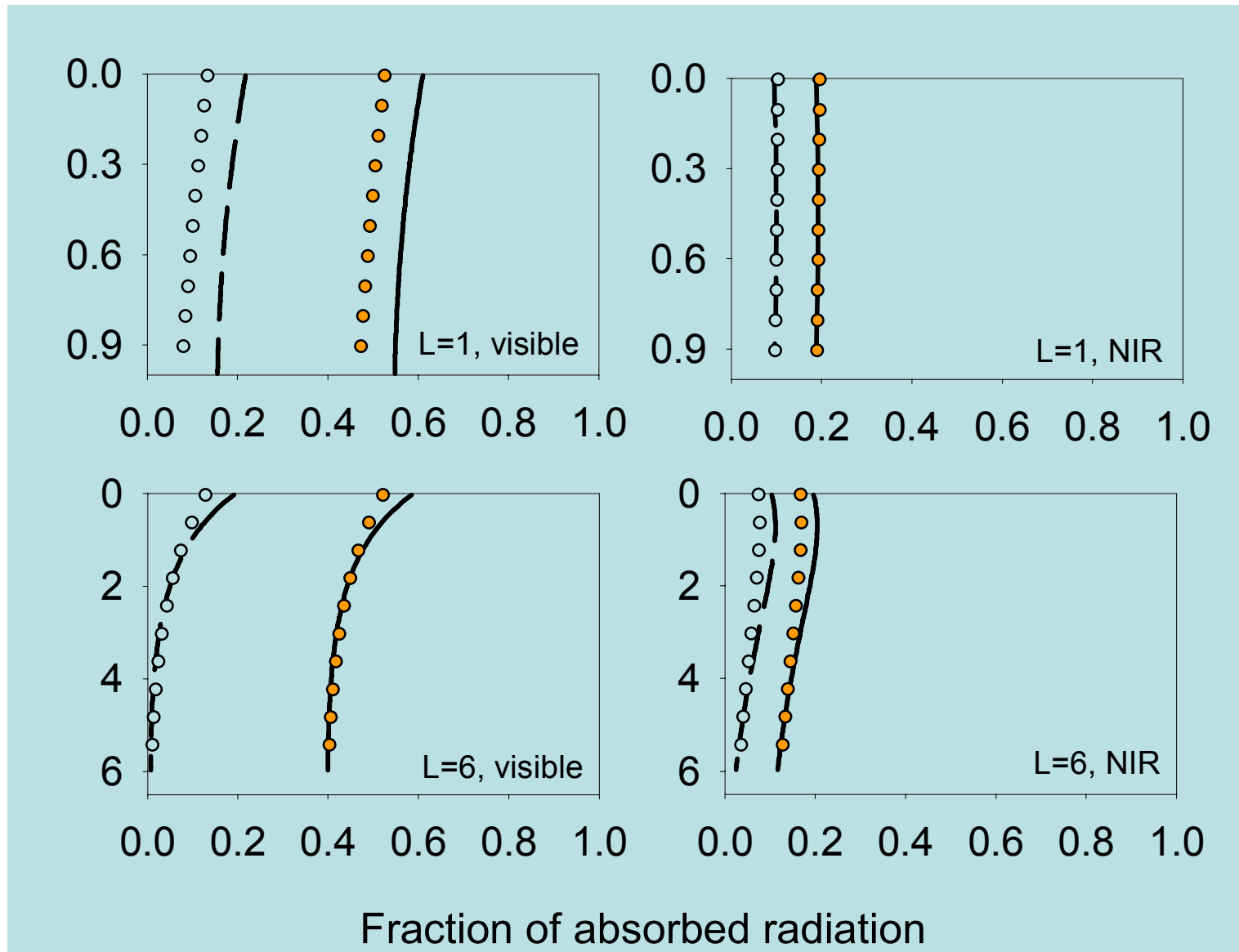
Examining results (case 41)



Examining the results (case 4)



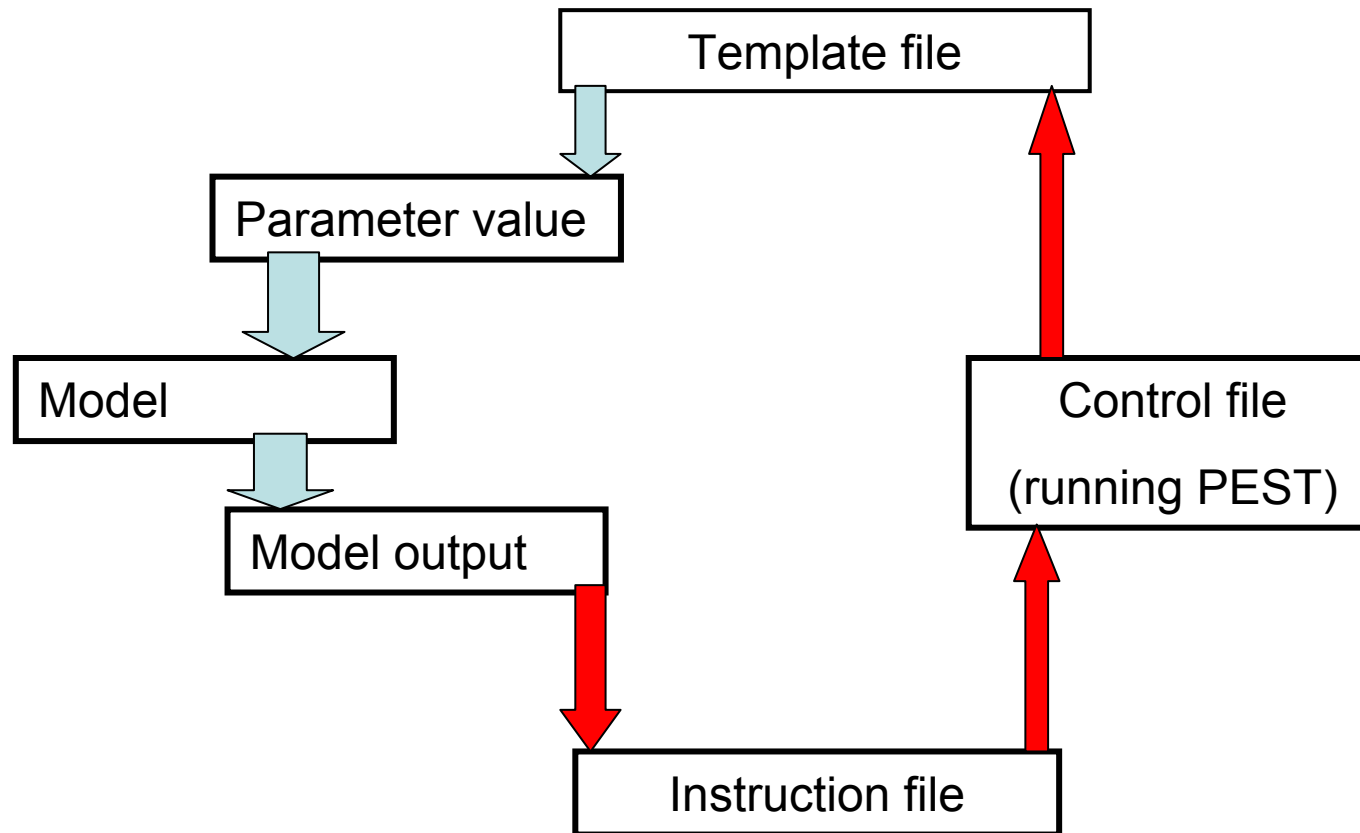
Radiation absorbed in a canopy



Introduction to PEST

- PEST is model-independent, nonlinear parameter estimation package. It is a widely used, free download software.
- It provides stable solution to most nonlinear inversion problems, with the capability of powerful predictive analysis and regularization.
- It communicates to users and models by text files that can be modified by users

How PEST works?




```
pcf
* control data
RSTFLE PESTMODE
NPAR NOBS NPARGP NPRIOR NOBSGP
NTPLFLE NINSFLE PRECIS DPOINT NUMCOM JACFILE MESSFILE
RLAMBDA1 RLAMFAC PHIRATSUF PHIREDLAM NUMLAM
RELPARMAX FACPARMAX FACORIG
PHIREDSWH
NOPTMAX PHIREdstp NPHISTP NPHINORED RELPARSTP NRELPAR
ICOV ICOR IEIG
* parameter groups
PARGPME INCTYP DERINC DERINCLB FORCEN DERINCMUL DERMTHD
(one such line for each of the NPARGP parameter groups)
* parameter data
PARNME PARTRANS PARCHGLIM PARVAL1 PARLBNd PARUBND PARGP SCALE OFFSET DERCOM
(one such line for each of the NPAR parameters)
PARNME PARTIED
(one such line for each tied parameter)
* observation groups
OBNME
(one such line for each observation group)
* observation data
OBSNME OBSVAL WEIGHT OBNME
(one such line for each of the NOBS observations)
* model command line
write the command which PEST must use to run the model
* model input/output
TEMPFLE INFLE
(one such line for each model input file containing parameters)
INSFLE OUTFLE
(one such line for each model output file containing observations)
* prior information
PILBL PIFAC * PARNME + PIFAC * log(PARNME) ... = PIVAL WEIGHT OBNME
(one such line for each of the NPRIOR articles of prior information)
```

Template file

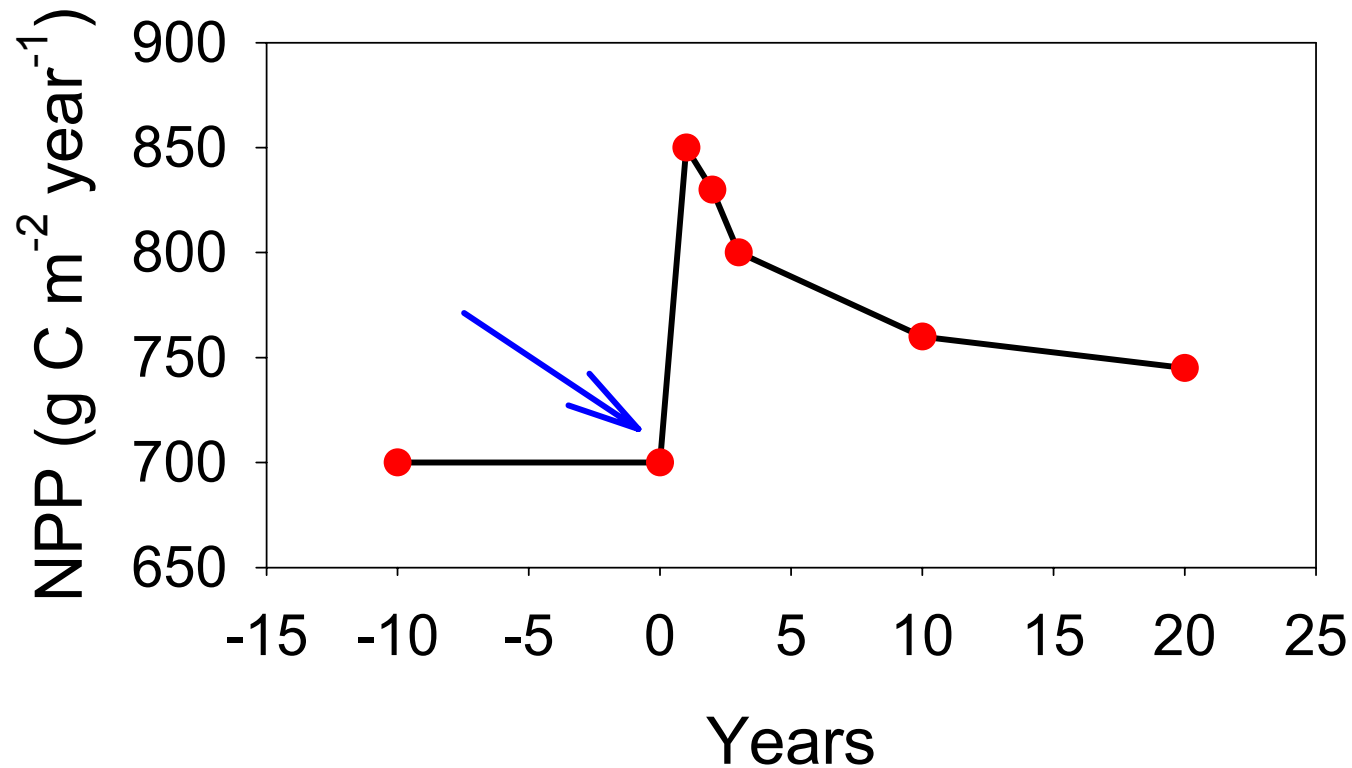
```
ptf #  
#    ratioRL    resprcl    tempcoef1    tempcoef2  
#    ratioRL    #,#    resprcl    #,#    tempcoef1    #,#    tempcoef2    #
```

Instruction file

```
pif #  
L1 (A00000001) 13:22  
L1 (A00000002) 13:22  
L1 (A00000003) 13:22  
L1 (A00000004) 13:22  
L1 (A00000005) 13:22  
L1 (A00000006) 13:22  
L1 (A00000007) 13:22  
L1 (A00000008) 13:22  
L1 (A00000009) 13:22  
L1 (A00000010) 13:22  
L1 (A00000011) 13:22  
L1 (A00000012) 13:22  
L1 (A00000013) 13:22  
L1 (A00000014) 13:22  
L1 (A00000015) 13:22  
L1 (A00000016) 13:22  
L1 (A00000017) 13:22  
L1 (A00000018) 13:22  
L1 (A00000019) 13:22  
L1 (A00000020) 13:22  
L1 (A00000021) 13:22  
L1 (A00000022) 13:22
```

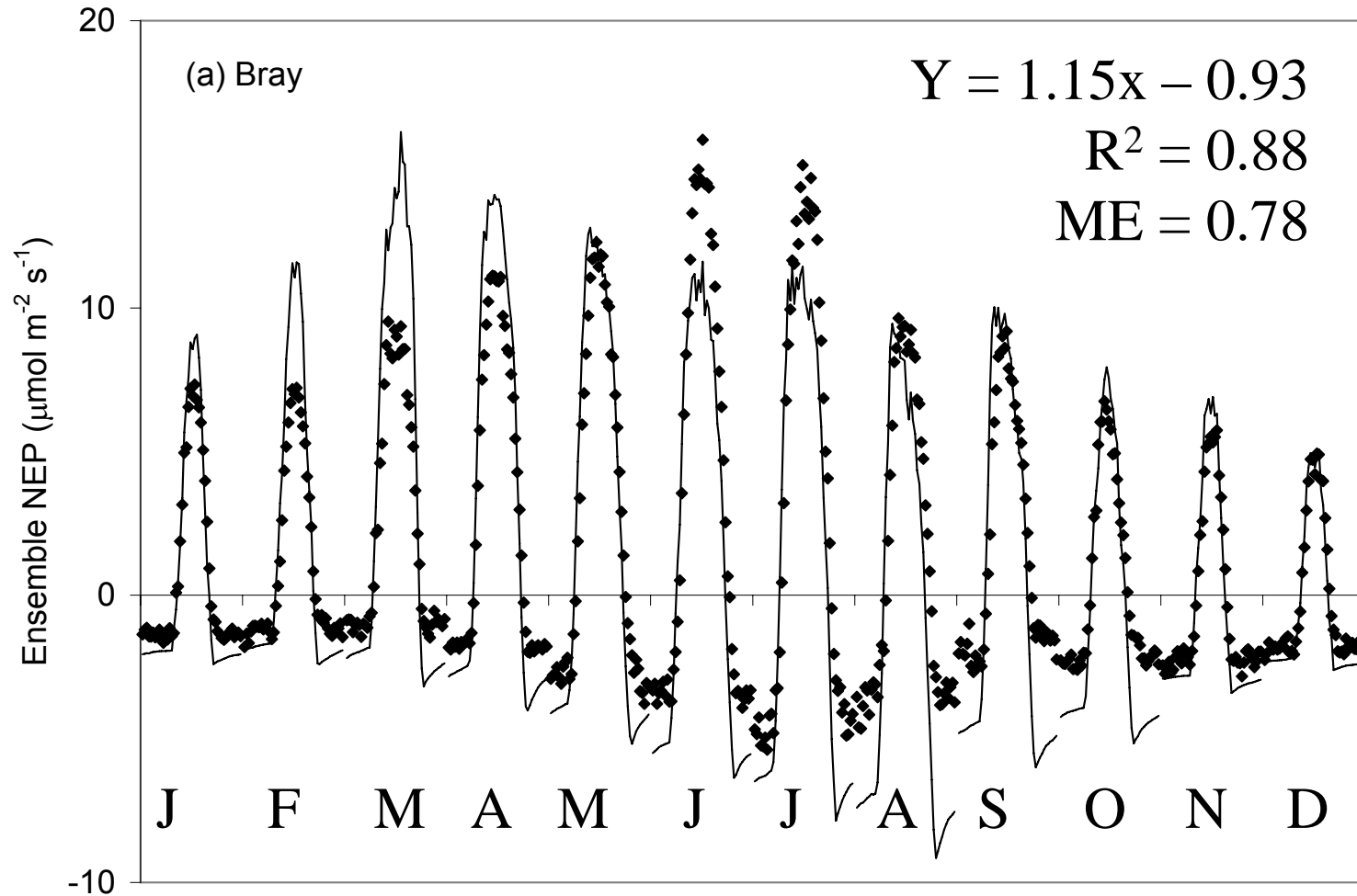
Application I: interpretation

Response of NPP to CO₂ doubling



See Wang, McMurtrie, Medlyn and Pepper (2006)

Application II: calibration



Application III: predictive analysis

