IN-CANOPY TRANSFER : A KEY FOR UNDERSTANDING ATMOSPHERE-SURFACE INTERACTIONS

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M2 CLUES – 16 Oct. 2018

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OUTLINE

- **Introduction**
  - Examples showing the role of in-canopy transfer
- **Key concepts of in-canopy turbulence**
  - Turbulence (Reynolds number & scales)
  - Momentum flux
  - Turbulence statistic in the canopy
- **Key concepts of in-canopy transfer**
  - Evidence for non-diffusive transfer
  - Diffusive transfer approximation (K-theory)
  - Resistance analogy
- **Concept of transport and chemical time scales**
  - The transport time scale
  - The chemical time scale
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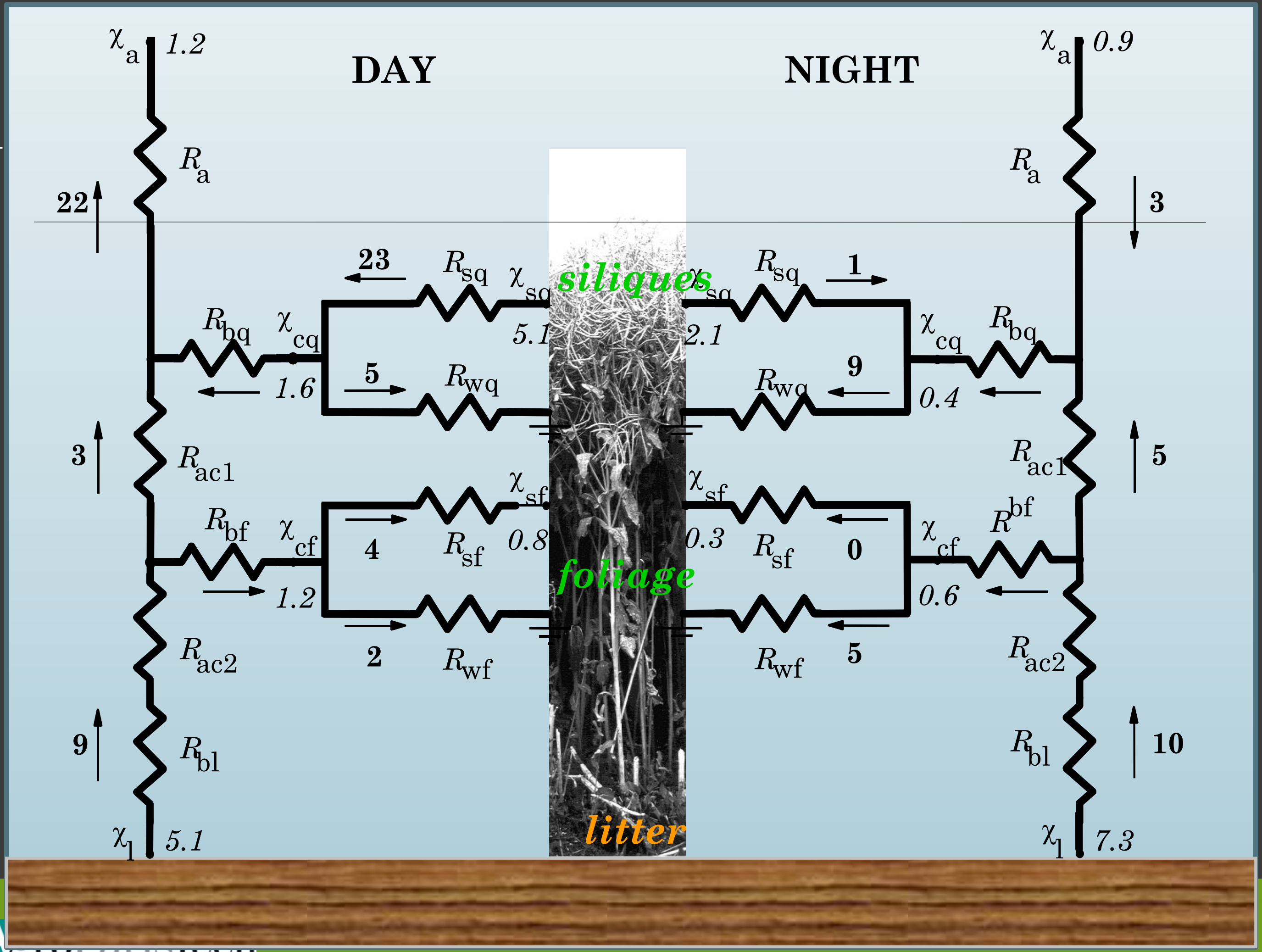
  - In canopy Lagrangian Stochastic Dispersion models
  - A simple Random Walk advection diffusion model in R
  - An example use for inferring methanol sources in a canopy

IMPORTANCE OF IN-CANOPY TRANSFER:
In canopy cycling of nitrogen (ammonia)

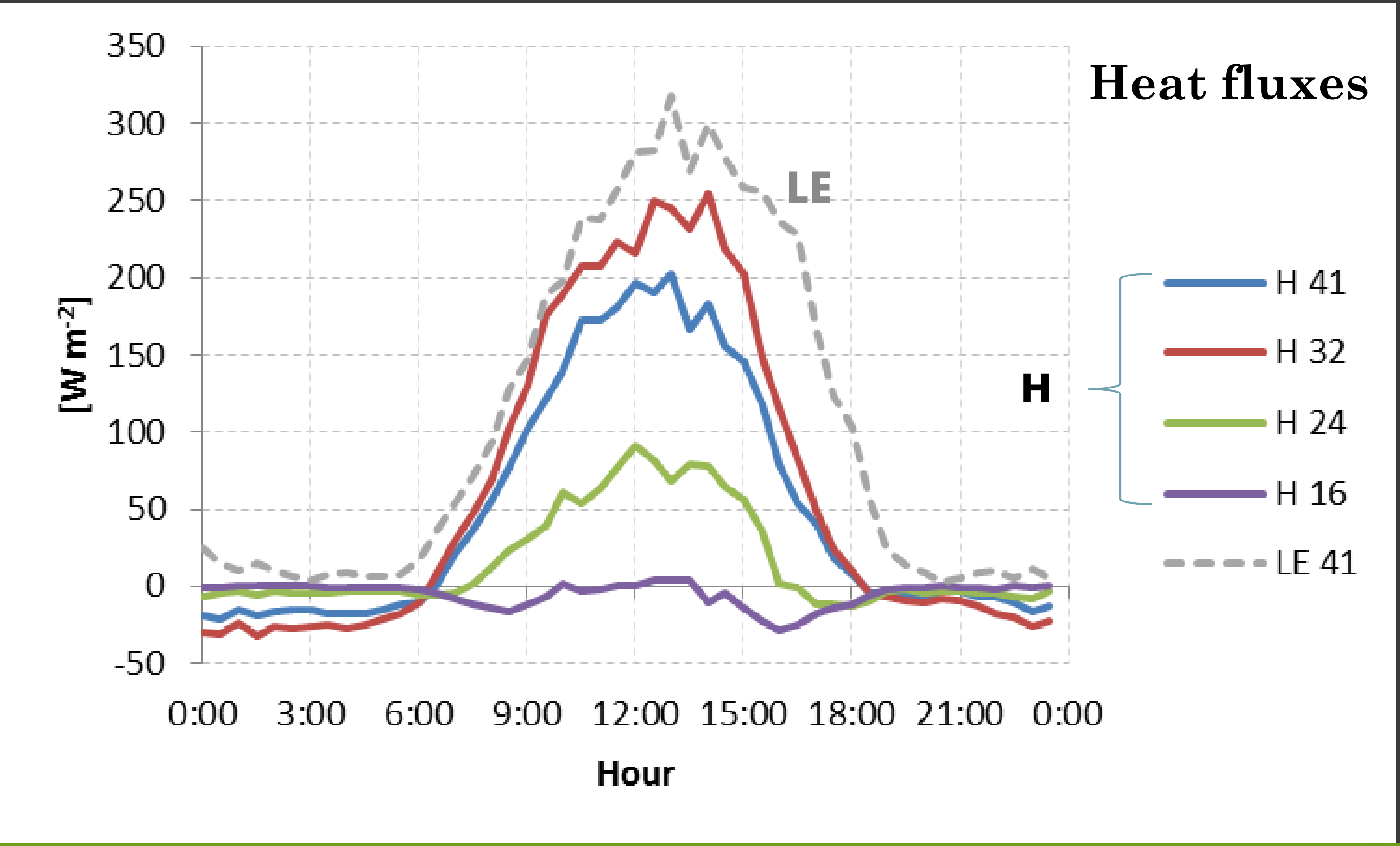
NH_3

µg NH_3 m-2 s-1



(Nemitz et al., 2000)

IMPORTANCE OF IN-CANOPY TRANSFER: In-canopy fluxes evolve quickly (large sources)



IMPORTANCE OF IN-CANOPY TRANSFER:
The role of in-canopy chemistry (NO_2, O_3)

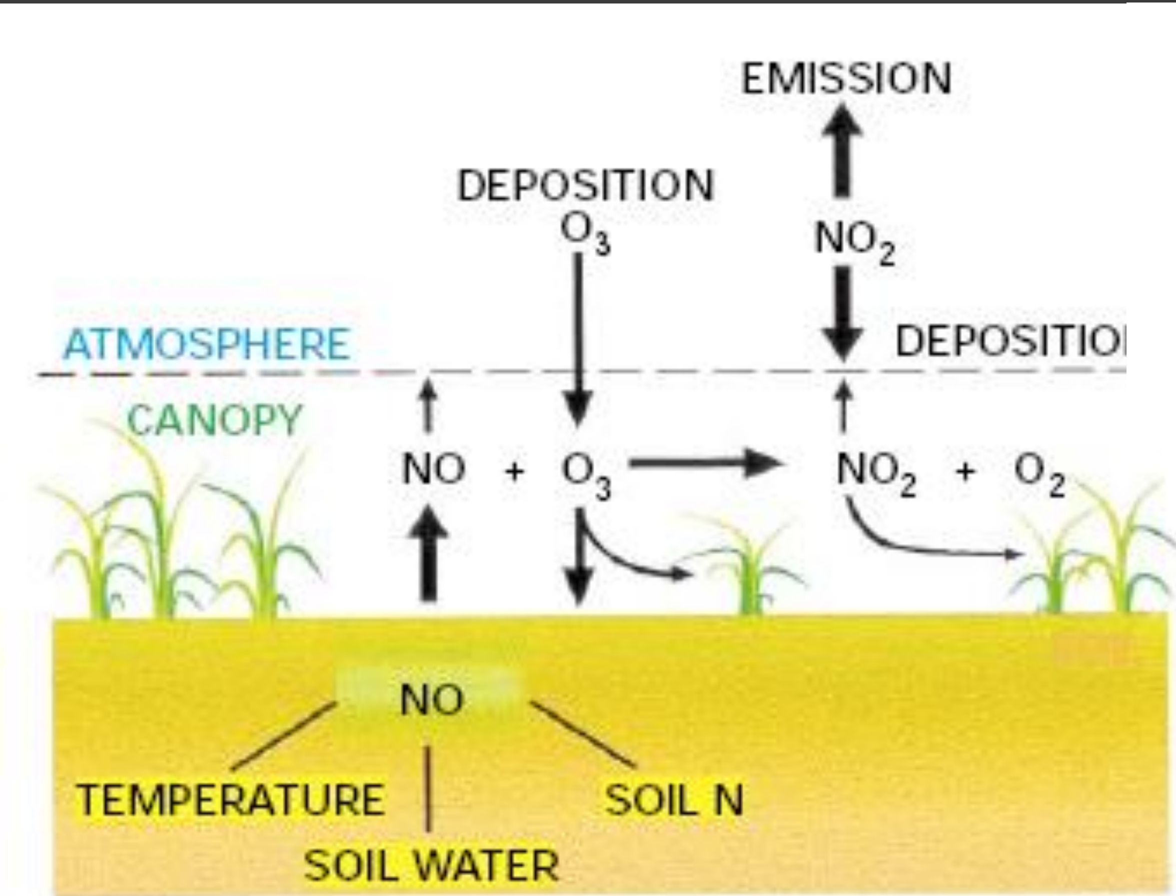


Figure 8. Interactions between soil NO emission, and the deposition of NO_2 and O_3 in crop canopies.

$$NO_2 + h_\nu (\lambda < 400\ \text{nm}) \xrightarrow{j} NO + O(^3P),$$

$$O_3 + NO \xrightarrow{k} NO_2 + O_2,$$

$$O(^3P) + O_2 \xrightarrow{\text{fast}} O_3,$$

$$[O_3] = \frac{j.[NO_2]}{k[NO]},$$

$$\left(\frac{\text{flux}}{\delta z}\right) = k[NO][O_3] - j[NO_2].$$

IMPORTANCE OF IN-CANOPY TRANSFER: The role of in-canopy chemistry: Secondary organic aerosols formation

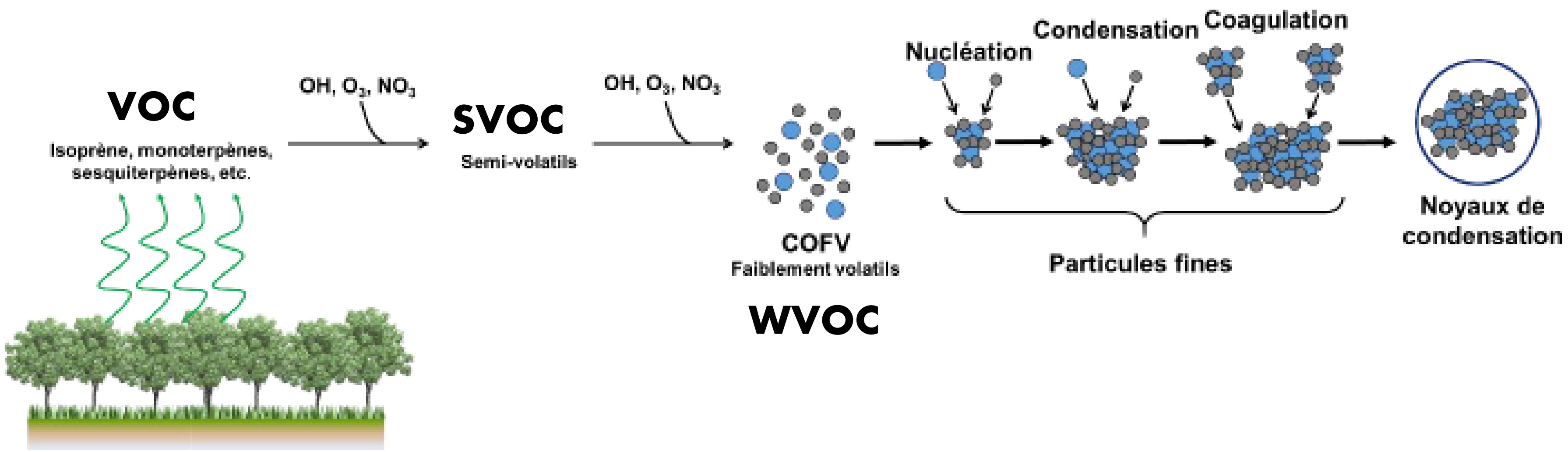


Figure 1-5 : Représentation schématique des processus impliqués dans la formation d'AOS en milieu forestier (d'après Delmas *et al*. 2005).

Delmas et al., 2005, Kammer et al. 2016

IMPORTANCE OF IN-CANOPY TRANSFER: The location of the sources and sinks: Secondary organic aerosols formation

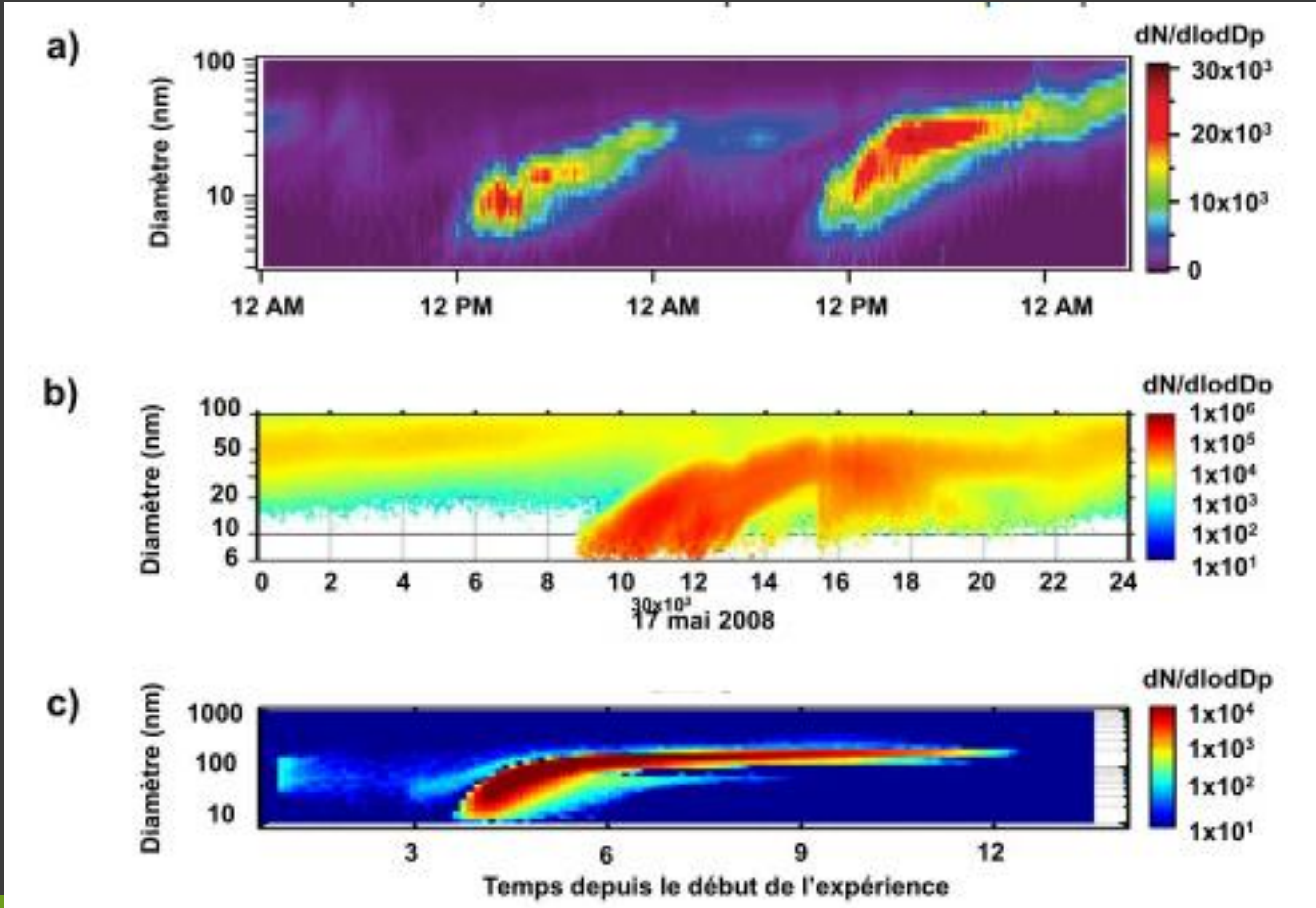
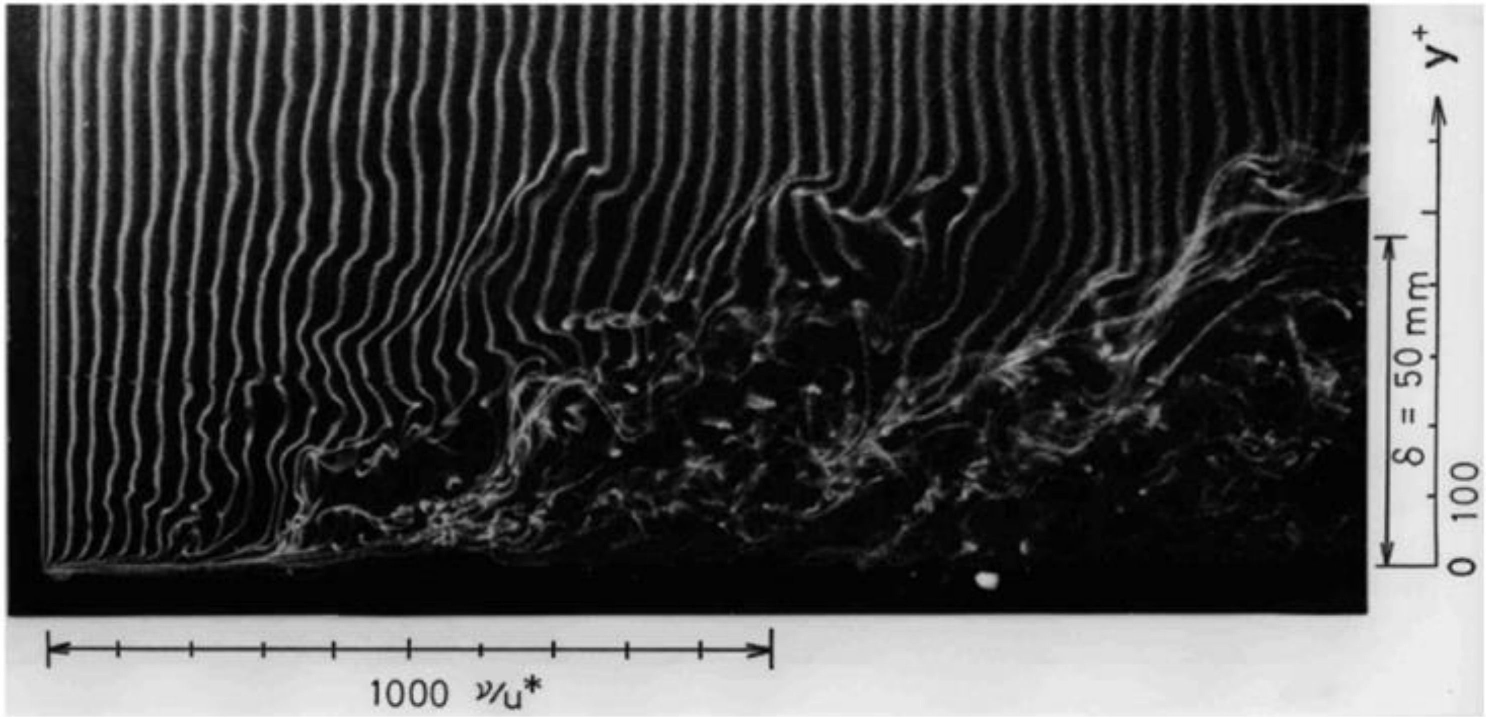


Figure 1-6 : Exemples d'épisodes de formation de nouvelles particules observés en forêt et en laboratoire. Ces phénomènes ont été observés a) en forêt boréale sur le site d'Hyytiälä en Finlande les 18 et 19 avril 2011 (Pennington et al., 2013), **b)** dans une forêt de feuillus près de la ville de Bloomington, Ind. - USA (Pryor et al., 2011), et c) en laboratoire suite à l'ozonolyse du d-limonène (Ortega *et al.*, 2012).

Kammer et al. 2016

KEY CONCEPTS: TURBULENCE

Transition from Laminar to Turbulent Flows



http://www.thtlab.t.u-tokyo.ac.jp/index.html

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KEY CONCEPTS: TURBULENCE

- Atmospheric turbulence
  - Non-linear (Navier-Stokes equations) : Chaotic
  - Non-Gaussian : Skew and Kurtosis
  - 3-dimensional (vortex in 3 directions)
  - Dissipative : continuum motion -> internal and heat
  - Diffusive: efficient mixing
  - Multiple scales : from atmospheric layer to Kolmogorov scale

KEY CONCEPTS: TURBULENCE

- Reynolds number

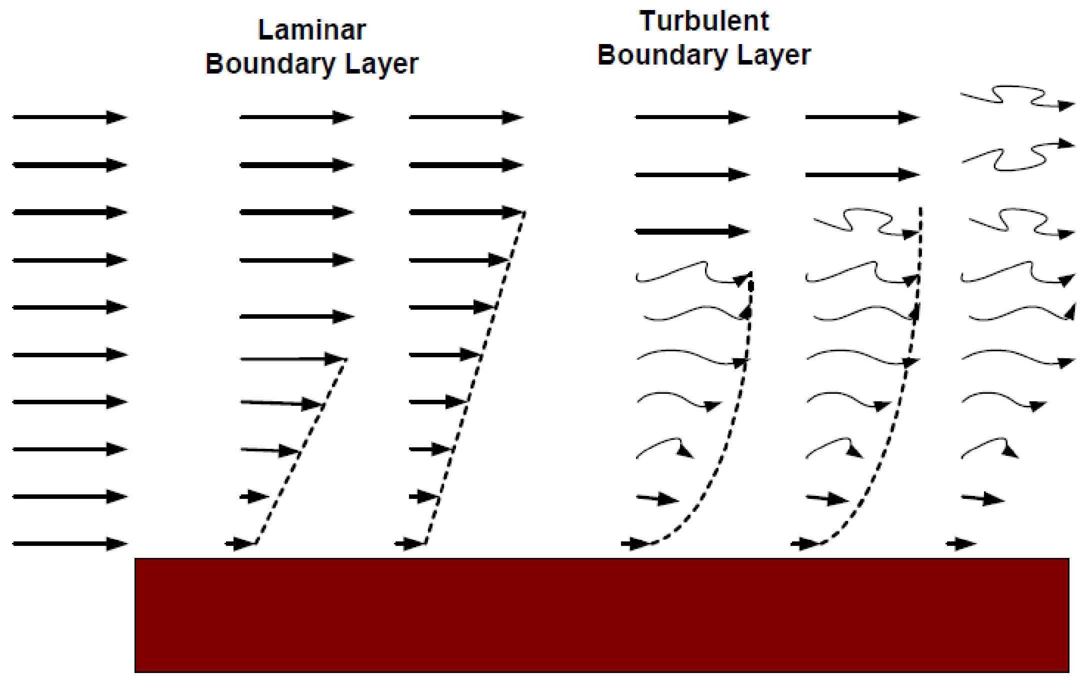


Figure 2 Evolution of boundary layers as wind blows over a surface

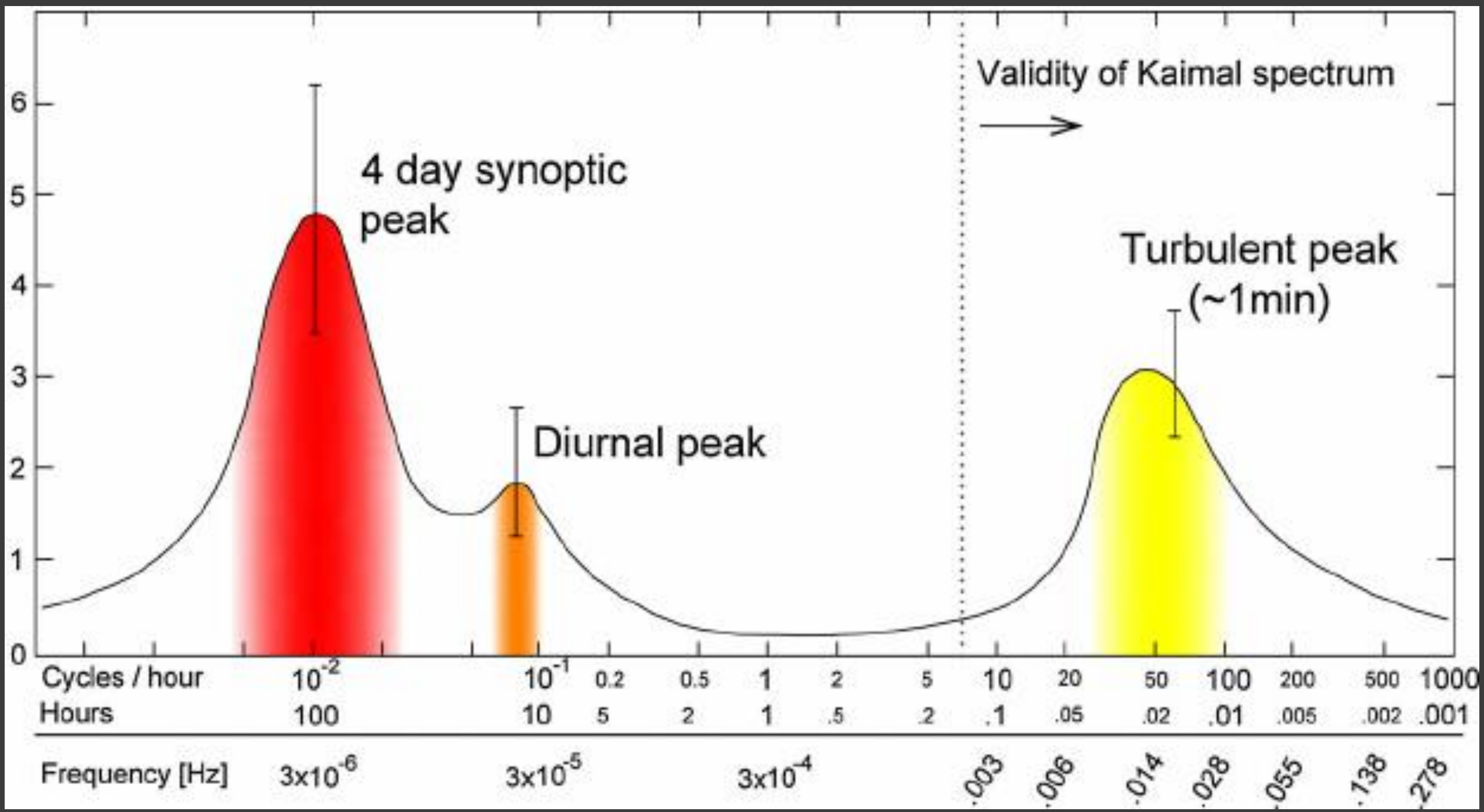
$$Re = \frac{d \cdot u}{\nu}$$

Ratio between momentum and viscous forces

d : characteristic length
u : wind velocity
ν : viscosity

KEY CONCEPTS : TURBULENT SCALES

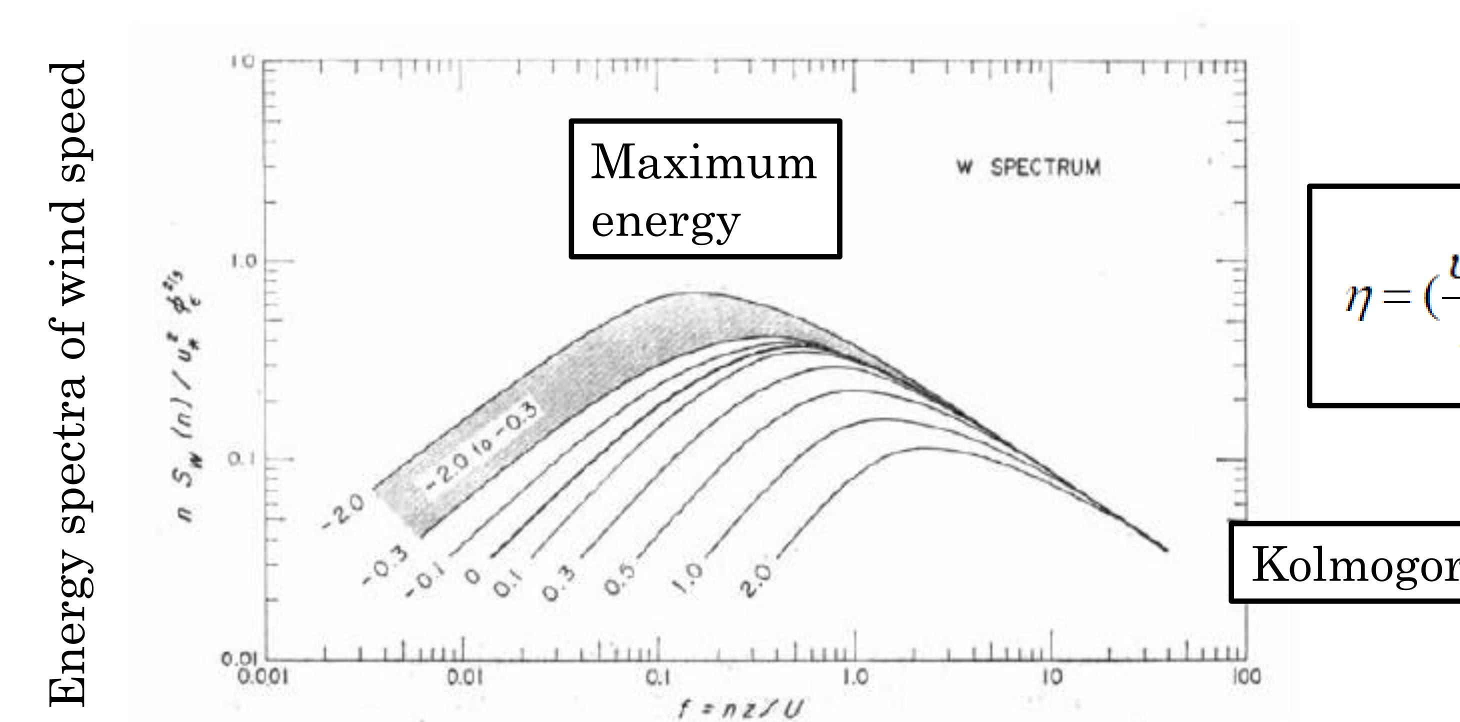
Energy spectra of wind speed



Van der Hoven, 1957

KEY CONCEPTS : TURBULENT SCALES

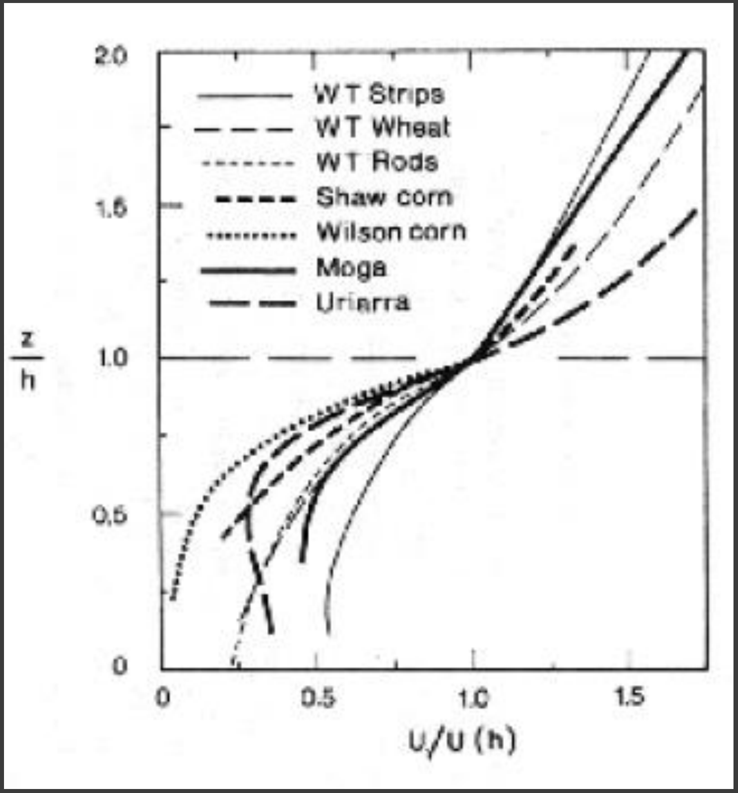
- Kolmogorov microscale : η
- Kinematic viscosity : ν
- Dissipation rate of kinetic energy : ε



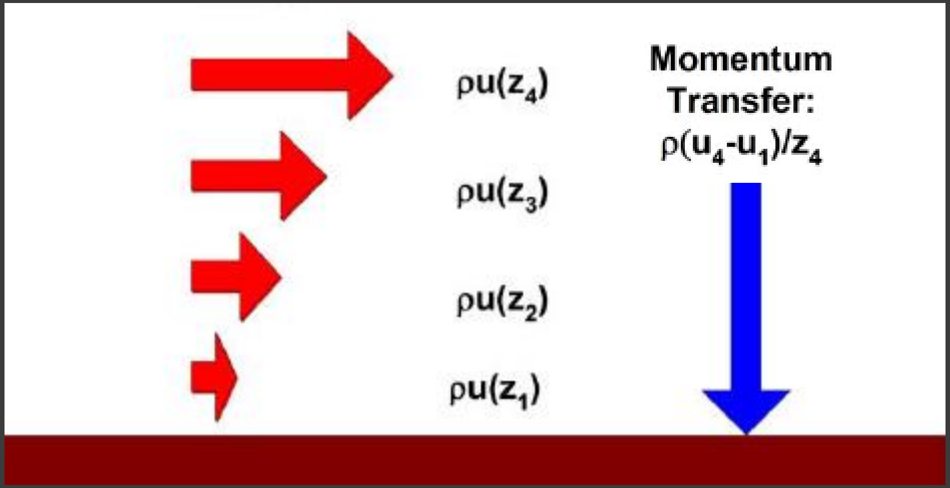
$$\eta = \left(\frac{\upsilon^3}{\varepsilon}\right)^{1/4}$$

Figure 4. Generalized *w* spectrum for *z/L* … +2·0 to −2·0. Stippling indicates absence of any … th *z/L*.

MOMENTUM FLUX TOWARDS THE SURFACE



$$\tau = \overline{u'w'} = -u_*^{\ 2}$$



τ : shear stress - u_* : friction velocity

u' and w' : fluctuation around the mean of the horizontal and vertical wind velocity components

MOMENTUM FLUX DUE TO DRAG ON VEGETATION

$$\frac{\partial \tau}{\partial z} = -\rho C_d a |\overline{u}| \overline{U}$$

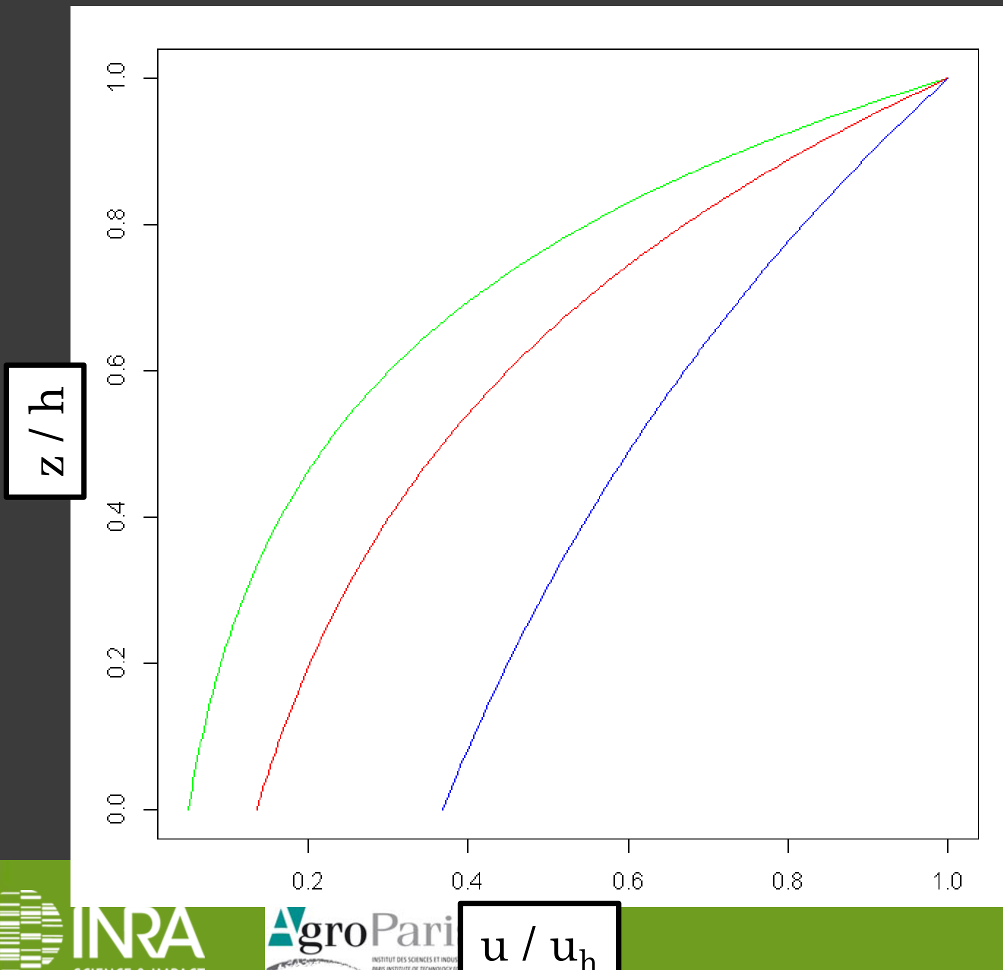
τ : shear stress
Cd : drag coefficient
a : leaf area density
U : wind velocity
z : height
h : canopy height

$$\tau(z) = \tau(h) - \rho \int_z^h C_d a(z) u(z)^2 \, dz$$

Raupach; Thom 1981

WIND VELOCITY IN CANOPY

- The exponential model



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

$$\alpha = \frac{haC_d^{'}}{2C_d}$$

h : canopy height
z : height
u : wind speed
u_h : wind speed at h
C_d : drag coefficient
a : leaf area density

TURBULENT STATISTICS IN THE CANOPY

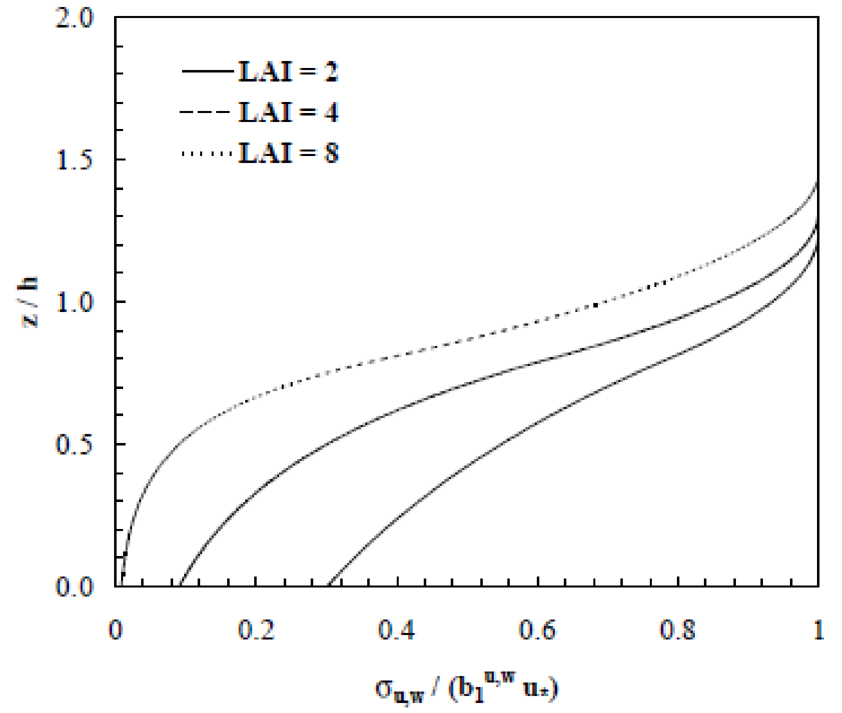


Figure III.4. Profils normalisés d'écart-types des composantes horizontales et verticales de la vitesse du vent, $\sigma_u / (b_u u_*)$ et $\sigma_w / (b_w u_*)$, dans le couvert, pour différentes valeurs de *LAI*. Les profils correspondent aux Eqns. III.53a,b,c.

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Loubet, 2000

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EVIDENCE OF NON-LOCAL TRANSPORT

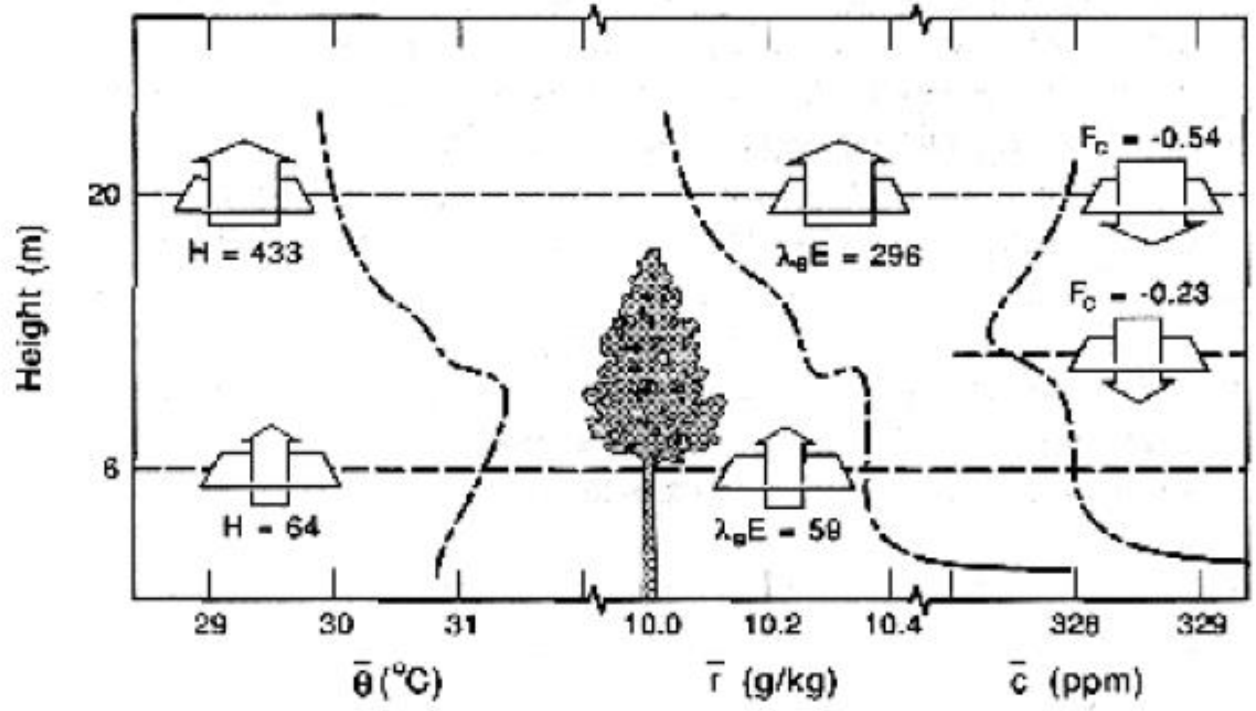
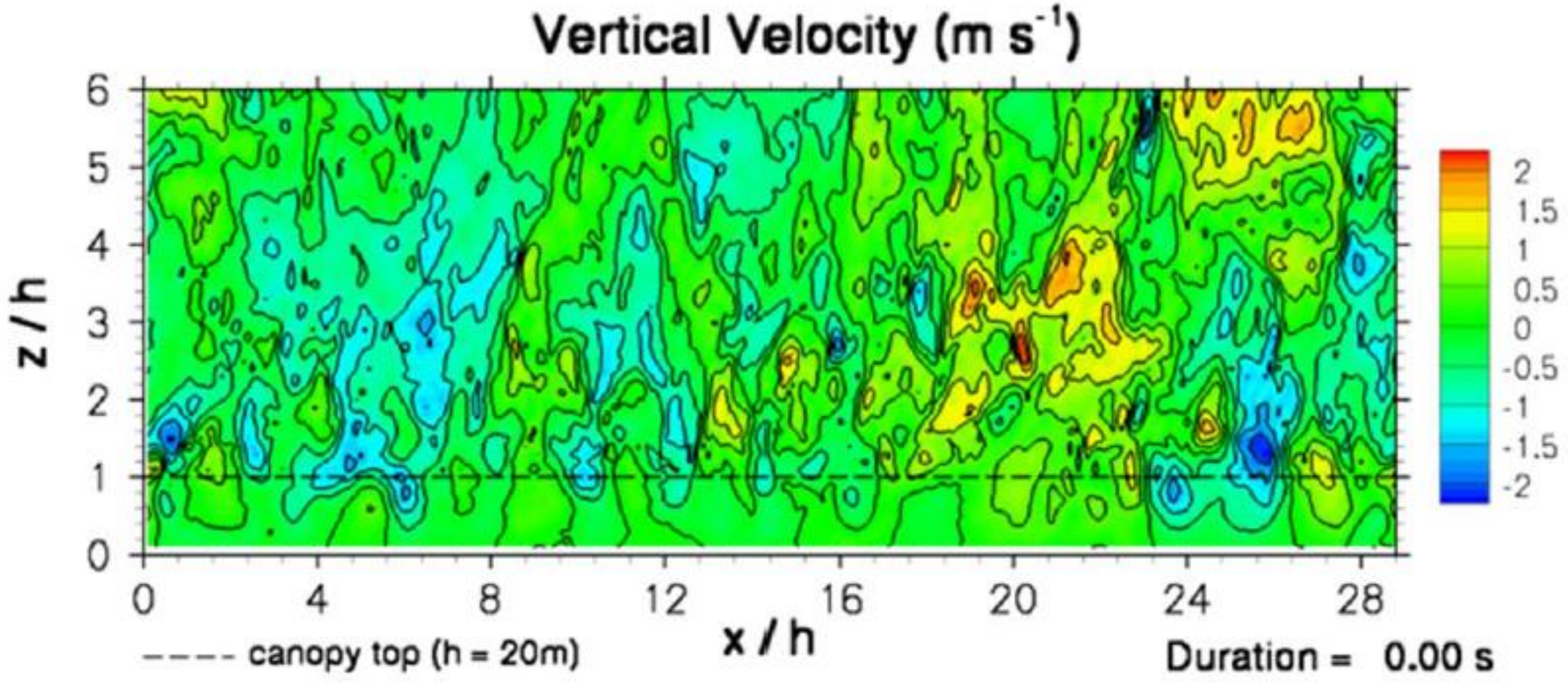


Figure II.19. Profils de température moyenne ($\overline{\theta}$) , rapport de mélange en vapeur d'eau ($\overline{r}$), concentration en CO_2 ($\overline{c}$), et flux turbulents à deux niveaux (W m^{-2} pour $\lambda_o E$ et H), observés dans une forêt sur une période de 1 heure, à midi. D'après Denmead et Bradley (1985).

NON-LOCAL TRANSPORT SHOWN BY LARGE EDDY SIMULATIONS



LES simulation of Ned Patton, NCAR

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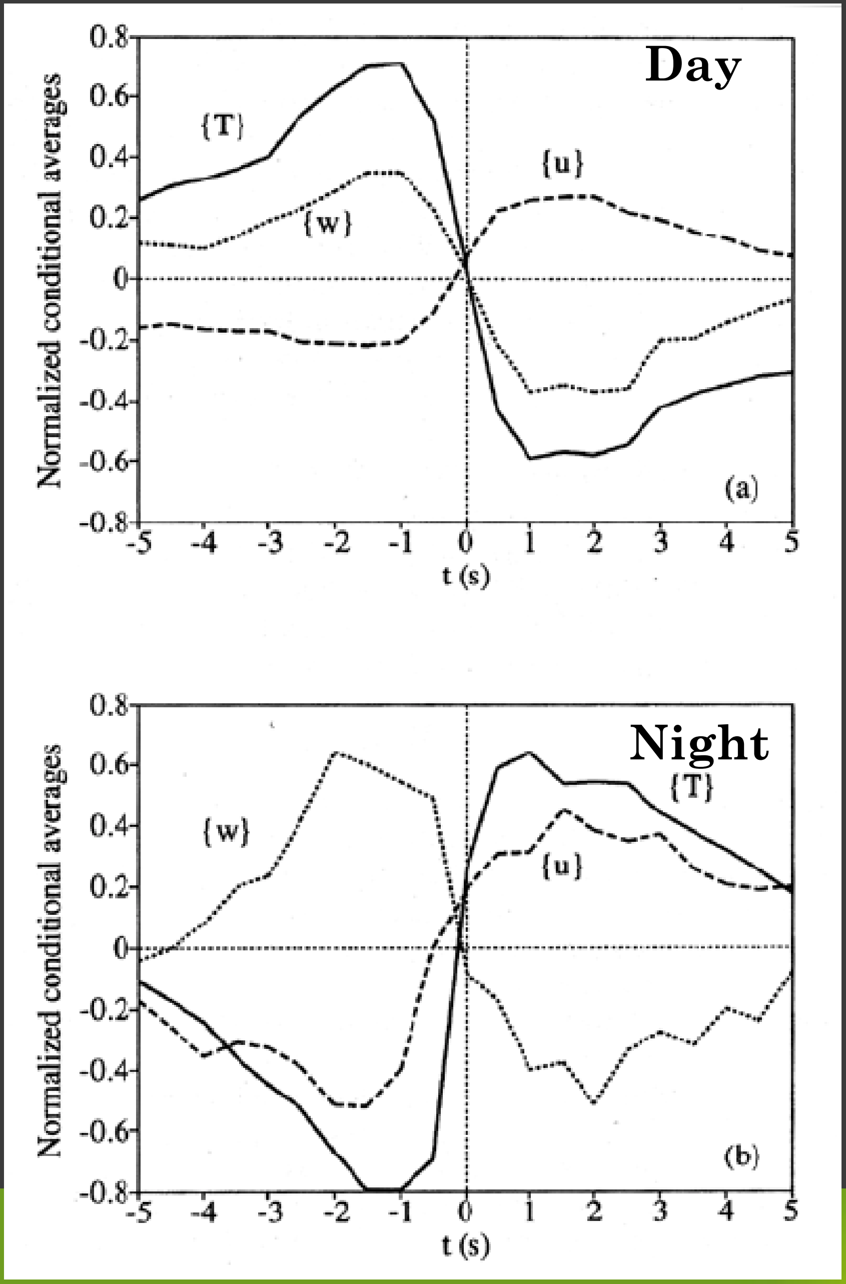
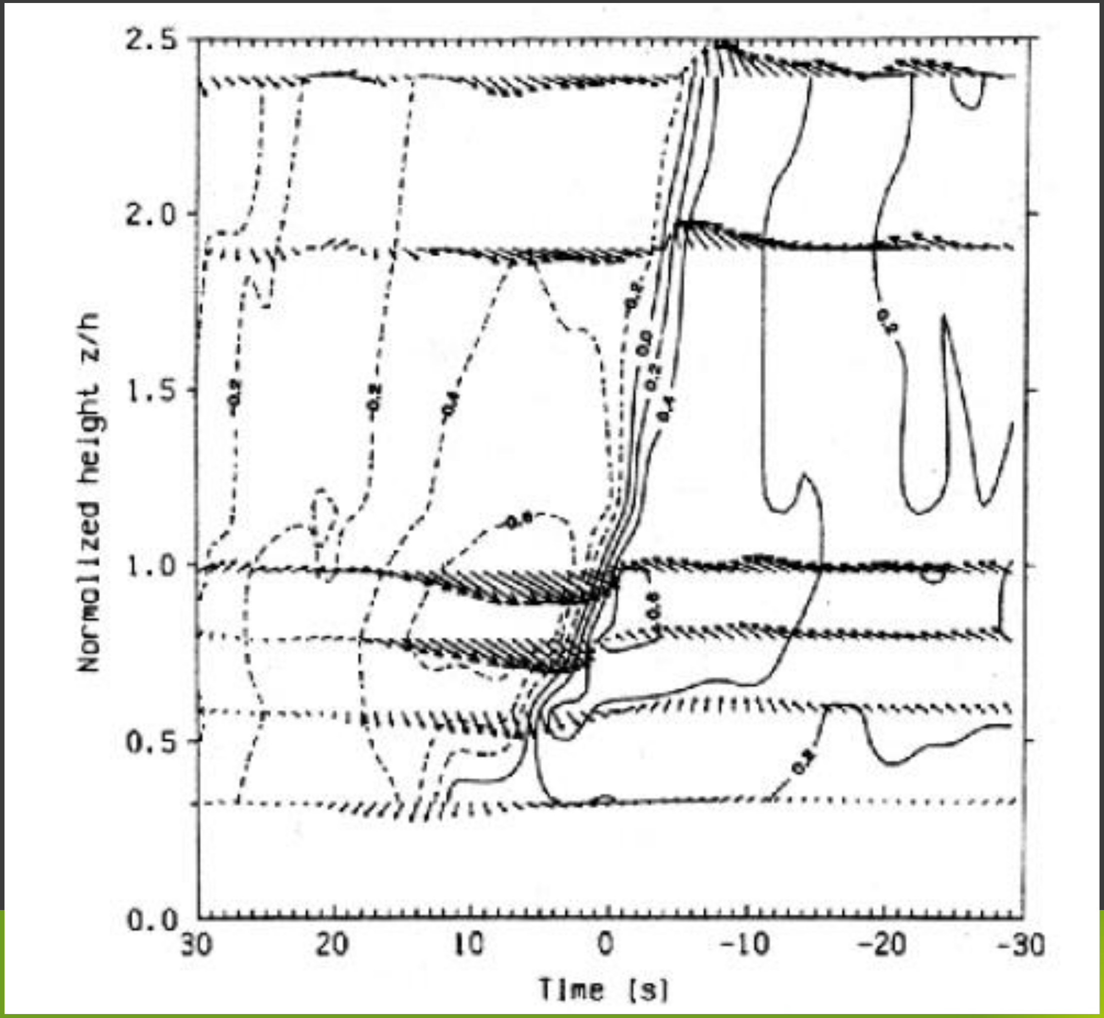
NON-LOCAL TRANSPORT SHOWN BY WAVELET ANALYSIS



Brunet and Collineau, 1994

NON-LOCAL TRANSPORT SHOWN BY PROFILE MEASUREMENTS



DIFFUSIVE TRANSFER APPROXIMATION (K-THEORY) IN THE CANOPY

$$\frac{\partial \bar{c}}{\partial t} + \bar{u_i}\frac{\partial \bar{c}}{\partial x_i} = -\frac{\partial F_i}{\partial x_i} + S(x_i)$$

Storage   Advection   Flux divergence   Sources

$$F_i = -K_i \frac{\partial \bar{c}}{\partial x_i}$$

Analogy to molecular diffusion

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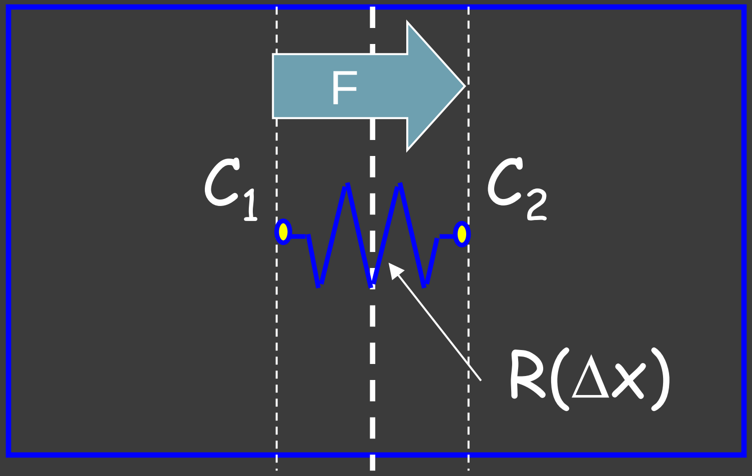
RESISTANCE ANALOGY

Integration with a
constant flux hypothesis



R(Δx) ~ Δx / K

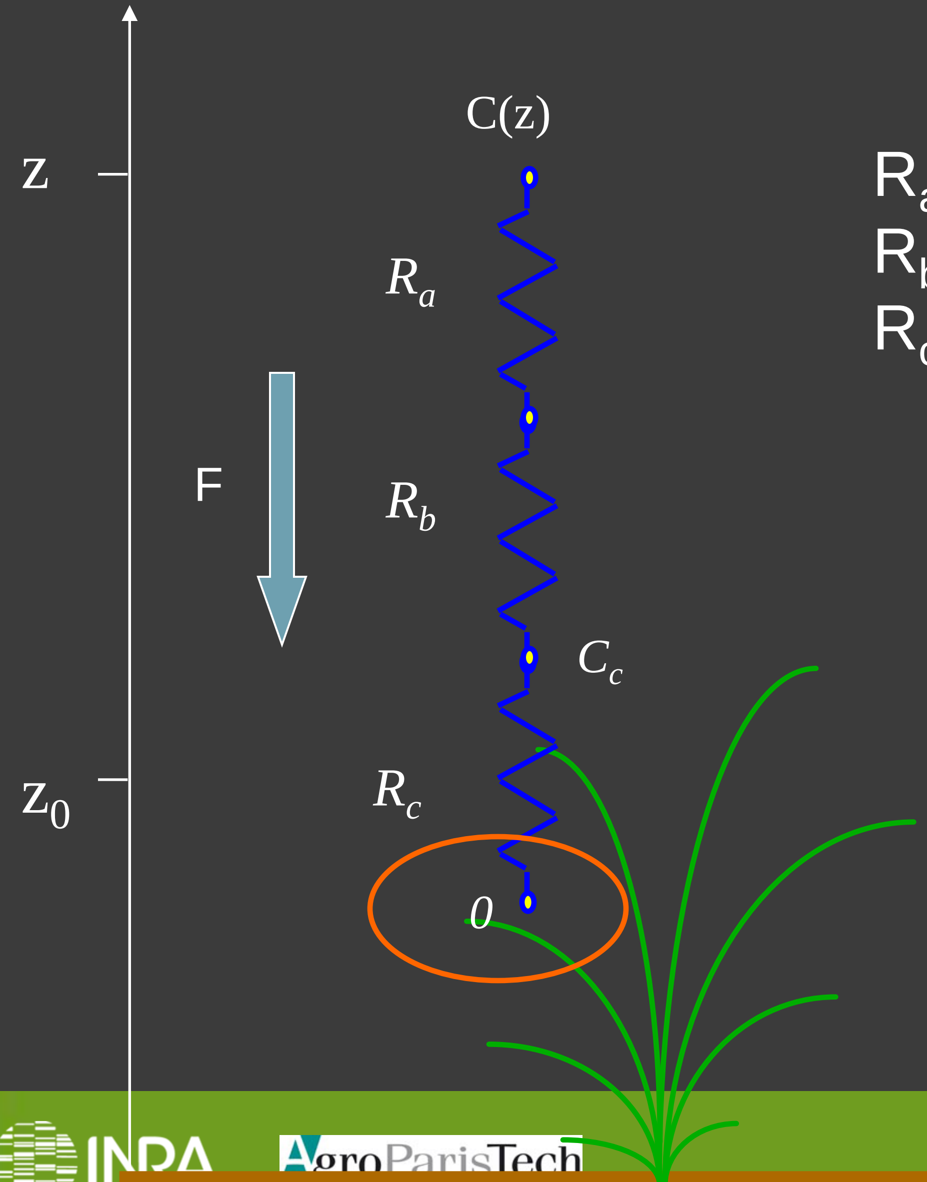
Fick

$$F_i = -K_i \frac{\partial \bar{c}}{\partial x_i}$$

Ohm

$$F_i = -\frac{\bar{c}_2 - \bar{c}_1}{R(\Delta x_i)}$$

RESISTANCE ANALOGY: THE BIG LEAF MODEL EXAMPLE



R_a = aerodynamic resistance
R_b = boundary layer resistance
R_c = canopy resistance

Deposition only

$$Vd = 1 / (R_a(z) + R_b + R_c)$$

$$F = - C(z)\ V_d(z)$$

$$V_{max} = 1 / (R_a(z) + R_b)$$

TRANSPORT TIME: A key in chemical processes in the canopy

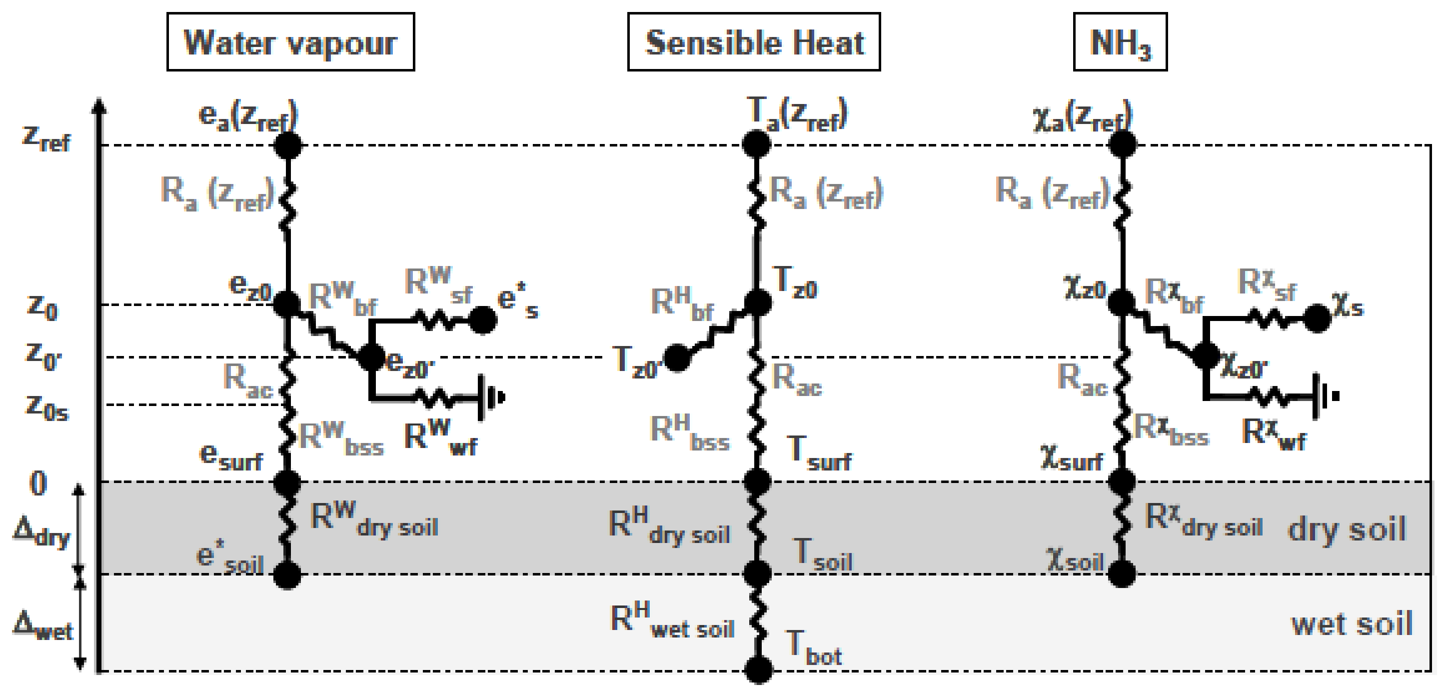


Figure 17. Resistance scheme for water vapour, heat, and NH_3 exchange models as in the Surfatm-NH_3 model. (Personne et al., 2009).

Personne et al. 2009

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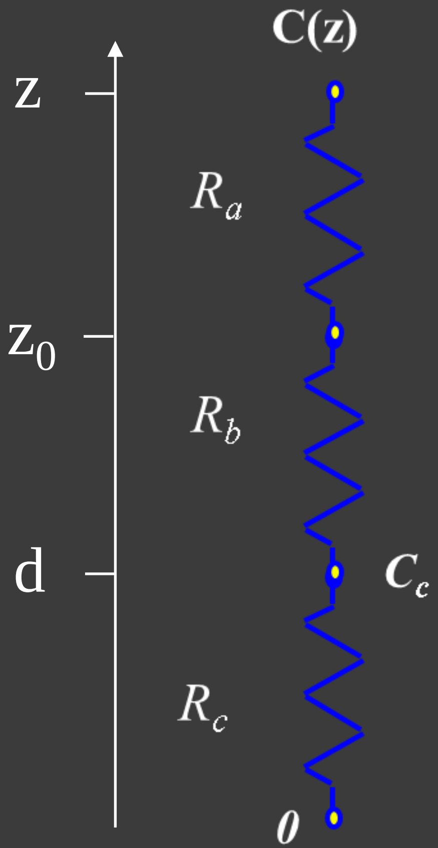
TRANSPORT TIME

- The transport time concept

$$T_{transport} = R \quad \times \Delta z$$



TRANSPORT TIME: A key in chemical processes in the canopy

- The transport time above the canopy

$$\tau_{trans} = R_a(z) \times (z_m - z_0) + R_b \times (z_0 - z_{0'}) \approx R_a(z) \times (z_m - z_0)$$

$$R_a(z) = \frac{u(z)}{u_*^2} - \frac{\Psi_H\left(\frac{z}{L}\right) - \Psi_M\left(\frac{z}{L}\right)}{k u_*}$$

$$R_b = (B_{St} u_*)^{-1}$$

Stella et al. (2011)

- The transport time in a canopy of height *h*

$$T_{transport} = R_{ac} \times h$$

TRANSPORT TIME: A key in chemical processes in the canopy

- The chemical time scale

$$NO + O_3 \rightarrow NO_2 + O_2 \qquad k_r(T_a)$$

$$NO_2 + O_2 + h\nu \rightarrow NO + O_3 \qquad J_{NO2}$$

$$\tau_{chem} = 1 / (k_r^* [NO])$$

$$\tau_{chem} = \left[j_{NO_2}{}^2 + k_r^{*2} ([O_3] - [NO])^2 + 2 j_{NO_2} k_r^* ([O_3] + [NO] + 2[NO_2]) \right]^{-0.5}$$

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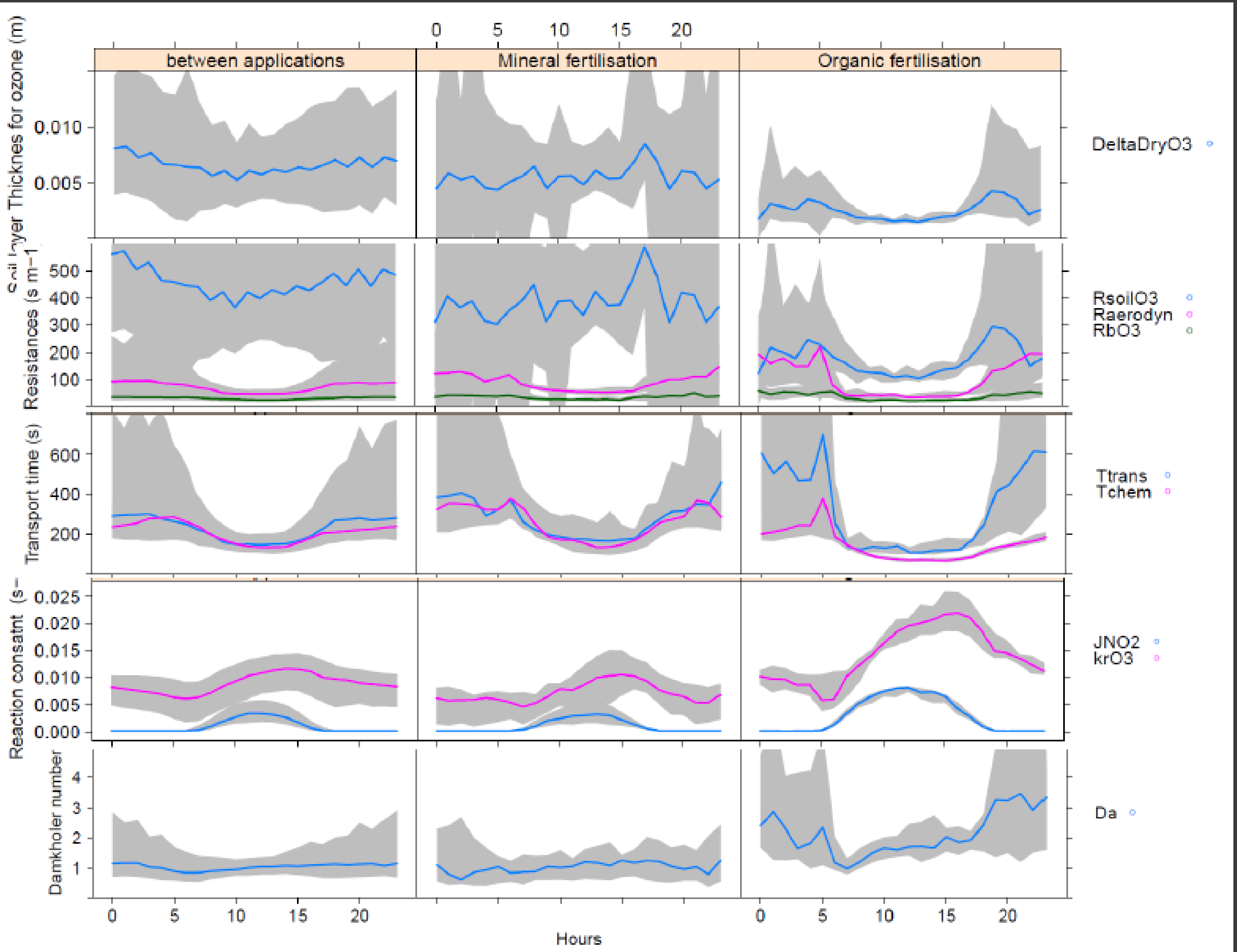
Loubet et al. 2011



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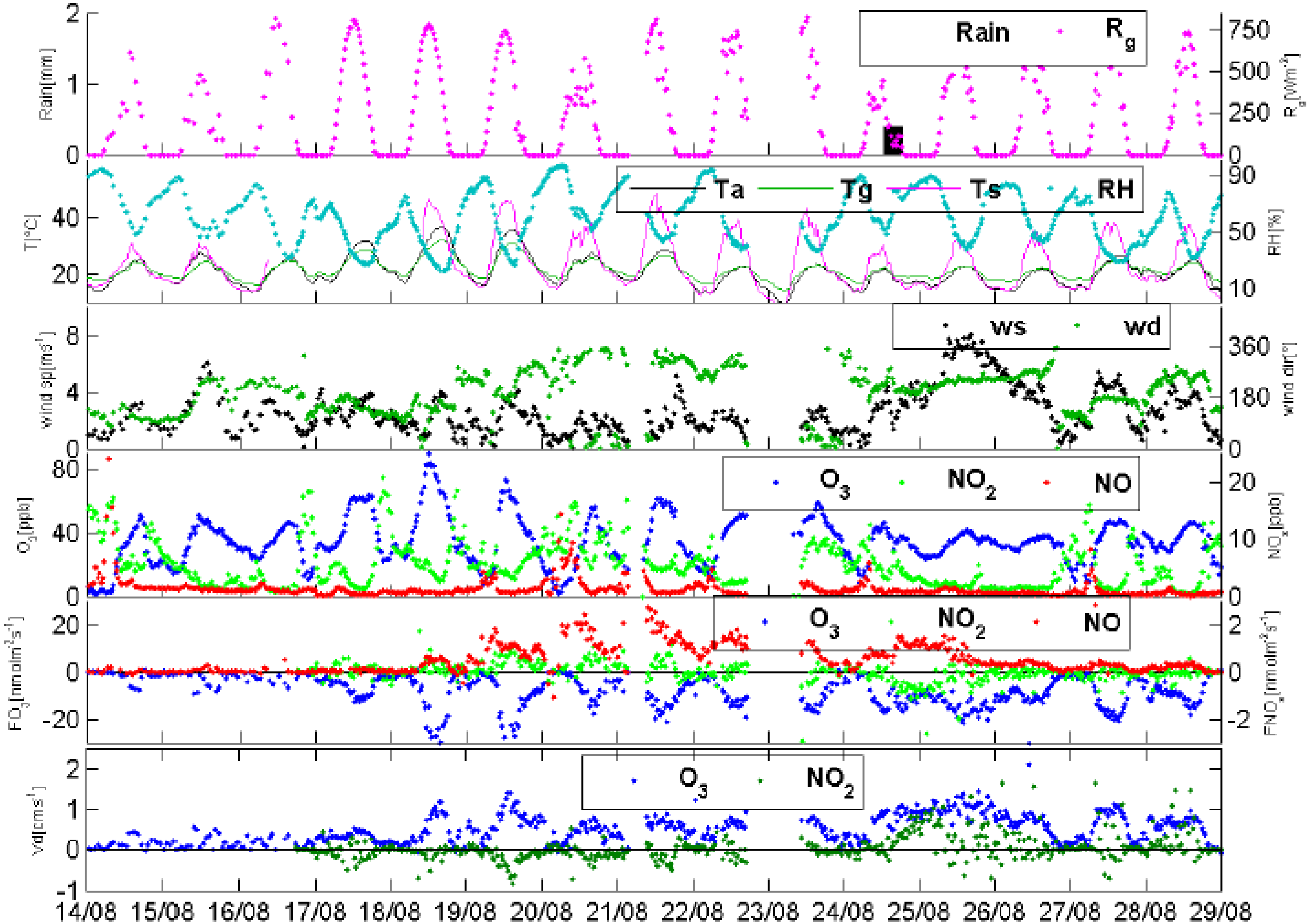
http://www.biogeosciences-discuss.net/bg-2016-199/


Rain
Rg
Rain[mm]
Rg[Wm-2]
Ta
Tg
Ts
RH
T[°C]
RH[%]
ws
wd
wind sp[ms-1]
wind dir[°]
O3
NO2
NO
O3[ppb]
NOx[ppb]
FO3[nmolm-2s-1]
FNOx[nmolm-2s-1]
Vd[cms-1]
14/08
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IN CANOPY LAGRANGIAN STOCHASTIC DISPERSION MODELS

Particle trajectory Differential equation

$$\begin{cases} dw = -w/\tau_L \, dt + b \times d\varepsilon(t) \\ dz = (w - w_s)dt \end{cases}$$

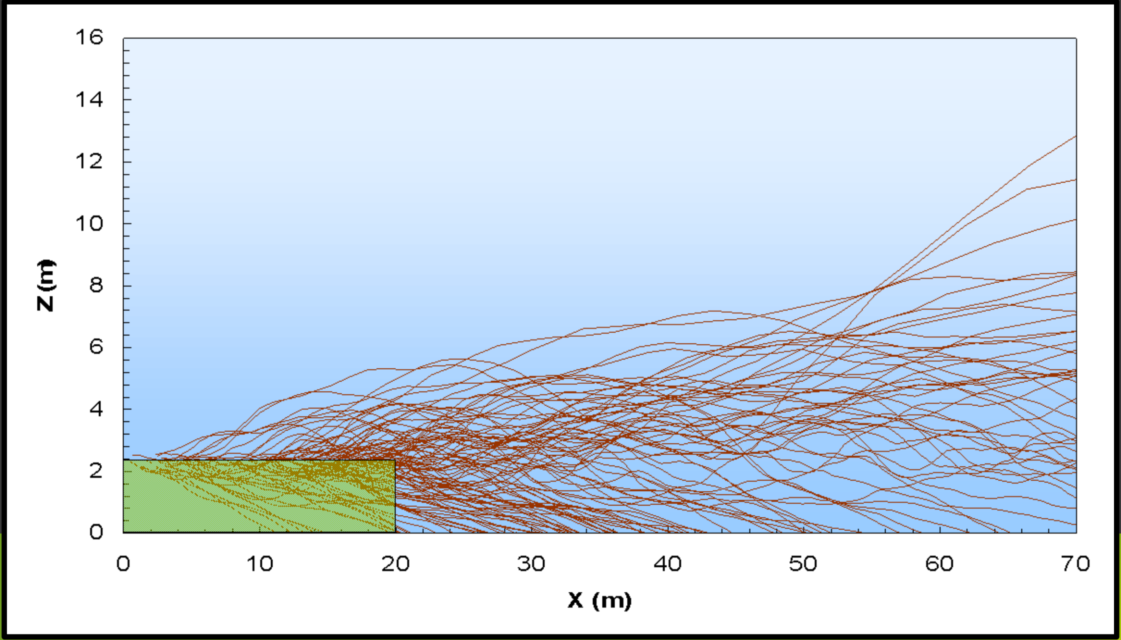
Random acceleration

Vertical wind velocity *w*

Settling velocity

Non-local and non-diffusive transport

Jarosz et al. 2004-2006



IN CANOPY RANDOM WALK MODELS

Particle trajectory Differential equation

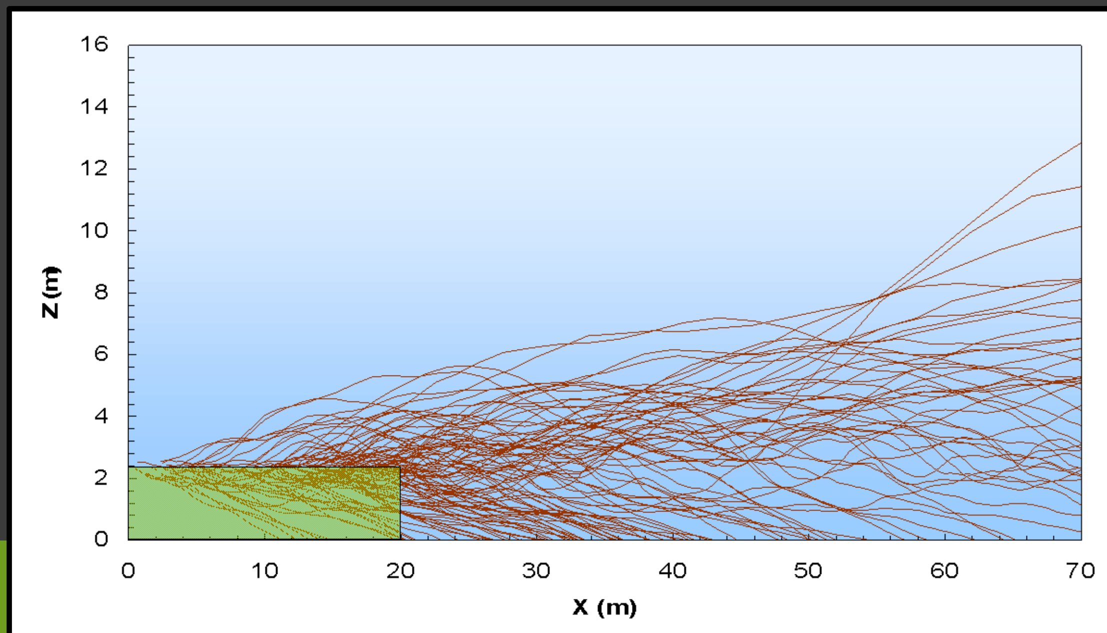
$$dz = (W + dKz / dz)\, dt + (2Kz)^{1/2}\, d\theta z(t)$$

$$dx = (U + dKx / dz)\, dt + (2Kx)^{1/2}\, d\theta z(t)$$

Velocity

Diffusivity

Analog to diffusive transport



Jarosz et al. 2004-2006

RANDOM WALK MODELS

- Differential stochastic equation (DSE)

$$dx = q(\mathbf{x},t)\,dt + d(\mathbf{x},t)\,d\theta(t)$$

$d\theta(t)$ is a Wiener process

$$\begin{cases} \overline{\theta} = 0 \\ \mathrm{var}(\theta) = dt \end{cases}$$

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RANDOM WALK MODELS

What do the different terms mean?

$$dx = q\,(\mathbf{x},t)\,dt + d\,(\mathbf{x},t)\,d\theta\,(t)$$

$$\Rightarrow \quad \overline{\frac{dx}{dt}} = \overline{q(x,t)} + \overline{d(x,t)d\theta(t)}$$

$\overline{q(x,t)}$ = average particle velocity

$\overline{d(x,t)d\theta(t)}$ = dispersion around the mean

RANDOM WALK MODELS FOR PARTICLES

The case of particle transport: accounting for settling and inertia

$$\mathrm{d}Z_\mathrm{p} = (W - V_\mathrm{s})\mathrm{d}t + (2K_\mathrm{p})^{1/2}\mathrm{d}\xi$$

Inertia

$$K_p(z) = \frac{K_{gas}(z)}{\sqrt{1+\left(\frac{1.6 \cdot Vs}{u_*}\right)^2}}$$

Settling

$$V_s^2 = \frac{4gd_\mathrm{p}\rho_\mathrm{p}}{3C_\mathrm{D}\rho_\mathrm{a}}$$

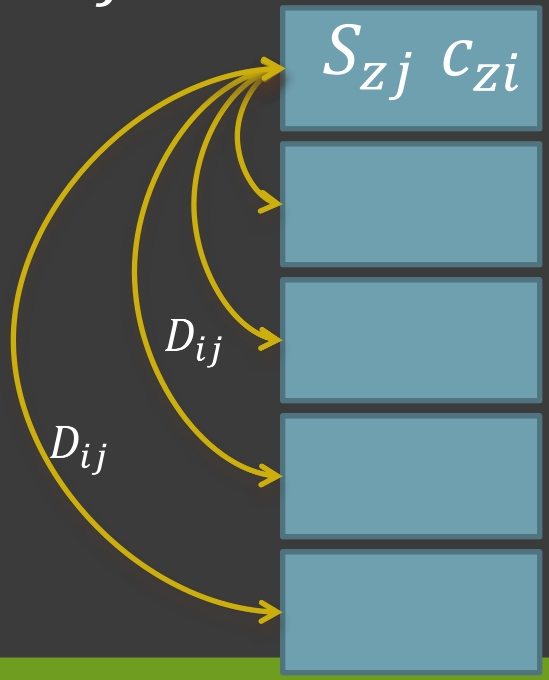
$$C_\mathrm{D} = \frac{24}{Re_\mathrm{p}}\left(1 + 0.158Re_\mathrm{p}^{2/3}\right)$$

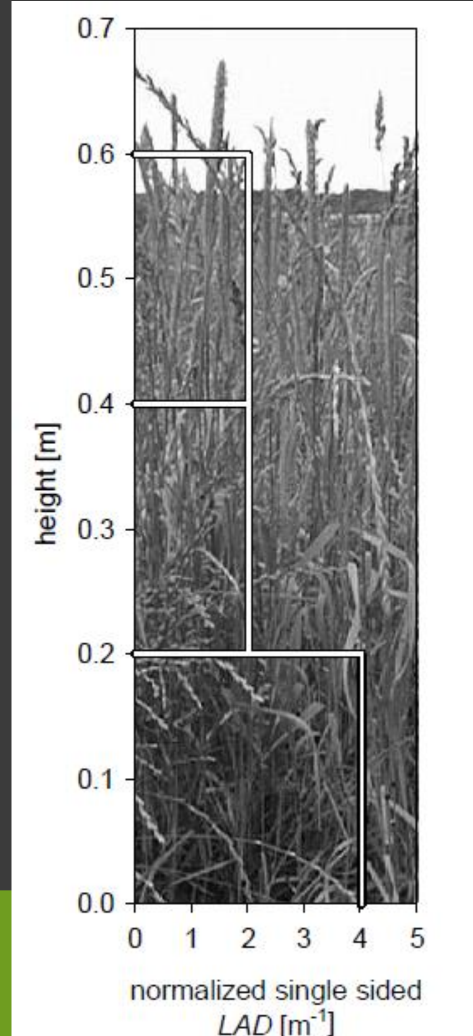
Jarosz et al. 2003

RANDOM WALK MODELS : APPLICATION FOR INFERRING SOURCES IN THE CANOPY

$$c_{zi} - c_{ref} = D_{ij} \times S_{zj}$$

Retreive S_z from c_z implies inverting the equation





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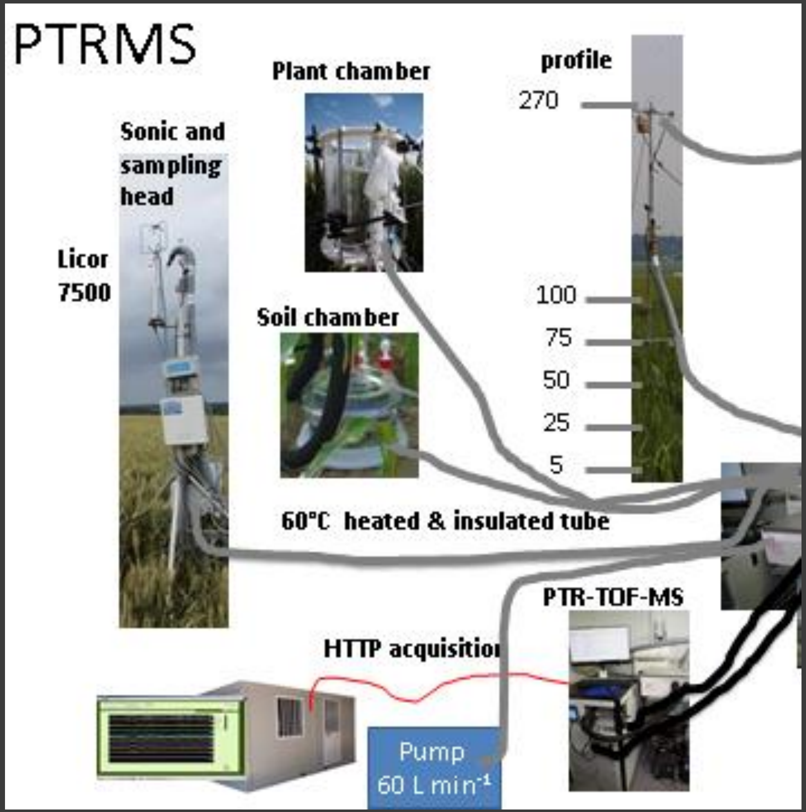
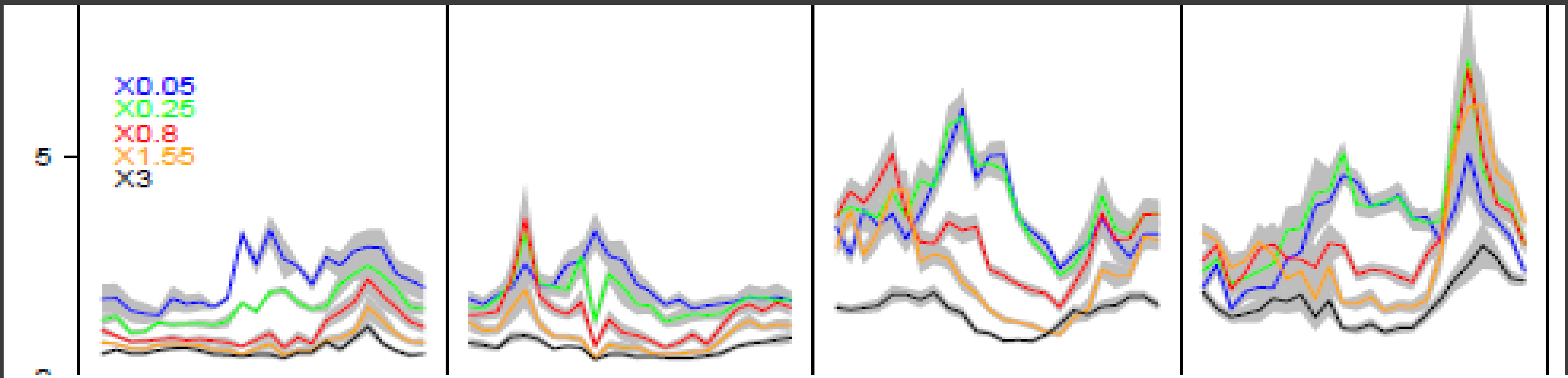
APPLICATION FOR INFERRING SOURCES IN THE CANOPY : EXAMPLE

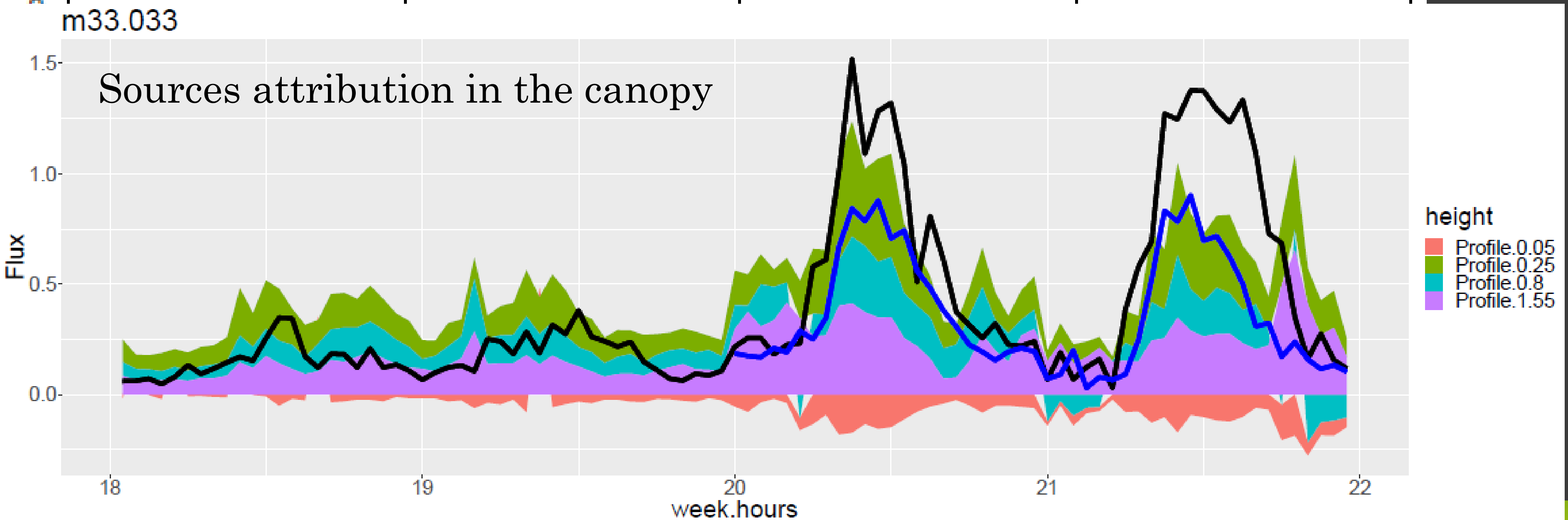


https://www6.inra.fr/cov3er

In canopy concentrations



Sources attribution in the canopy



CONCLUSIONS

- In-canopy turbulence essential for surface-atmosphere transfer
- Non-local transport is an important feature
- Lagrangian stochastic models and LES useful in this context

SUPPORT DE COURS

Site web de l'unité Environnement et Grandes Cultures

http://www6.versailles-grignon.inra.fr/ecosys

(aller dans l'onglet Productions / Cours)

Cours de Denis Baldocchi

@ Nature.berkeley.edu

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RÉFÉRENCES BIBLIO

- Raupach, M.R., 1988. Canopy transport processes. In: W.L. Steffen and O.T. Denmead (Editors), Flow and transport in the natural environment: advances and applications. Springer, Berlin, pp. 95-129.
- Nemitz, E., Sutton, M.A., Schjørring, J.K., Husted, S. and Wyers, G.P., 2000. Resistance modelling of ammonia exchange over oilseed rape. Agric. For. Meteorol., 105(4): 405-425.
- Dupont, S., Brunet, Y. and Jarosz, N., 2006. Eulerian modelling of pollen dispersal over heterogeneous vegetation canopies. Agric. For. Meteorol., 141(2-4): 82-104.
- Jarosz, N., 2003. Etude de la dispersion atmosphérique du pollen de maïs Contribution à la maîtrise des risques de pollinisation croisée. PhD Thesis, Institut National Agronomique Paris-Grignon, Paris, 125 pp.
- Jarosz, N., Loubet, B. and Huber, L., 2004. Modelling airborne concentration and deposition rate of maize pollen. Atmos. Environ., 38(33): 5555-5566.
- Loubet, B., Jarosz, N., Saint-Jean, S. and Huber, L., 2007. A method for measuring the settling velocity distribution of large biotic particles. Aerobiologia, 23(3): 159-169.
- Vuolo, R.M., Loubet, B., Mascher, N., Gueudet, J.C., Durand, B., Laville, P., Zurfluh, O., Ciuraru, R., Stella, P. and Trebs, I., 2017. Nitrogen oxides and ozone fluxes from an oilseed-rape management cycle: the influence of cattle slurry application. Biogeosciences, 14(8): 2225-2244.
- Loubet, B., 2000. Modélisation du dépôt sec d'ammoniac atmosphérique à proximité des sources. Thèse de doctorat Thesis, Université Paul Sabatier, Toulouse. (http://tel.ccsd.cnrs.fr/documents/archives0/00/00/32/50/index_fr.html), 330 pp.

RANDOM WALK MODELS : TO GO BEYOND

Differential stochastic calculation is specific :

« Since the variance of an infinitesimal increase is dt instead of dt^2, this results in a differing differentiation scheme »

$$dg(x,t) = \frac{\partial g}{\partial t}\,dt + q\,\frac{\partial g}{\partial x}\,dt + d\,\frac{\partial g}{\partial x}\,d\theta + \frac{1}{2}\,d^2\,\frac{\partial^2 g}{\partial x^2}\,dt$$

Rodean et al., 1996

RANDOM WALK MODELS : TO GO BEYOND

Calculating a plume width

$$g(x,t) = x^2$$

$$dx^2 = 0 \cdot dt + 2qxdt + 2dxd\theta + d^2dt$$

$$dx^2 = (2qx + d^2)dt + 2dxd\theta$$

$$d\overline{x^2} = \overline{(2qx + d^2)}dt + \overline{2dx} \cdot \overline{d\theta}$$

=0

RANDOM WALK MODELS : TO GO BEYOND

Application to calculating a plume width: σ_x

$$\frac{d\sigma_x^2}{dt} = 2\overline{qx} + \overline{d^2}$$

If no drift

$$\sigma_x^2 = \overline{d^2}t$$

d^2 is hence proportional to a diffusivity

RANDOM WALK MODELS : TO GO BEYOND

Fokker-Planck equation: probability of presence of air parcels

$$dx_i = q_i(\mathbf{x},t)\,dt + d_{ij}(\mathbf{x},t)\,d\theta_j(t)$$

$$\frac{\partial p}{\partial t} = -\frac{\partial q_i p}{\partial x_i} + \frac{1}{2}\frac{\partial^2 d_{ik} d_{jk} p}{\partial x_i \partial x_j}$$

RANDOM WALK MODELS : TO GO BEYOND

Analogy between advection-diffusion equation: identifying q_i et d_{ij}

$$\frac{\partial p}{\partial t} = -\frac{\partial q_i p}{\partial x_i} + \frac{1}{2}\frac{\partial^2 d_{ik} d_{jk} p}{\partial x_i \partial x_j}$$

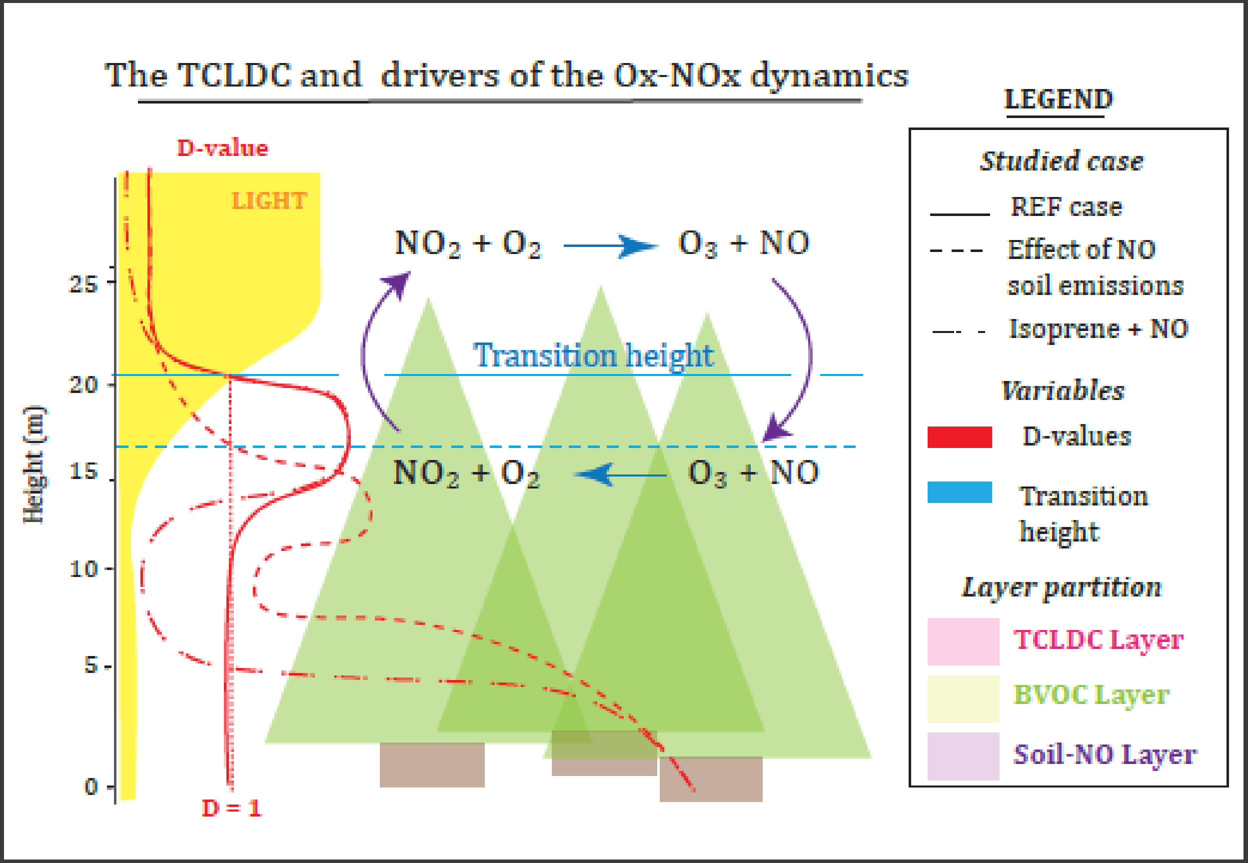
$$\frac{\partial \bar{c}}{\partial t} + \bar{u}_i \frac{\partial \bar{c}}{\partial x_i} = -\frac{\partial K_i c}{\partial x_i} + S(x_i)$$

⇨

$$dz = (W + dKz / dz)\, dt + (2Kz)^{1/2}\, d\theta z(t)$$

$$dx = U\, dt$$

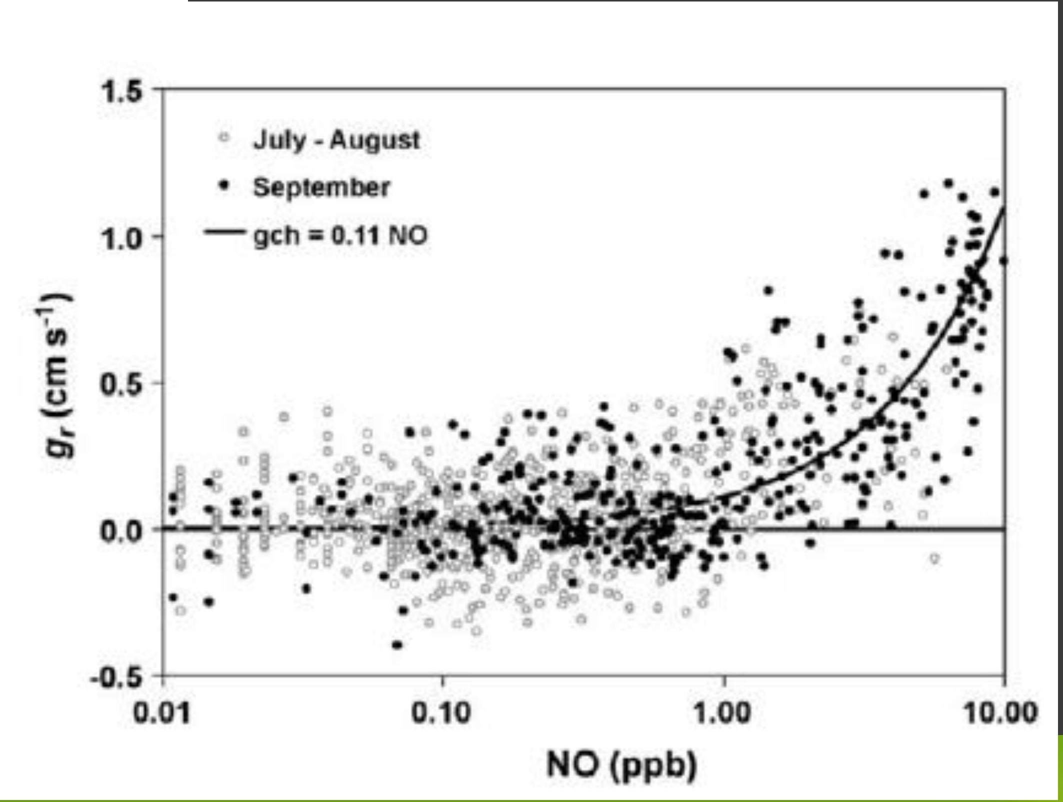
IMPORTANCE OF IN-CANOPY TRANSFER: The role of in-canopy chemistry (NO_2, O_3)



Applying the 1D-ESX model at *Bosco Fontana* (Italy) in order to explore the fate and interaction of NOx and O_3 in the canopy of a Mediterranean deciduous forest

TRANSPORT TIME: EQUIVALENT CONDUCTANCE TO CHEMICAL TRANSFER

$$g_{chem} = h_c / \tau_{chem} = k_r \times [NO] \times h_c$$



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loubet B. (2011)