IFIN-HH

Approaches in modelling tritium uptake by crops

EMRAS II
Approaches for Assessing Emergency Situations
Working Group 7
“Tritium” Accidents

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History

Different models and equations have been proposed to express the uptake kinetics of tritiated water.The first is

$$C_{TFWT} = C_{\infty}(1 - e^{-k.t})$$

- C_{TFWT} :HTO concentration in the plant at the considered time t (Bq L^{-1})
- C_{∞} : steady-state TFWT concentration (Bq L^{-1})
- k : rate constant for HTO uptake (h^{-1})
- t : time after the beginning of exposure (h)
- But $C_{\infty} = 1.1 * \rho_a / \rho_s C_{ah}$
- ρ_s is water vapor density in leaf stomatal pore (g /m3), ρ_a is the water vapor density in atmosphere (g /m3), C_{ah} *is the air water HTO concentration (Bq/L)*
- $k = \rho_s /(1.1*W*r)$
- W water content of leaf (g /m2), r leaf resistance to water transport (h/m)
- The above relationships were used to interpet experimental dat aon various plants and environmental conditions. Many results will follow

Table 2
D_2O uptake kinetics in plant leaves

		Rate constant k (h^{-1})	Steady-state conc. C_{max} (ppm)	Initial uptake rate $C_{max}k$ (ppm h^{-1})	Stomatal resistance r (s cm^{-1})	Rate constant k'^{a} (h^{-1})
Day '95	Komatsuna	0.95 ± 0.16	$10\,080 \pm 910$	9580	1.2–9.4	0.31–2.63
	Orange	0.25 ± 0.08	$17\,040 \pm 4580$	4260	3.1–44	0.07–1.19
Day '96	Komatsuna 1[b]	0.74 ± 0.16	$17\,130 \pm 1320$	12700	0.8–3.8	0.73–3.91
	Komatsuna 2[b]	0.84 ± 0.19	$17\,820 \pm 1240$	15000	0.8–3.8	0.73–3.91
	Radish 1[b]	0.91 ± 0.17	$19\,070 \pm 1230$	19000	1.3–3.9	0.79–2.4
	Radish 2[b]	1.38 ± 0.38	$18\,610 \pm 1630$	25700	1.3–3.9	0.79–2.4
	Tomato[b]	1.03 ± 0.14	$16\,430 \pm 770$	16900	1.6–10	0.25–1.73
	Rice[b]	3.63 ± 0.31	$20\,310 \pm 430$	73700	—	—
Night '95	Komatsuna	0.65 ± 0.19	$15\,780 \pm 2850$	10300	5.7–40	0.06–0.44
	Orange	0.06 ± 0.29	$278\,00 \pm 127810$	1670	49–55	0.04–0.05
Night '96	Komatsuna	0.20 ± 0.04	$18\,300 \pm 1330$	3660	2.7–3.2	0.82–0.97
	Radish	0.31 ± 0.05	$20\,600 \pm 1590$	6390	2.6–3.4	0.72–0.95
	Tomato	0.12 ± 0.02	$19\,160 \pm 1630$	2300	6.9–15	0.16–0.36

[a] Rate constant calculated using porometer data, $k' = \rho_s/(aWr)$.
[b] Komatsuna 1, Radish 1 and Tomato were exposed on 8/24 and Komatsuna 2, Radish 2 and Rice were exposed on 8/25 in 1996, respectively.

Atarashi 1997

From Ichimasa

Table 2 Rate constant (k) and steady state concentration ratio (C_{Rmax}) of D_2O uptake from air to vegetation

	Daytime release		Nighttime release	
	k (hr^{-1})	C_{Rmax}	k (hr^{-1})	C_{Rmax}
Rice plant leaf	2.384±0.965	0.541±0.022	0.429±0.039	0.562±0.018
Unhulled rice	0.636±0.124	0.217±0.010	0.055±0.114	0.750±1.283
Rice plant leaf (flooding)	2.269±0.760	0.440±0.016	0.551±0.067	0.544±0.020
Unhulled rice (flooding)	0.378±0.072	0.216±0.014	0.355±0.059	0.247±0.018
Soybean leaf	2.951±1.668	0.562±0.022	0.671±0.319	0.428±0.057
Soybean pea	0.230±0.375	0.273±0.224	0.071±0.002	0.210±0.004
Soybean hull	0.069±0.083	0.534±0.510	0.046±0.002	0.307±0.012

$C_{Rp} = C_{Rmax}(1-e^{-kt})$

Table 3 Rate constant (k)[*1] and half time ($t_{1/2}$)[*2] of TFWD loss from vegetation

	Daytime release		Nighttime release	
	k (hr^{-1})	$t_{1/2}$ (hr)	k (hr^{-1})	$t_{1/2}$ (hr)
Rice plant leaf	1.155±0.204	0.6	0.514±0.042	1.3
Unhulled rice	0.452±0.087	1.5	0.214±0.039	3.2
Rice plant leaf (flooding)	1.041±0.212	0.7	0.582±0.061	1.2
Unhulled rice (flooding)	0.388±0.087	1.8	0.202±0.033	3.4
Soybean leaf	1.058±0.155	0.7	0.547±0.117	1.3

*1, $C_p = C_0 e^{-kt}$ *2, $e^{-kt1/2} = 1/2$

From Ichimasa

Table 2 Rate constant (k) and steady state concentration ratio (C_{rmax}) of D_2O uptake from air to soybean

		Daytime release		Nighttime release	
Exp. No.	Sample, Exp.	k (hr^{-1})	C_{rmax}	k (hr^{-1})	C_{rmax}
I	Leaf, Aug. 99	3.0±1.7	0.6±0.0	0.7±0.3	0.4±0.1
I	Bean, Aug. 99	0.2±0.4	0.3±0.2	0.1±0.0	0.2±0.0
I	Hull, Aug. 99	0.1±0.1	0.5±0.5	0.1±0.0	0.3±0.0
II	Leaf, Aug. 00	1.5±0.3	0.5±0.0	0.4±0.2	0.8±0.2
III	Leaf, Sept. 00	0.9±0.4	0.7±0.0	1.6±0.6	1.0±0.0
IV	Leaf, Apr. 02	1.4±0.4	0.8±0.1	0.6±0.1	1.0±0.0
V	Leaf, Aug. 02	6.1±1.5	0.8±0.0		
VI	Leaf, Sept. 02	5.7±1.9	0.7±0.0	0.5±0.1	1.1±0.1

$$C_p/C_a = Cr_{rmax}(1-e^{-kt})$$

C_p : TFWD concentration in plant (ppm)

C_a : D_2O concentration in air moisture (ppm)

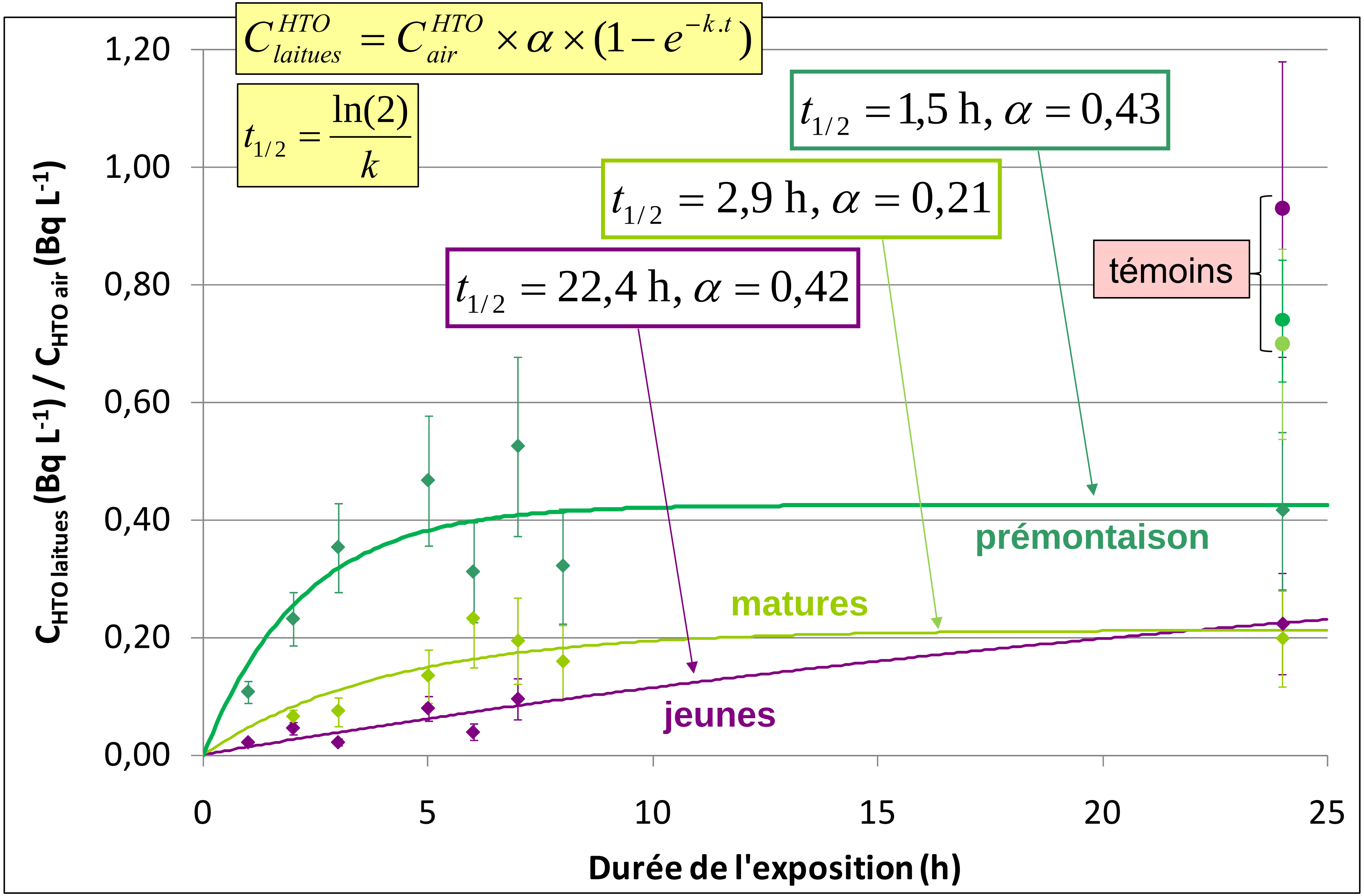
Cr_{rmax} : Steady state concentration ratio (C_p/C_a)

k : Rate constant of D_2O uptake from air

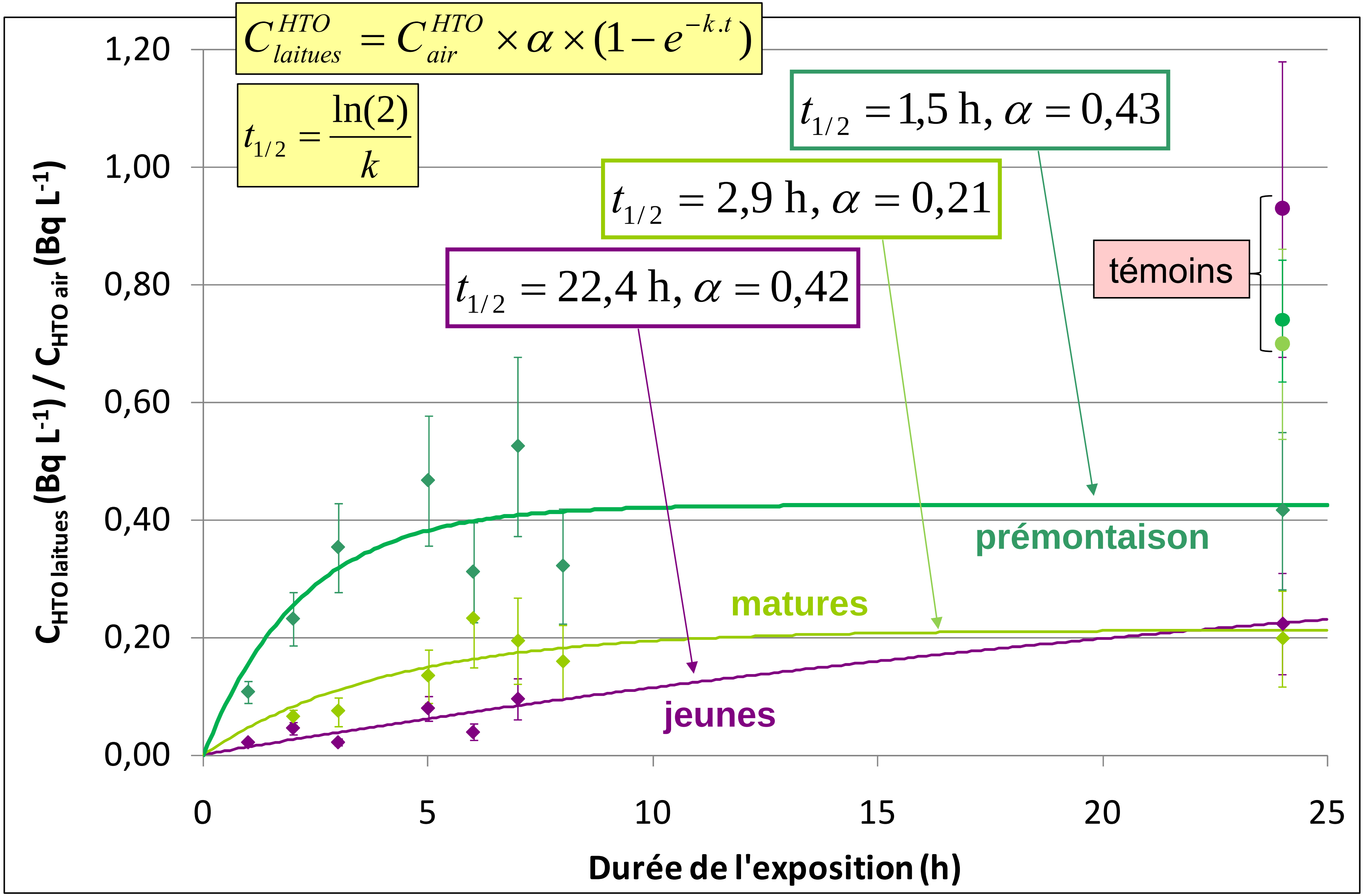
t : Time after the start of exposure (h)

Other values in Cecile Boyer thesis and paper

Mesures dans l'eau tissulaire : conditions d'éclairement



Mesures dans l'eau tissulaire : conditions d'éclairement



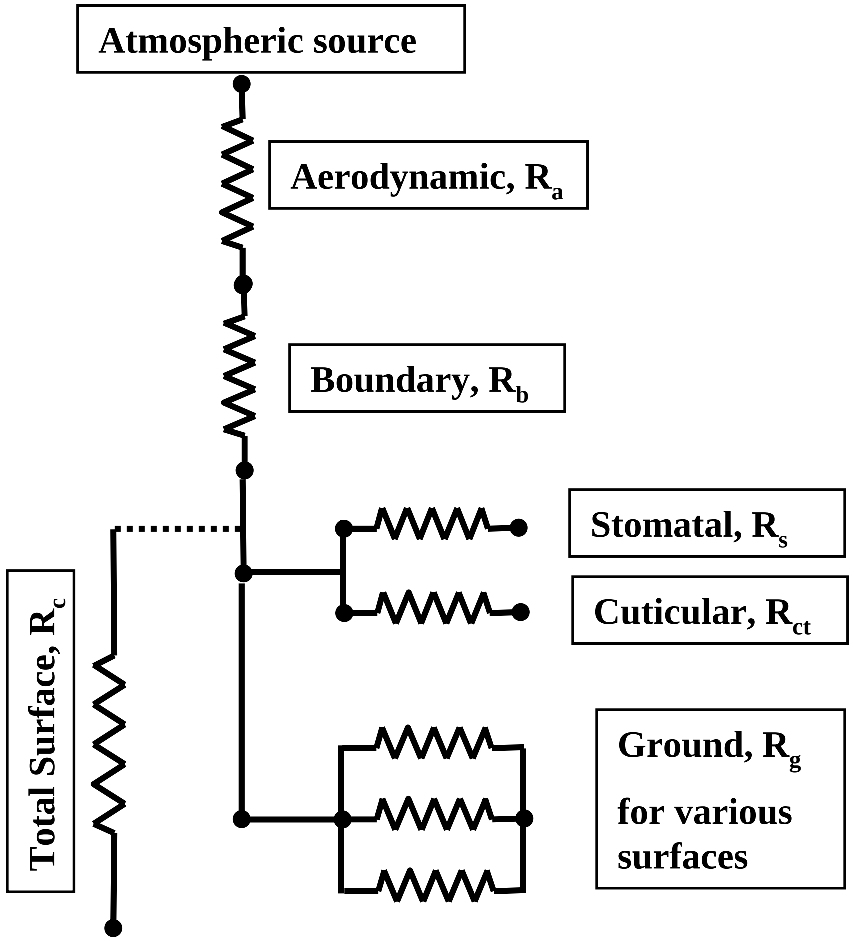
Rate constant k shows a large variability between plants and environmental conditions.
Clearly depends on light, temperature, humidity and development stage of plants
We must asses the uptake by the vegetation canopy, not for a single leaf

Keum use a single value for morning, all plants,
Gazaxi (2002) use single values for day and night
ETMOD (1994) use seasonal value of leaf resistance by macro plants categories (binome)
UFOTRI scale leaf resistance to canopy by dividing leaf resistance to leaf area index

In land atmosphere interaction, exchange velocity is used (inverse of resistance) due to atmospheric resistance, boundary layer resistance and canopy resistance

Follows excerpts form a lecture last year (A Melintescu)

Resistance Approaches to Deposition and Exchange



- Similitude between water vapour transport and electric circuits, because in both cases the transport is due to specific gradients:
  - specific humidity for water
  - electric potential for electricity
- Resistance to environmental transport is defined by analogy with resistance in electric circuits, both of them being the ratio between potential difference and flux
- Aerodynamic resistance R_a depends on turbulence and wind speed
- Boundary layer resistance R_b depends on turbulence, wind speed and surface properties
- Total surface resistance R_c can be split up into canopy and ground related resistance
- Canopy resistance depends on surface properties, temperature, photosynthetically active radiation (PAR), humidity, water content in soil
- For HT deposition, ground resistance depends on the rates of diffusion and oxidation in soil, and is much lower than the canopy resistance

Deposition velocity=1/(R_a+R_b+R_c)

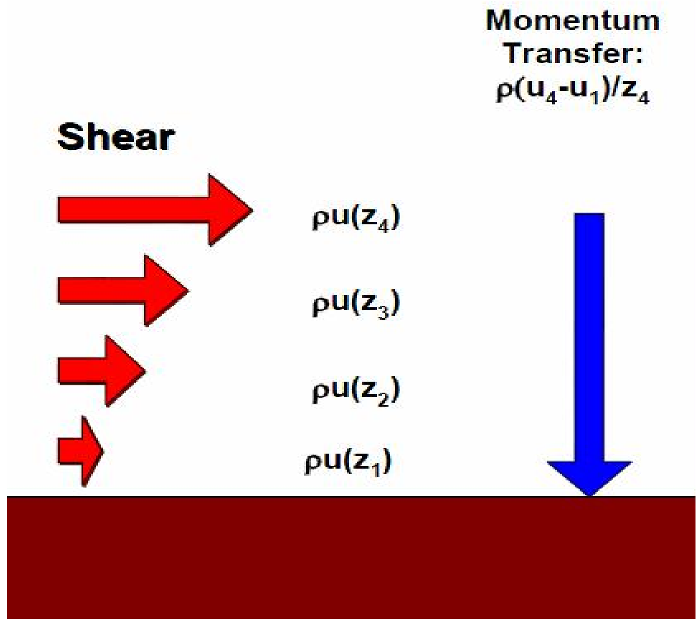
This is also an exchange velocity at air to plant (soil) interface

Turbulent eddies are responsible for transporting material through the surface boundary layer

Transport processes associated with the transfer of heat, mass and momentum modify the properties of the the atmosphere. A distinct aspect of the boundary layer is its turbulent nature.

Momentum must be transferred downward**.**

A **force** is needed to change momentum transfer from one level to another. This **drag force** or shear stress is also equivalent to the **momentum flux density**

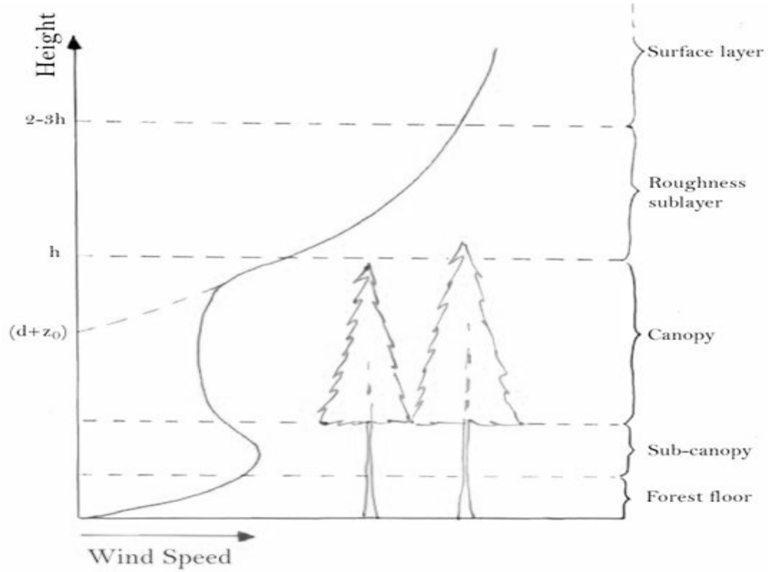


Visualization of momentum transfer

Logarithmic wind profile

$$u(z) = \frac{u_*}{k} \ln\left(\frac{z}{z_0}\right)$$

u* - friction velocity
K – von Karmann's constant (=0.40)
z - height above the ground
z_0 – **roughness parameter**. It defines the effectiveness of a canopy to absorb momentum; valid only for very short vegetation and for a neutrally stratified atmosphere
d - **Zero-Plane Displacement Height**. It represents the level at which surface drag acts on the roughness elements or level which would be obtained by flattening out all the roughness elements into a smooth surface.



- Turbulent eddies are responsible for transporting material through the surface boundary layer.
- The aerodynamic resistance determines the rate that momentum, and other scalars, are transported between a given level in the atmosphere and the vegetation's effective surface sink.
- The aerodynamic resistance is expressed as:

$$R_a = \frac{1}{ku^*} \ln \frac{z - d}{z_o} - \psi_c$$

ψc - adiabatic correction function

- Surrounding the leaf and covering the surface of the soil is a thin skin of unperturbed air - the ***boundary layer***
- Heat and water vapor must be transferred through this layer through molecular diffusion (conduction).
- The long timescale involved can be represented by a large resistance - the *boundary layer resistance*.
- The magnitude of this resistance depends mainly on the depth of the boundary layer and is proportional to leaf size/wind speed.

$$R_b = \frac{1}{ku^*} \ln \frac{z_o}{z_c} = \frac{const}{ku^*} (Sc / Pr)^{2/3}$$

z_c - scalar roughness length,

Sc - Schmidt number

Pr – Prandtl number.

constant is often assumed to equal 2 over closed canopies, but can be much greater over rough incomplete canopies

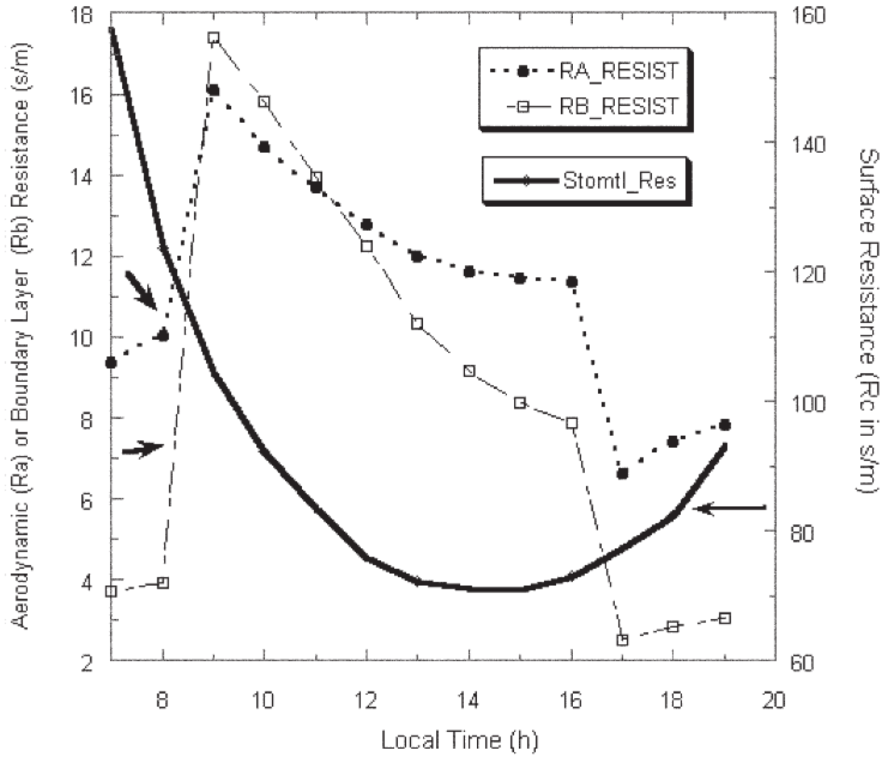
R_a, R_b - affected by wind speed, crop height, leaf size, and atmospheric stability;
- decrease with increasing wind speed and crop height

- Smaller resistances are expected over tall forests than over short grass and under unstable atmospheric thermal stratification, than under neutral and stable stratification.
- When wind speeds are 4 m s^{-1} theoretical boundary layer resistances over a 0.1 m tall grass, a 1.0 m crop and a 10 m conifer forest are about 60, 20 and 10 s m^{-1}, respectively
- Experimental measurements show that both R_a and R_b are less than 20 s m^{-1} during the day over a temperate deciduous forest.
- Greater R_a values (up to 150 s m^{-1}) occur at night when turbulent mixing is reduced.

- **Canopy resistance is predominant**

FOREST

Sample time history of simulated aerodynamic (Ra), boundary layer (Rb), a (Rc) resistances using a photosynthesis-based biophysical model. Effects of changes and the dominance of the canopy resistance term is clearly seen



R_a and R_b vary between 4 -18 s/m
Surface resistance, mainly canopy, varies between 70 – 160 s/m

Relative magnitudes of r_a, r_b, and r_c

$$\nu_d = \frac{1}{r_T} = \frac{1}{r_a + r_b + r_c}$$

Z_o =	0.1 m	Grass	$r_a \simeq$ 60 s/m	Windspeed = 4 m/s
=	0.1 m	Crop	$\simeq$ 20 s/m	
=	10 m	Conifer forest	$\simeq$ 10 s/m	

Day time, $r_a \longrightarrow$ low, except very reactive species such as HNO_3, HCl and NH_3

Night time, $r_a \longrightarrow$ high, can be over 150 s/m over land

Stable conditions, low winds: $r_a \longrightarrow$ dominates dry deposition

Neutral and unstable conditions: $r_a \longrightarrow$ small

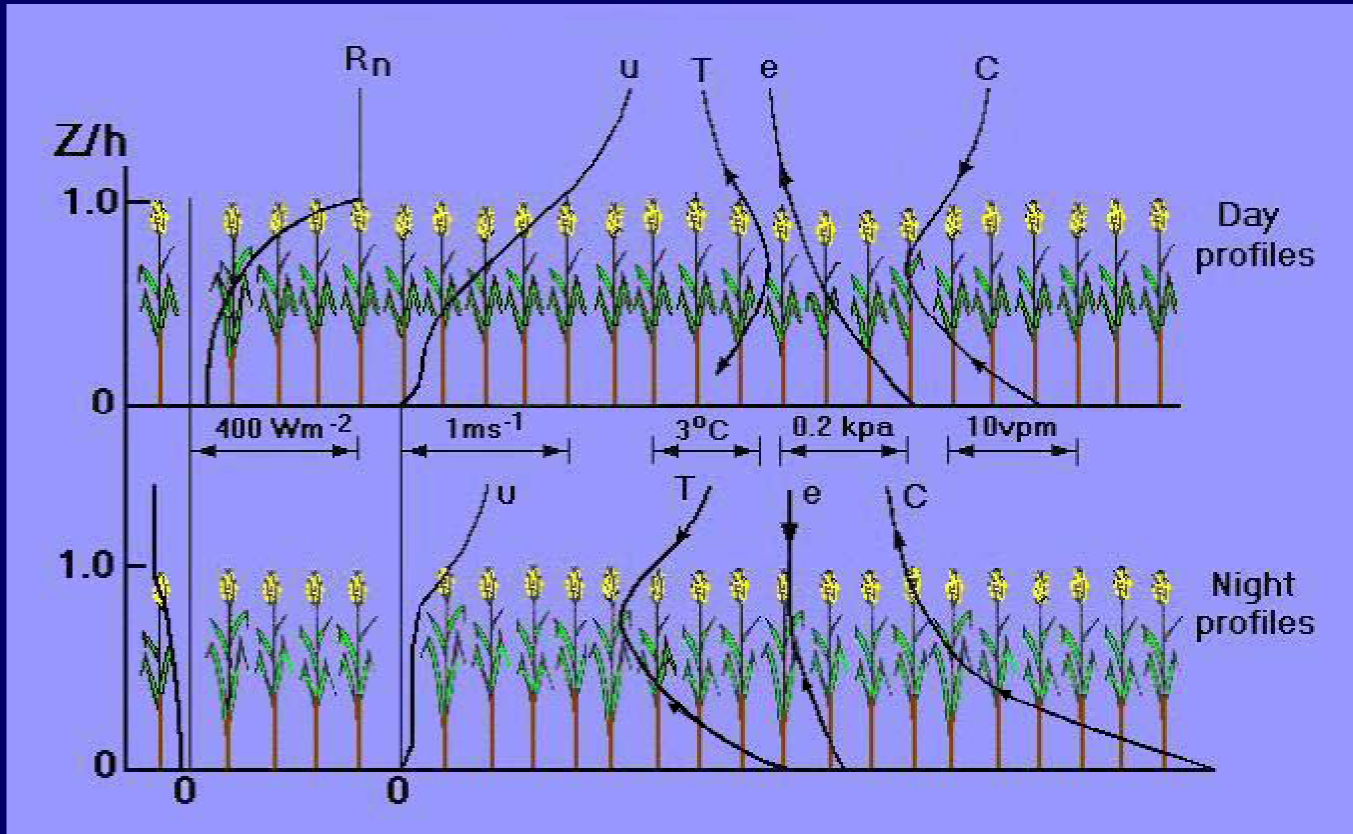
Pojanie Khummongkol

r_b does not change significantly over most condition

r_c is large over barren landscapes, sea
$\longrightarrow$ low deposition

r_c is small under highly unstable conditions over transpiration vegetation
$\longrightarrow$ greatest deposition velocities

Pojanie Khummongkol



Profiles of net radiation(R_n), windspeed (u), air temperature (T), vapor pressure (e) and CO_2 concentration (C) in a field crop growing to a height h plotted as a function of z/h

Canopy resistance – physiological models

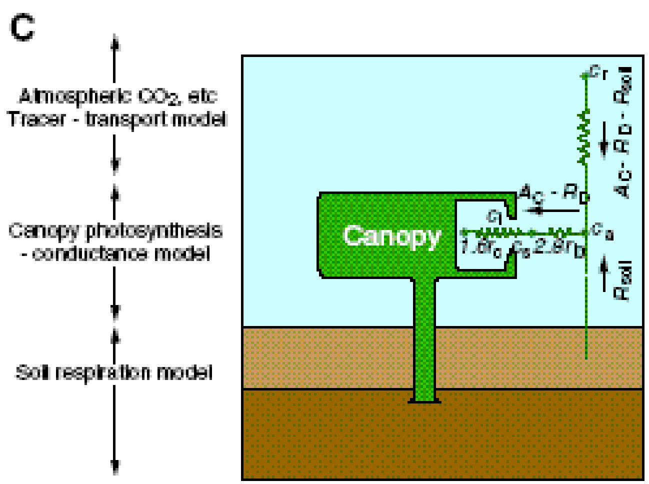
- The canopy resistance (R_c) is a function of the canopy stomatal resistance (R_{stom}), the canopy cuticle resistance ($R_{cuticle}$), and the soil resistance (R_{soil}).
- These resistances are affected by leaf area, stomatal physiology, soil pH, and the presence and chemistry of liquid drops and films.
- The stomatal, leaf surface (cuticle) and soil resistances act in parallel, causing R_c to be formulated as:

$$\frac{1}{R_c} = \frac{1}{R_{stom}} + \frac{1}{R_{soil}} + \frac{1}{R_{cuticle}}$$

- 'Big-Leaf' resistance models have electrical analogy - current flow (mass or energy flux density) is equal to the ratio between a potential and the sum of the resistances to the flow:

$$F_c = \frac{C_a - C_0}{R_a + R_b + R_c}$$

C_a – concentration of a scalar in the atmosphere over the vegetation
C_0 – 'internal' concentration



Stomatal cavity → common pathway for water and CO_2

Leaf = Σ stomata

$$E = \rho_a \frac{q_{in} - q_{air}}{r_a + r_c}$$

E – evaporation
ρ_a – air density
q_{in} – saturated air vapour at leaf temperature
q_{air} – air vapour in atmosphere

Scalling from leaf to canopy
-classic: $R_c = R_{leaf}/LAI$
-big leaf: integral over all canopy as a single leaf
-physiological approach

Jarvis Scheme vs Ball-Berry Scheme

Jarvis scheme

$$R_c = \frac{R_c\_\min}{LAI \times F1 \times F2 \times F3 \times F4}$$

LAI – Leaf Area Index,
F1 ~ f (amount of PAR)
F2 ~ f(air temperature: heat stress)
F3 ~ f(air humidity: dry air stress)
F4 ~ f(soil moisture: dry soil stress)

Fundamental difference: evapotranspiration as an 'inevitable cost' the foliage incurs during photosynthesis or carbon assimilation

A_n: three potentially limiting factors:
1. efficiency of the photosynthetic enzyme system
2. amount of PAR absorbed by leaf chlorophyll
3. capacity of the C3 and C4 vegetation to utilize the photosynthesis products

Ball-Berry scheme in GEM (Gas Exchange Model)

$$g_s = m\frac{A_n}{C_s}h_s p_s + b \qquad R_c = \frac{1}{g_s}$$

hs – relative humidity at leaf surface
ps – Surface atmospheric pressure
An – net CO2 assimilation or photosynthesis rate
Cs – CO2 concentration at leaf surface
m and b are linear coeff based on gas exchange consideration

GEM model reference: Niyogi, Alapaty, Raman, Chen, 2007: JAMC, in revision.

Jarvis approach – light, temperature, water vapour deficit, and soil water deficit behave independently as modifying factors (0, 1)

- minimal leaf resistance R_{c-}min is plant characteristic

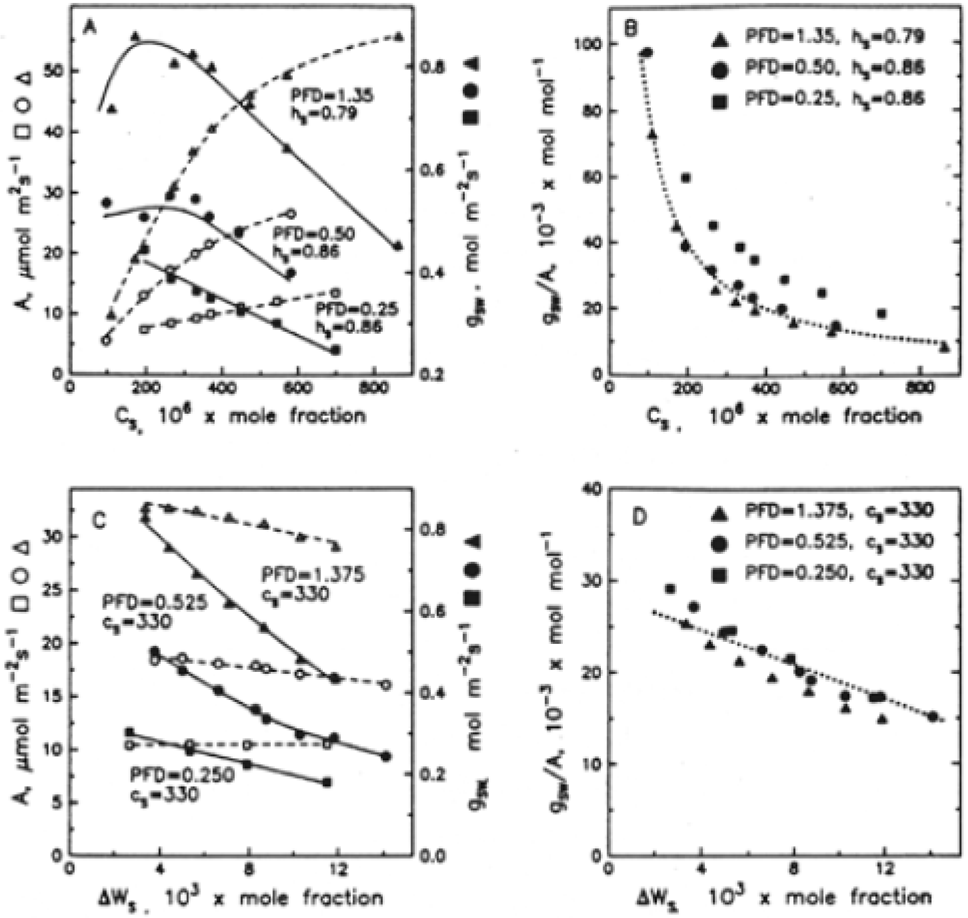
Physiological approach – link between water and CO_2 pathway to photosynthesis (A_n), taking into account different diffusion coefficients

Ball-Berry scheme uses m and b as semi-empirical coefficients → inconvenience

Multiple Environmental Effects

on Stomatal Conductance

PFD = "photon flux density" (light)
c_s = CO_2 at leaf surface
h_s = relative humidity at leaf sfc



Tim Ball (PhD thesis, 1988)

- Interactions among environmental forcing variables produce complicated responses
- Scaling g_s by photosynthetic assimilation rate (A) collapsed much of variability

Leuning, improvement of Ball Berry

$$g_s = g_{\min,c} + m\left(1 - \frac{D_s}{D_0}\right)\frac{A_n}{C_s - C_i}$$

with D_0 set to 45 g kg^{-1}.

Cs - the CO2 concentration at the leaf surface
Ci - the CO2 concentration in the plant interior
An - the net assimilation rate- leaf

MOSES

$$A_n = g_{l,c}(C_s - C_i) = \frac{g_{l,w}}{m}(C_s - C_i)$$

$$f = \frac{C_i - \Gamma}{C_s - \Gamma} = F_0\left\{1 - \frac{D_s}{D_c}\right\}$$

$g_{l,c}$ and $g_{l,w}$ are leaf conductance for CO2 and water vapor

Jacobs-Calvet-Ronda (preferred and tested)

- assumes that C conductance is determined by ratio between photosynthetic rate and the concentration difference of CO_2 for leaf surface and leaf interior

$$g_{l,c} = g_{\min,c} + \frac{a_1 A_g}{(C_s - \Gamma)\left(1 + \dfrac{D_s}{D_*}\right)},$$

$$\frac{C_i - \Gamma}{C_s - \Gamma} = f_0\left(1 - \frac{D_s}{D_0}\right) + f_{\min}\frac{D_s}{D_0},$$

$g_{\min,c}$ - the cuticular conductance
A_g - the gross assimilation rate- leaf
D_s - the vapour pressure deficit at plant level
C_s - the CO_2 concentration at the leaf surface
C_i - the CO_2 concentration in the plant interior
f_0 - the maximum value of $(C_i - \Gamma)/(C_s - \Gamma)$
D_0 - the value of *Ds* at which the stomata close
Γ – CO_2 compensation point

$$g_{l,c} = \frac{g_{l,w}}{1.6} \Rightarrow g_{c,c} = \frac{g_{c,w}}{1.6}.$$

$g_{l,c}$ – leaf C conductance;
$g_{l,w}$ – leaf water conductance;
$g_{c,c}$ – C canopy conductance;
$g_{c,w}$ - water canopy conductance

For canopy - integrate on LAI
We use gross canopy photosynthesis rate from WOFOST;
Data base exist → advantage

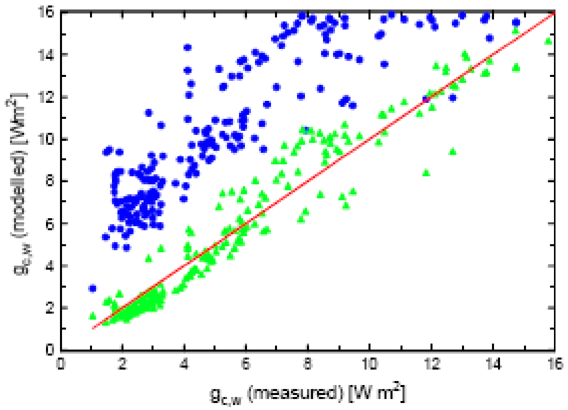


Figure 1: Scatter plot of modelled against measured canopy conductance for FIFE-KANSAS: simulated with physiology based model (green) and with JS-model (blue).

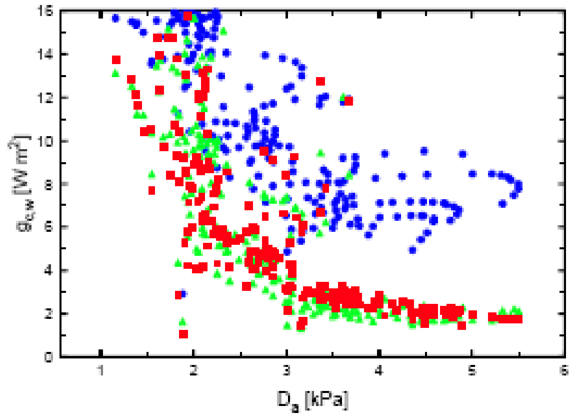


Figure 2: Scatter plot giving the canopy conductance as function of D_a; measurements (red), physiologically based model (green) and JS-model (blue).

Water vapor deficit and soil water deficit

$$\frac{C_i - \Gamma}{C_s - \Gamma} = f_0 - a_d D_s,$$

$$D_0 = \frac{f_0 - f_{\min}}{a_d}.$$

Vegetation type	f_o	a_d (kPa^{-1})
Low vegetation C3	0.89	0.07
Low vegetation C4	0.85	0.015
Lobos	0.093	0.12
Rice and phalaris grass	0.89	0.18
Forest temperate	0.875	0.06
Boreal forest	0.4	0.12

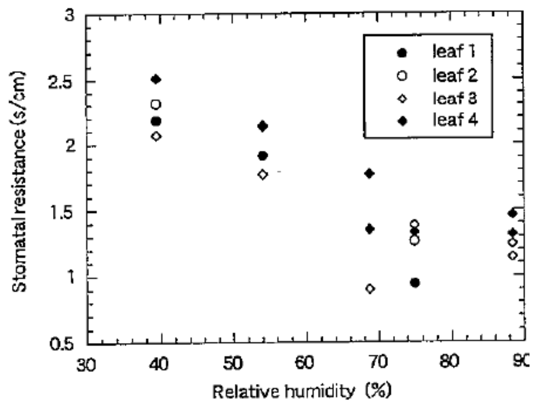
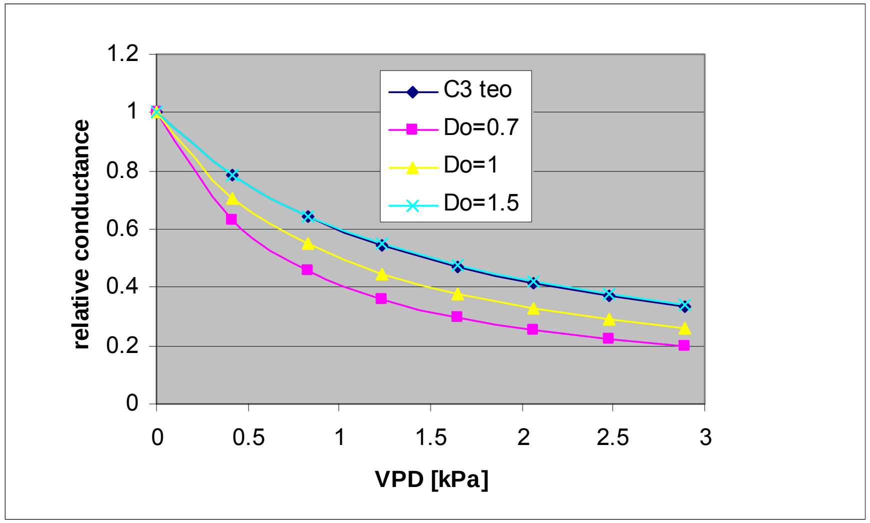
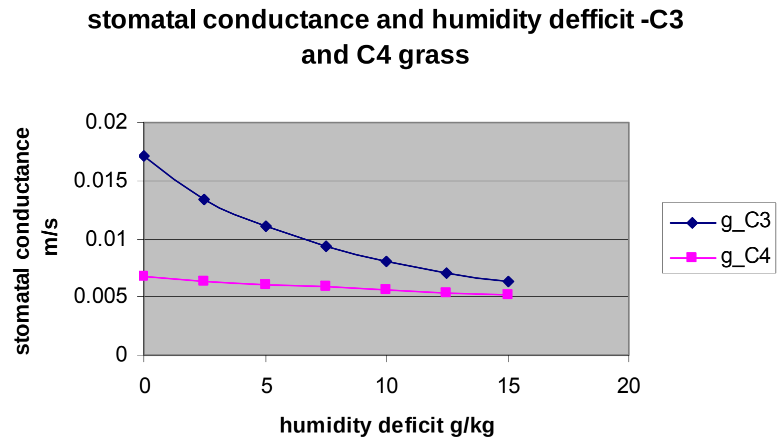


Fig. 4 Stomatal resistance of radish leaves





$$A_g = A_g^*[2\beta(\overline{\theta}) - \beta^2(\overline{\theta})].$$

$$\beta(\overline{\theta}) = \max\left[0, \min\left(1, \frac{\overline{\theta} - \mathrm{WP}}{\mathrm{FC} - \mathrm{WP}}\right)\right].$$

$$\overline{\theta} = R_1\theta_1 + R_2\theta_2 + R_3\theta_3 + R_4\theta_4.$$

Photosynthesis, at canopy level

- Many approaches in literature
- Need to considers sun and shaded leaves, nitrogen influence on photosynthesis rate, leaf orientation, leaf area profile etc.
- Scaling from leaf to canopy
- We simplify using WOFOST
- In land atmosphere interaction they use Ball Berry and Farquar models

Photosynthesis and stomatal conductance (leaf scale)

Stomatal conductance is linearly related to photosynthesis:

Semi-empirical model of leaf conductance g_s
("Ball-Berry-Collatz")

Net CO_2 assimilation (photosynthesis)

RH at leaf surface

Atmospheric pressure

stomatal conductance

$$g_s = m \frac{A_n h_s}{c_s} p + b$$

g_{s_MIN} (C_3 ~ 0.01, C_4 ~ 0.04)

CO_2 at leaf surface

empirical coefficient (C_3 ~ 9, C_4 ~ 4)

Photosynthesis is controlled by three limitations
(The Farquhar-Berry model):

$$A_n = \min(A_C, A_L, A_S) - R_d$$

Dark respiration rate

Enzyme-limited rate ("RuBisCO")

Light-limited rate

Sink-limited rate

Photosynthesis and stomatal conductance (canopy sca

From previous slide: $g_s = f\left(A_n\right)$ (leaf scale)

Integrate for the entire canopy

Canopy top
Photosynthetically Active Radiation
Water vapor pressure deficit
Soil moisture

Canopy stomatal conductance

$$g_c = \int_{z_1}^{z_2} f(V_{\max 0}, PAR) f\left(p_{CO_2}, \delta e, T, W\right) \Pi dz$$

Canopy bottom
Max RuBisCO capacity at top canopy
CO_2 partial pressure
Temperature
PAR-use parameter

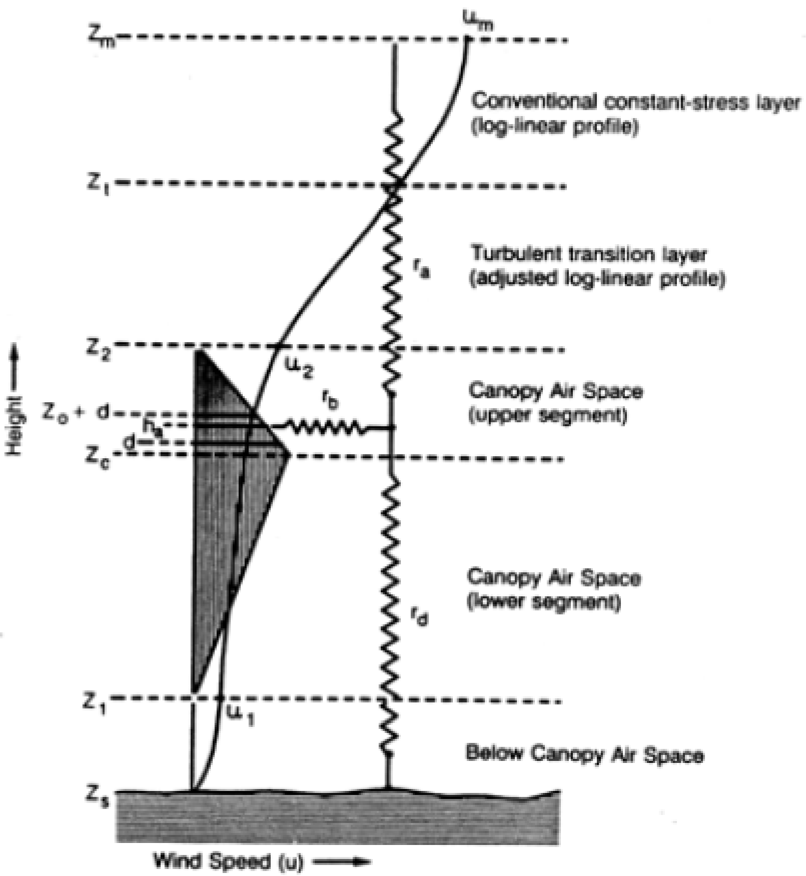
Photosynthesis-conductance model (e.g. SiB) directly links the plant transpiration with net assimilation (A_n)

Canopy transpiration rate
Saturated vapor pressure at canopy
Atmosphere vapor pressure
Density, specific heat of air
Fractional canopy wetted area

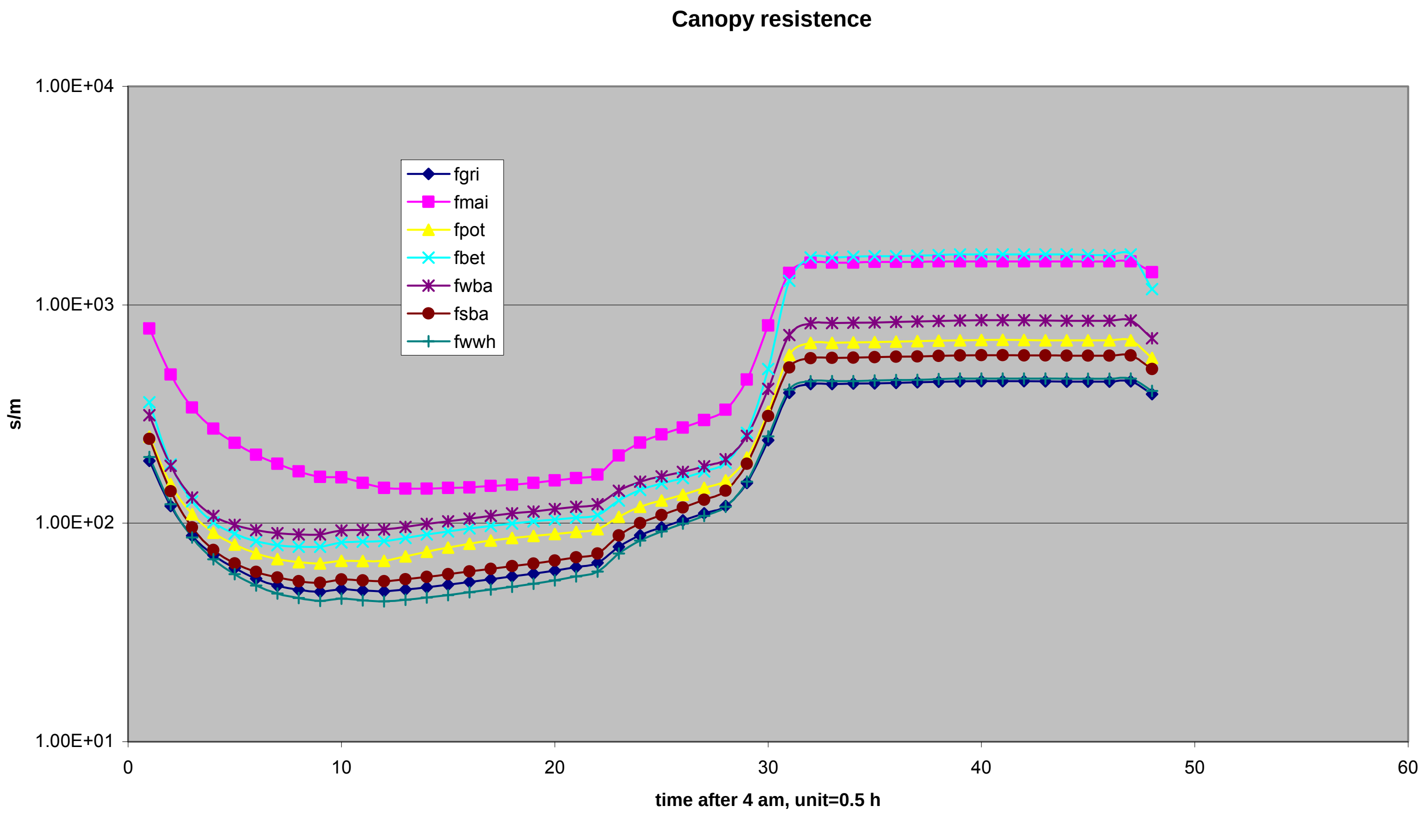
$$\lambda E_{ct} = \left[\frac{e^*(T_c) - e_a}{1/g_c + 2r_b}\right] \frac{\rho c_p}{\gamma} \left(1 - W_c\right)$$

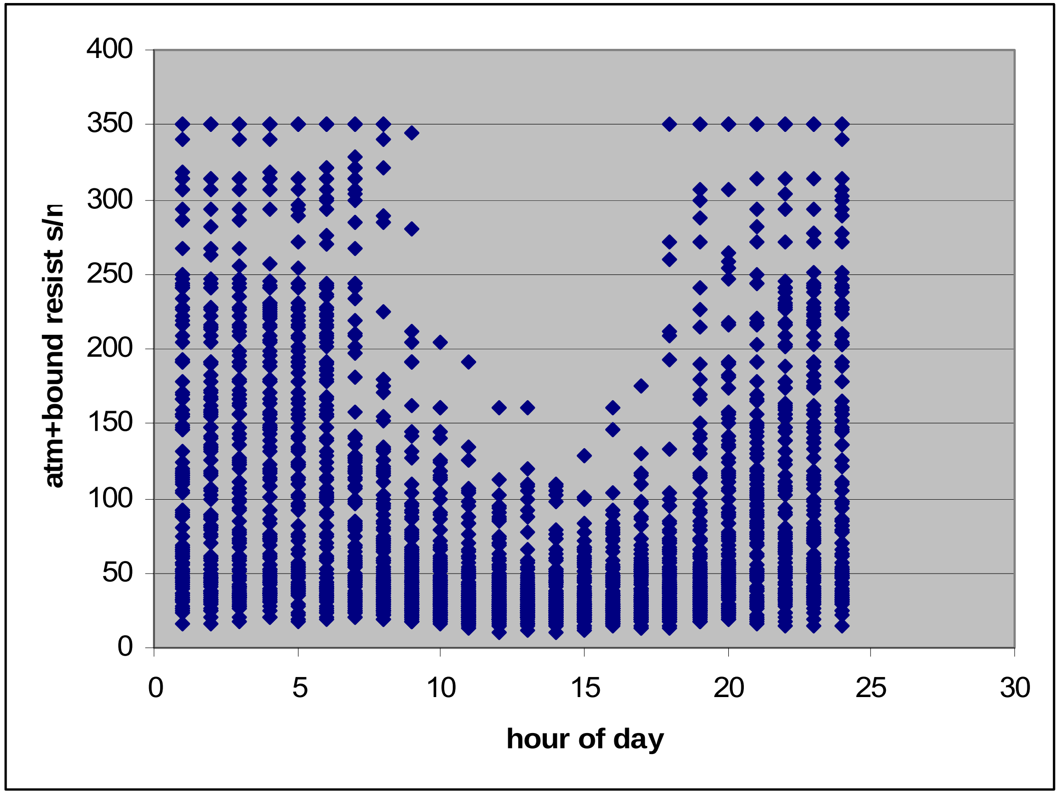
Canopy stomatal conductance
Plant to 'CAS" aerodynamic resistance
Psychrometric 'constant'

Aerodynamics in SiB2



- Compute resistances r_a, r_b, and r_d
- Assume log wind profile aloft, with transitional zone of enhanced turbulence near canopy top
- Strong damping within canopy
- Second log profile between canopy base and ground


Canopy resistence
1.00E+04
1.00E+03
1.00E+02
1.00E+01
s/m
0
10
20
30
40
50
60
time after 4 am, unit=0.5 h
fgri
fmai
fpot
fbet
fwba
fsba
fwwh



Sum of atmospheric and boundary layer resistances