Incorporation of Tritium Transport Processes into Atmosphere-soil-vegetation Model: SOLVEG

~OBT dynamics in plants using the SOLVEG code after an accidental tritium release~

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Outline of Study

Objectives

- ◻ Development of sophisticated land surface model including radionuclide (Tritium) transport processes
- ◻ Understand and predict behavior of radionuclide at land-surface by numerical experiment

Model development

- ◻ Step 1: Heat and water exchange processes
- ◻ Step 2: Canopy radiation and stomatal resistance → SOLVEG
- ◻ Step 3: CO_2 exchange processes → SOLVEG2

↓

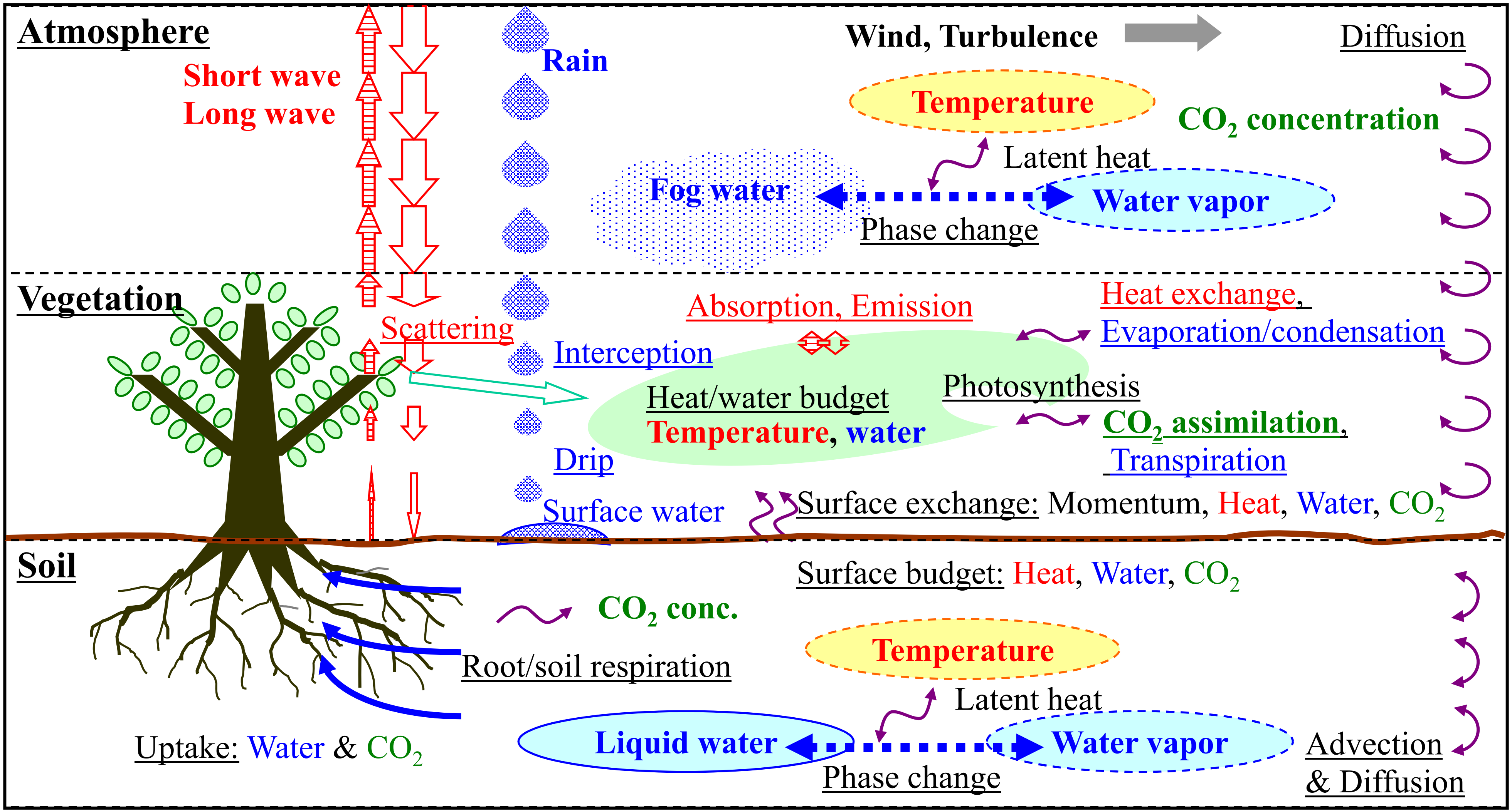
- ◻ EMRAS-II: Radionuclide transport processes (THO, OBT)

Land surface model SOLVEG2

Physical processes

Physical processes are calculated at each layer of vertical multi-layer model

Bold: main var., Underlined: processes, Red: heat/rad., Blue: water, Green: CO_2



Basic equations (1): heat, water, momentum

Atmosphere

Diffusion:
$$\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial z}K_z\frac{\partial\phi}{\partial z} + F_\phi \qquad \phi = u, v, \theta, q_a, e, e\lambda, w_f$$

Boundary condition

Source term

Soil

Heat:
$$\frac{\partial T_s}{\partial t} = \frac{\partial}{\partial z}K_T\frac{\partial T_s}{\partial z} + \frac{H_b}{C_s\rho_s} - \frac{C_w E_w}{C_s\rho_s}\frac{\partial T_s}{\partial z}$$

Liquid water:
$$\frac{\partial \eta_w}{\partial t} = -\frac{1}{\rho_w}\left(\frac{\partial E_w}{\partial z} + E_t + E_b\right)$$

Water vapor:
$$\frac{\partial[(\eta_{ws}-\eta_w)q_s]}{\partial t} = \frac{\partial}{\partial z}D_w f_a(\eta_w)\frac{\partial q_s}{\partial z} + \frac{E_b}{\rho}$$

Evaporation/condensation
$$H_b = -lE_b$$

Transpiration

Vegetation

Heat budget:
$$R_c = H_c + lE_c + H_p \qquad E_c = E_d + E_s$$

Leaf water:
$$\frac{dw_d}{dt} = E_{\text{int}} - E_d + E_{cap} - P_d$$

Water flux:
$$\frac{dP_r}{dz} = a\left(E_{\text{int}} - P_d\right) + E_{pr} - E_{col}$$

Radiation

(Next slide)

Net radiation

Short wave: Downward and upward transfer

Direct (visible + near-infrared) + Diffuse (visible + near-infrared)

Long wave: Downward and upward transfer

Radiation scheme (coefficients based on Verstraete 1987, 1988)

Short: (direct)

$$\frac{dS_d^{\downarrow}}{dz} = \left(aF_{rd} + a'_w + A'_w\right)S_d^{\downarrow},$$

⇩ (diffuse)

(visible)

(near-IR)

$$\frac{dS_s^{\downarrow}}{dz} = \left[aF_{rs}\left(1 - f_{sf}\right) + a'_w + A'_w\right]S_s^{\downarrow} - \left(aF_{rs} f_{sb} + A'_w\right)S_s^{\uparrow} - aF_{rd} f_{df} S_d^{\downarrow},$$

$$\frac{dS_s^{\uparrow}}{dz} = -\left[aF_{rs}\left(1 - f_{sf}\right) - a'_w + A'_w\right]S_s^{\uparrow} + \left(aF_{rs} f_{sb} + A'_w\right)S_s^{\downarrow} + aF_{rd} f_{db} S_d^{\downarrow}.$$

Scattering

Leaf projection cf.: F_{rd}

Scattering cf.:

f_{df} (forward),

f_{db} (backward)

Depend on solar angle and leaf surface angle

Long wave:

$$\frac{dL^{\downarrow}}{dz} = aF_{rs}\left[\left(1 - f_{sf}\right)L^{\downarrow} - f_{sb}L^{\uparrow} - \varepsilon_c \sigma T_c^4\right] + k_l w_l \left(L^{\downarrow} - \sigma T_a^4\right),$$

$$\frac{dL^{\uparrow}}{dz} = -aF_{rs}\left[\left(1 - f_{sf}\right)L^{\uparrow} - f_{sb}L^{\downarrow} - \varepsilon_c \sigma T_c^4\right] - k_l w_l \left(L^{\uparrow} - \sigma T_a^4\right).$$

Leaf projection cf.: F_{rs} Forward scattering cf.: f_{sf} Back scattering cf.: f_{sb}

Depend on leaf area density └Depend on leaf surface angle┘

Basic equations (3): CO_2, stomata resistance

CO_2 assimilation (A_n): Farquhar et al. (1980)

$$A_n = \min(w_c, w_e, w_s) - R_d$$

w_c, w_e, w_s, R_d : Depend on PAR, leaf CO_2 conc., temperature

Stomatal resistance (r_s): Collatz et al. (1991, 1992)

$$\frac{1}{r_s} = g_s = m \frac{A_n}{c_s} \frac{e_s}{e_{sat}(T_v)} p_a + b$$

m **(constant),** ***b*** **(minimum conductance)** ⇒ measured parameter

c_s	CO_2 partial pressure at leaf surface
$e_s/e_{sat}(T_v)$	Relative humidity at leaf surface
p_a	Atmospheric pressure

CO_2

2 options

No CO_2

Stomatal resistance (Jarvis scheme): BATS (Dickinson et al. 1993)

$$r_s = r_{s,\min} f_r f_s^{-1} f_m^{-1} f_t^{-1}$$

$\boldsymbol{r_{s,min}}$ ⇒ measured parameter

f_r, f_s, f_m, f_t : Functions of PAR, soil water, humidity, temperature

Basic equations (4): soil CO_2

Soil CO_2 conservation: Simunek and Suarez (1993)

$$\frac{\partial}{\partial t}V_E c_a = \frac{\partial}{\partial z}D_E\frac{\partial c_a}{\partial z} - \frac{\partial}{\partial z}E_E^* c_a - E_t^* K_H RTc_a + S$$

Volume: $V_E = (\eta_{ws} - \eta_w) + K_H RT\eta_w$,

Diffusion: $D_E = (\eta_{ws} - \eta_w)D_a + K_H RT\eta_w D_w$,

Advection: $E_E^* = E_a^* + K_H RTE_w^*$,

⇒ Treatment of CO_2 in gas and aqueous phase together by Henry's Law: $c_w = K_H RTc_a$

c_a CO_2 conc. in soil air

η_w Volumetric water content

E_t^* Root uptake (transpiration)

S CO_2 source term (= soil: S_s + root: S_r)

$$S_s = S_{s0}f_s(z)f_s(\eta_w)f_s(T)f_s(c_a)f_s(t)$$

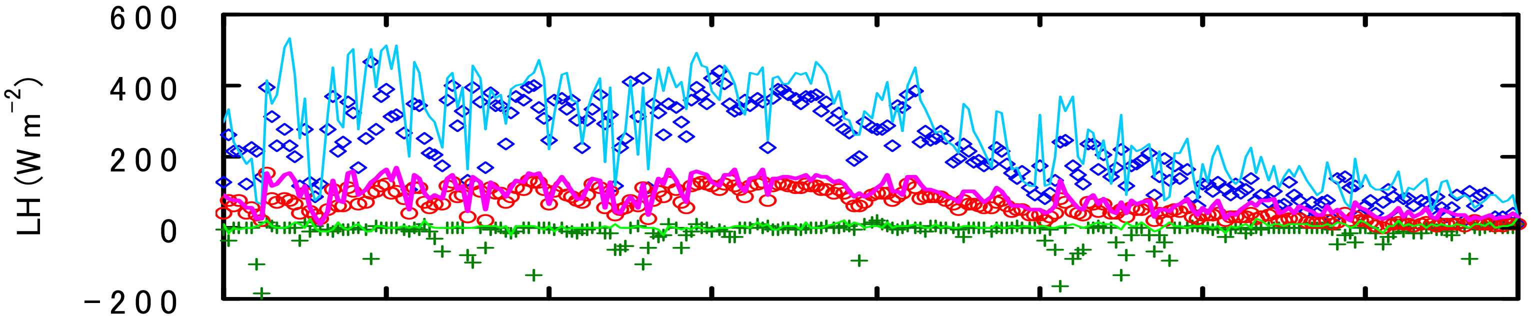
$$S_r = S_{r0}f_r(z)f_r(\eta_w)f_r(T)f_r(c_a)f_r(t)$$

Land surface model SOLVEG2

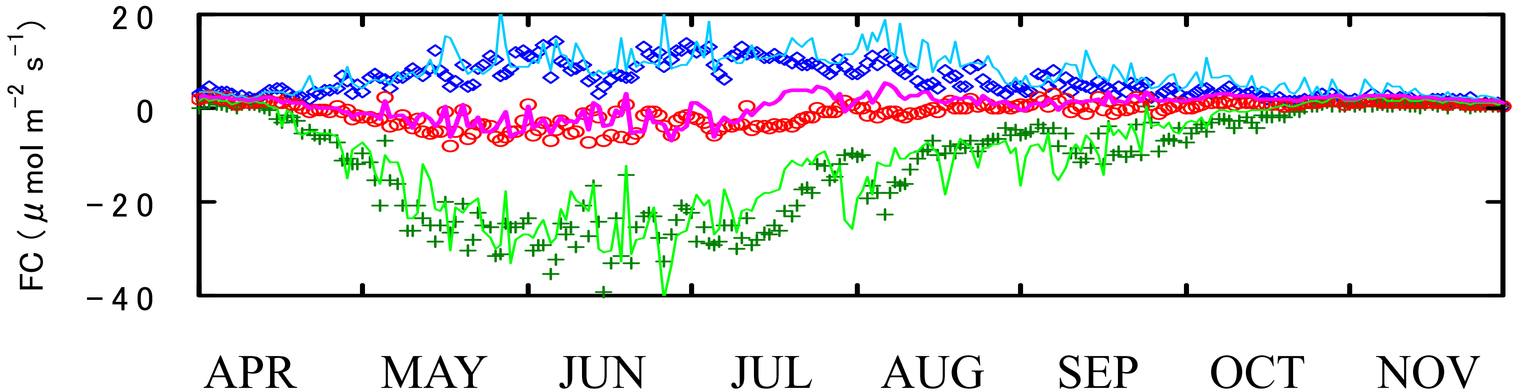
Water and CO_2 fluxes at grassland

- **Good performance for water and CO_2 exchanges at grassland (AmeriFlux data)**
  Diurnal variation and seasonal change are well reproduced.
  → It can be applied for detailed simulation of ^{3}H and ^{14}C transport.

Latent heat (water vapor) flux



CO_2 flux



Observation
○: daily mean
◇: daily max
+: daily min

Calculation
—: daily mean
—: daily max
—: daily min

Upward positive

Land surface model SOLVEG2

Incorporation of HTO transport processes

Concept

- Process based HTO transport model to simulate dynamic behavior of HTO in air-soil-plant system
- Explicit calculation of HTO transport in a similar way as water and vapor transport

Model development

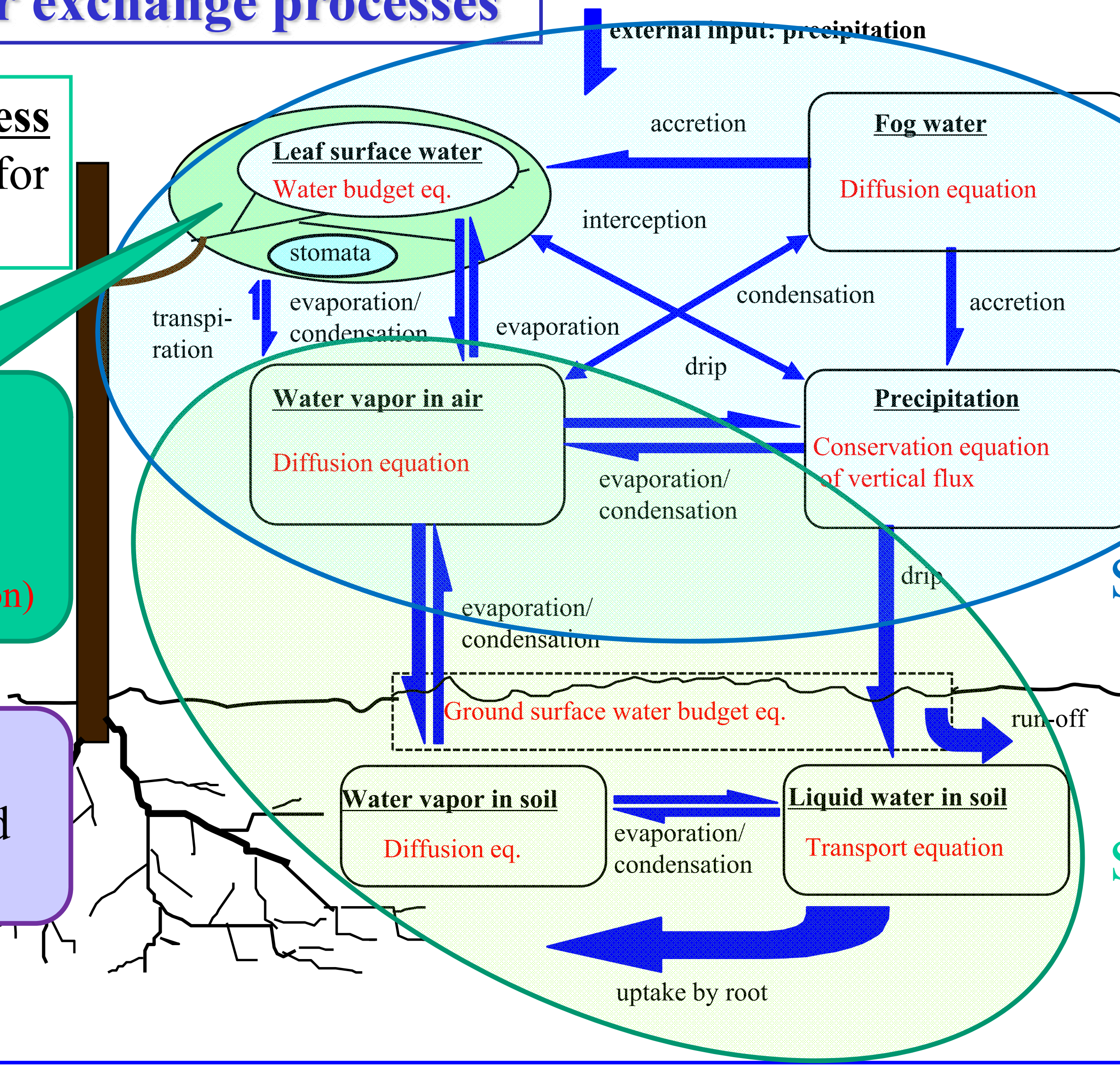
- Step 1: transport in the atmosphere and bare soil (no decay)
  - In-soil transport by Yamazawa (2001) applied for BIOMASS Theme 3-F (rise of HTO from contaminated groundwater)
  - Atmospheric transport for HTO vapor (1-D diffusion eq.)
  - Test calculation using met. data of AmeriFlux (previous slide)
- Step 2: inclusion of plant uptake processes
- Step 3: OBT formation and translocation

Land surface model SOLVEG2

Incorporation of HTO transport processes

Water and vapor exchange processes

HTO transport process
Calculate HTO conc. for each variable of water



New variable:
Plant water
Water budget eq.
(root uptake - transpiration)

Step 3
OBT formation and translocation

Land surface model SOLVEG2

In-soil HTO transport processes

Soil HTO transport: Yamazawa (2001) applied for BIOMASS theme 3

Liquid phase:
$$\frac{\partial}{\partial t}\eta_w \chi_w = -\frac{1}{\rho_w}\frac{\partial}{\partial z}E_w \chi_w + \frac{\partial}{\partial z}\left(D_{Tw}\frac{\partial \chi_w}{\partial z}\right) - e_b$$

Gas phase:
$$\frac{\partial}{\partial t}\left[(\eta_{ws} - \eta_w)\chi_{sa}\right] = \frac{\partial}{\partial z}\left[D_{Ta} f_{sa}(\eta_w)\frac{\partial \chi_{sa}}{\partial z}\right] + e_b$$

+: evaporation
-: Condensation

Surface B.C.:
$$-D_{Ta} f_{sa}(\eta_{w0})\frac{\partial \chi_{sa}}{\partial z}\bigg|_{z=0} + e_{b0} = c_{E0}|\mathbf{u}_r|(\chi_{sa0} - \chi_r)$$

Atmosphere-land exchange

χ_w, χ_{sa} , χ_r	HTO conc. in soil water (Bq/m^3-water), soil air and air (Bq/m^3-air)
η_w, η_{sw}	Volumetric soil water content and saturated value (m^3/m^3)
ρ_w	Density of soil water (kg/m^3)
E_w	Vertical liquid water flux (kg/m^2/s)
D_{Tw}, D_{ta}	Effective diffusivities of HTO in water and HTO vapor in air (m^2/s)
$f_{sa}(\eta_w)$	Tortuosity for diffusion in soil air
e_b	HTO conc. in soil air (Bq/m^3-air)
c_{E0}, $\lvert\mathbf{u}_r\rvert$	Bulk transfer coefficient for evaporation, wind speed (m/s)

HTO budget in leaf

HTO budget: $$\frac{\partial}{\partial t}\eta_v \chi_v = E_{stom} + E_{root} - E_{phot} + E_{res}$$

Stomata uptake: $$E_{stom} = \frac{1}{r_a + r_s}\left\{\chi_a - q_{sat}(T_c)\frac{\rho_a}{\rho_w}\chi_v\right\}$$

Root uptake: $$E_{root} = \int_0^{z_{btm}} E_r(z_s) f_{root}(z_s, z)\, dz_s$$

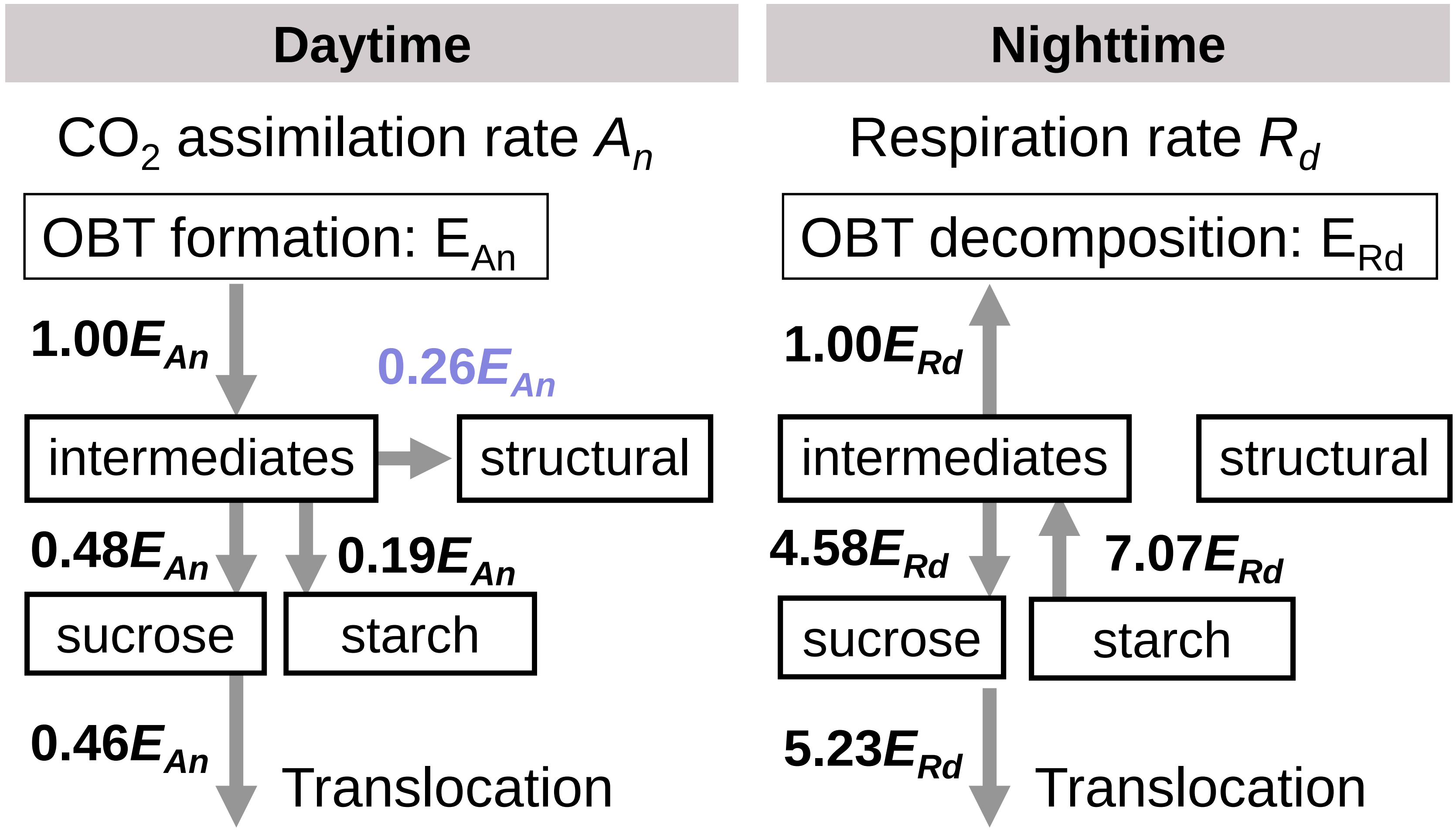
OBT formation: $$E_{phot} = \frac{\chi_v}{\rho_w} m_w A_g$$ (proportional to CO_2 assimilation rate)

OBT decomposition: $$E_{res} = S_{\mathrm{int}} m_{glu} \frac{1}{6} R_d$$ (proportional to respiration rate)

χ_v , χ_a	HTO conc. in leaf water (Bq/m^3-water) and air (Bq/m^3-air)
η_v	Leaf water content in unit leaf area (m^3/m^2)
r_a , r_s	Resistances (s/m) of leaf boundary layer and stomata
$q_{sat}(T_c)$	Saturated specific humidity (kg/kg) at leaf temperature (T_c)
ρ_a, ρ_w	Density of air and water (kg/m^3)
E_r	Root uptake rate of HTO ($Bq/m^3/s$)
$f_{root}(z_s,z)$	Distribution function of root uptake water
m_w , m_{glu}	Weight of 1 mol water and glucose (kg/mol)
A_g , R_d	Gross CO_2 assimilation rate and respiration rate (mol-CO_2/m^2/s)
S_{int}	OBT amount in intermediate pool (Bq/kg)

OBT formation and translocation

Carbohydrate formation and translocation processes
based on experimental result (Fondy & Geiger 1982)



Land surface model SOLVEG2

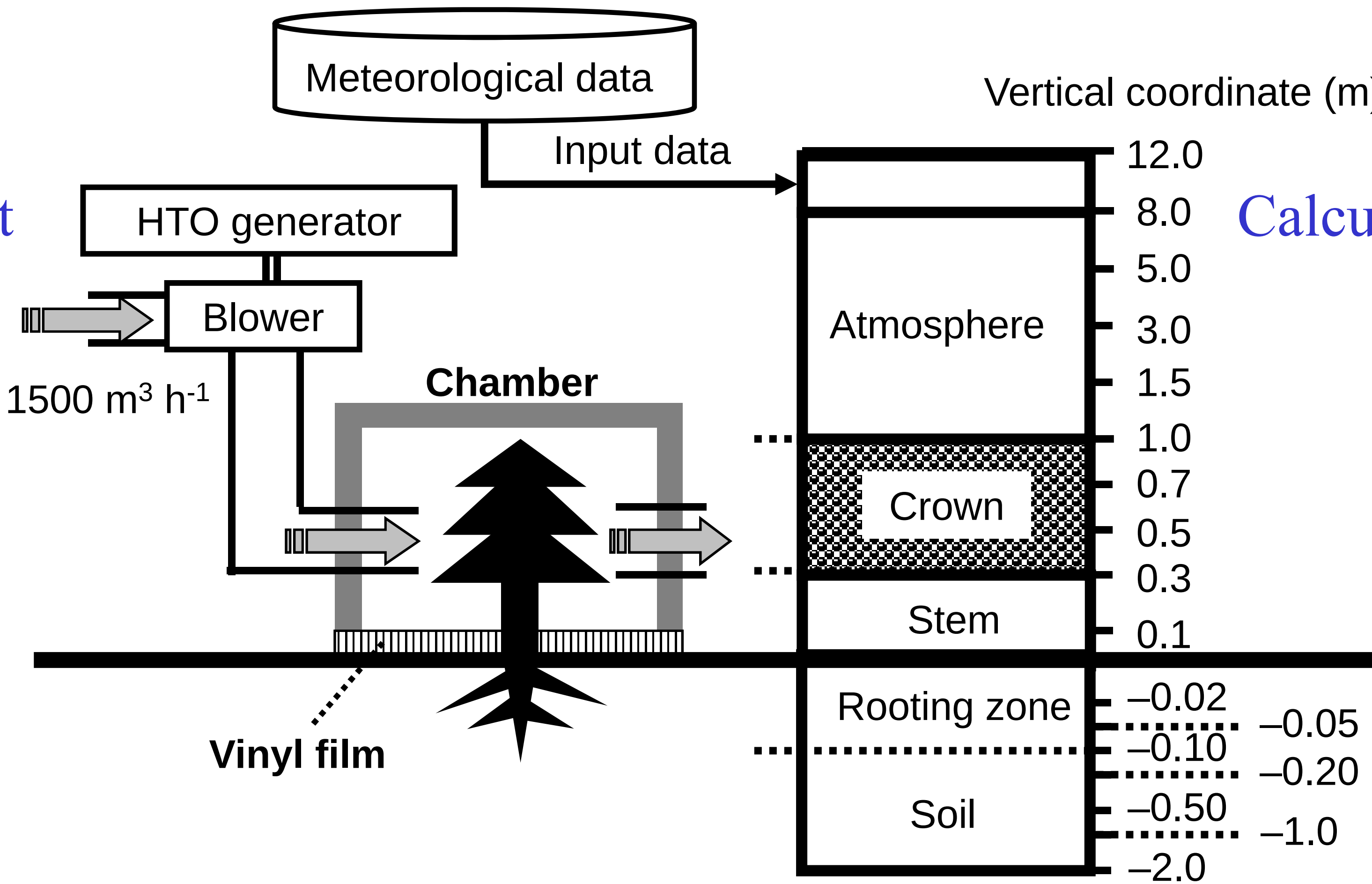
Test calculation

[Calculation setting]

- **Experiment: HTO exposure to blooming vine at Cadarache (Guenot and Belot 1984)**
- **Comparison with measurement of TWFT concentration and OBT amount in leaf**

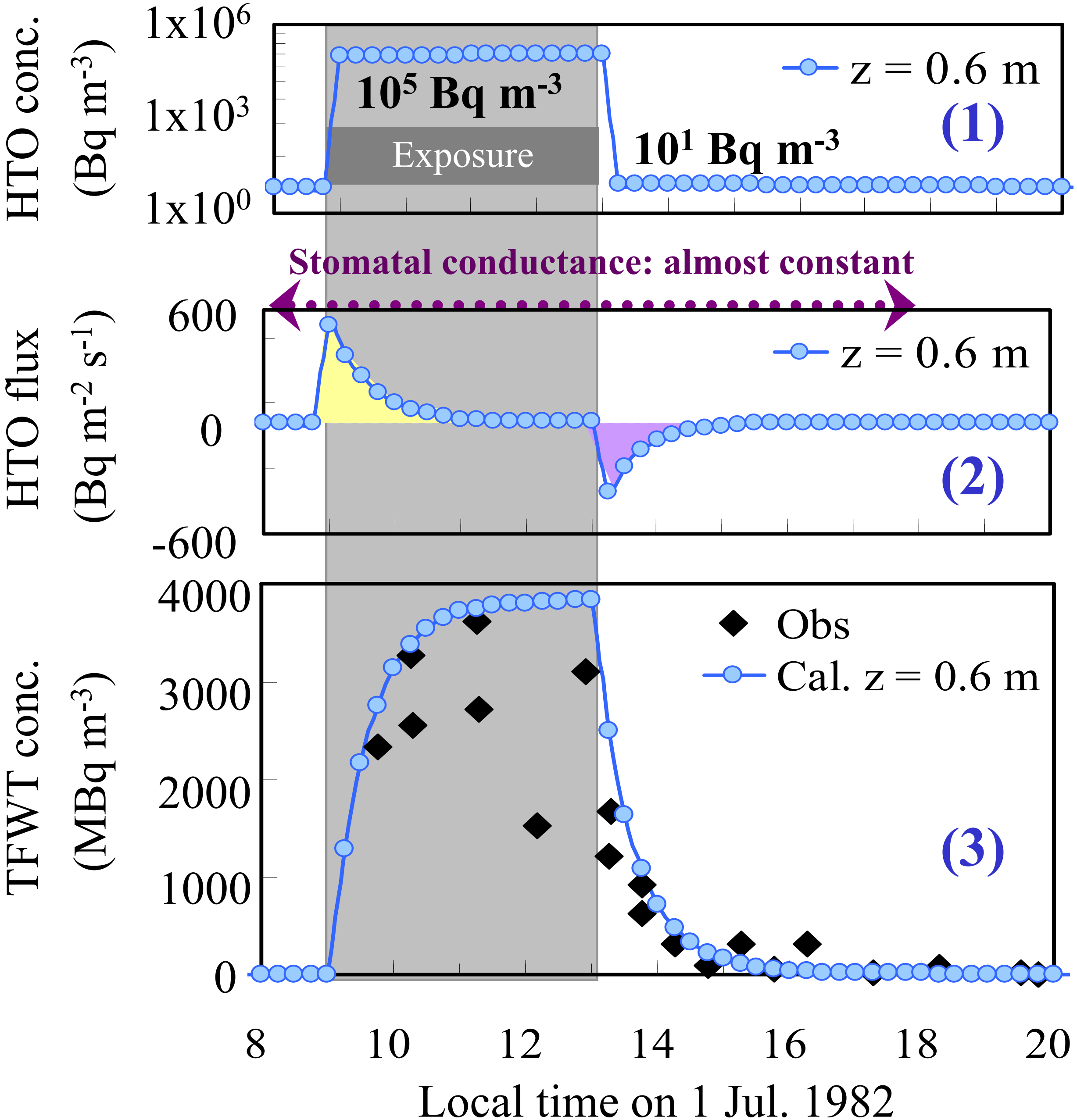
Experiment

HTO exposure from 09 to 13 LST



Calculation

TFWT concentration Cal. & Obs.



(1) Air HTO conc. (input)

(2) HTO flux

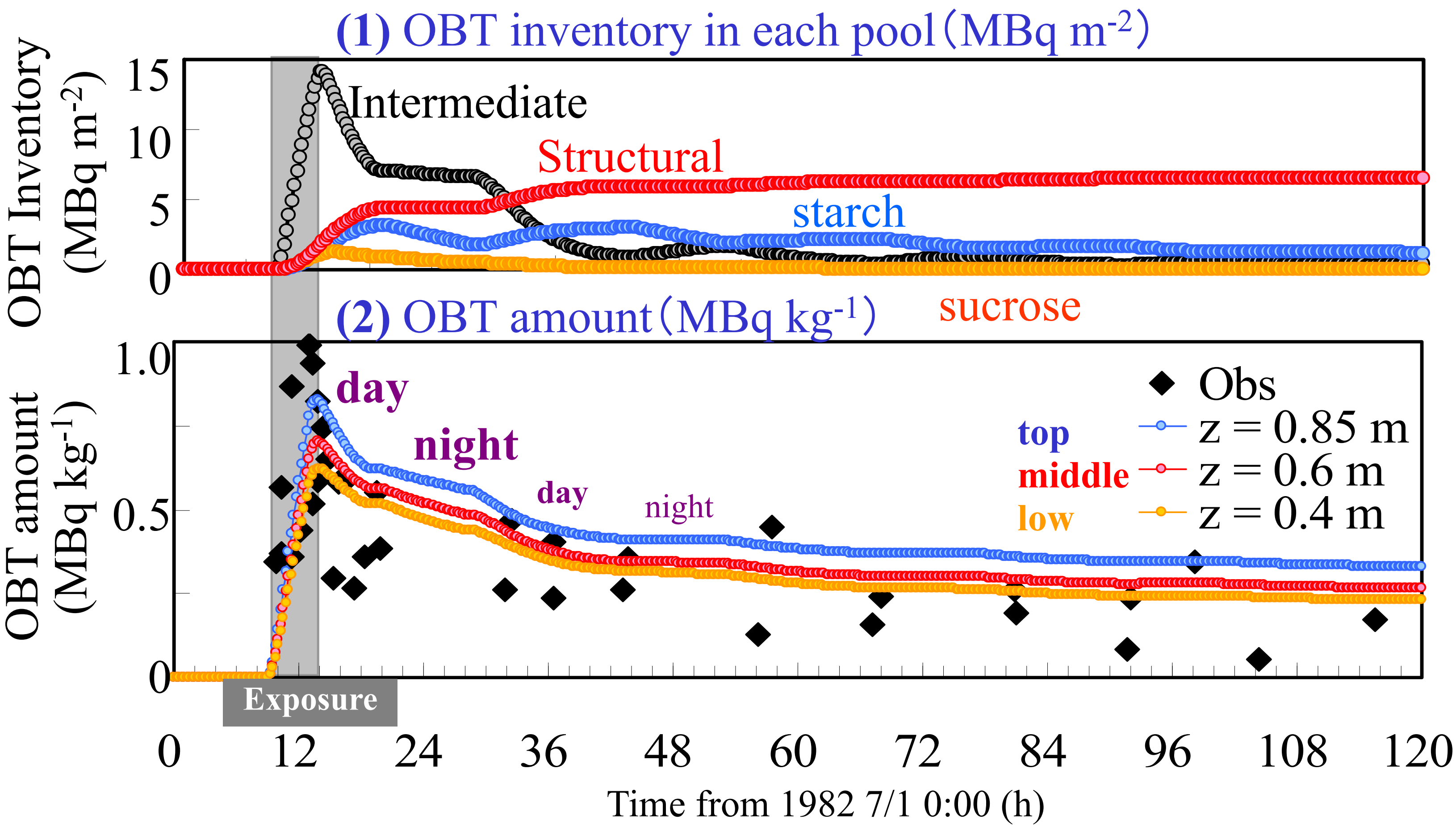
- Exposure start: Air→Leaf
- Exposure end: Leaf→Air

(3) TFWT conc.

- Come to equilibrium several hours after start/end of exposure

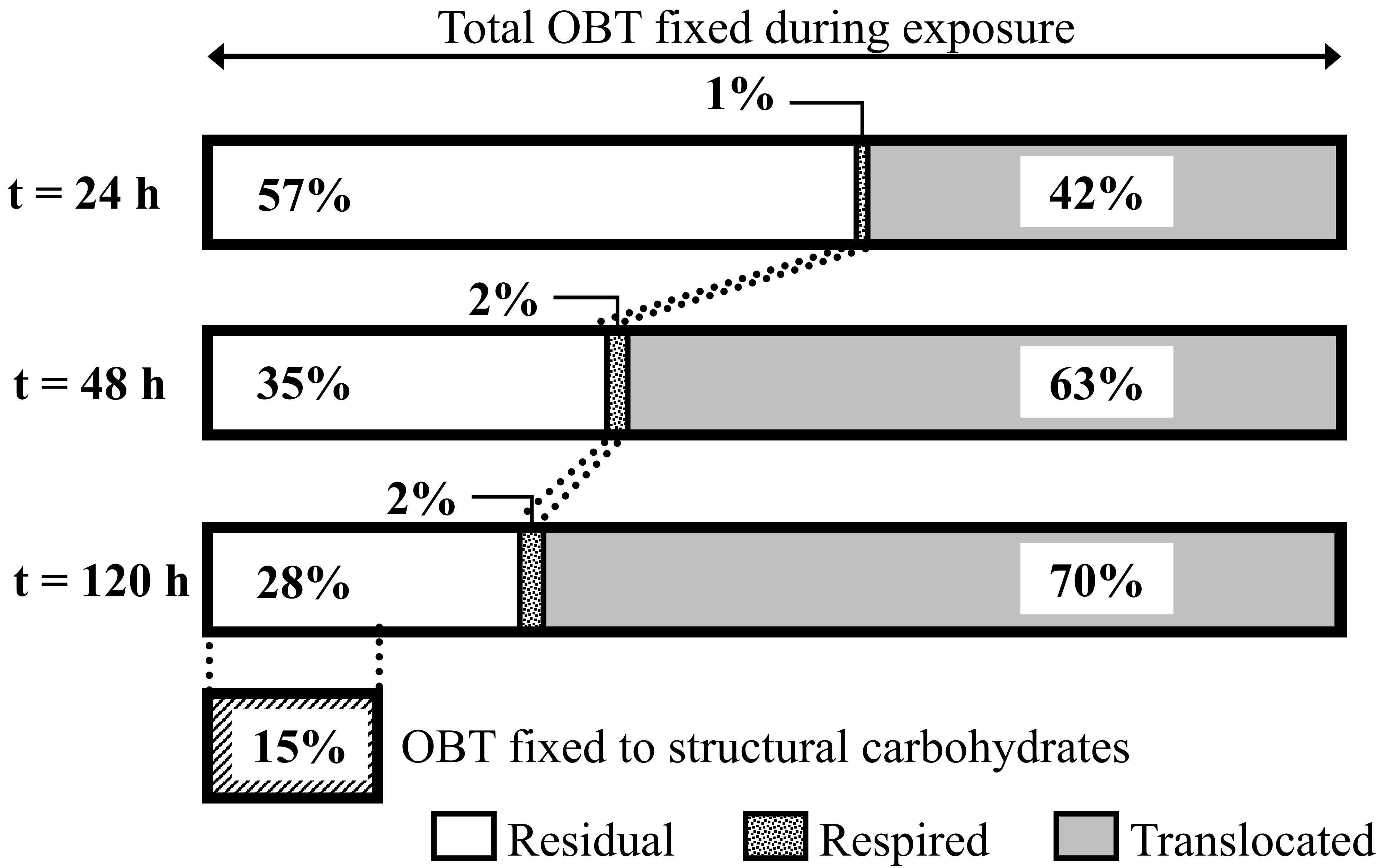
TFWT conc.: Cal. / Obs.	
9–13 h period	**1.3** (n = 8)
13–120 h period	**0.5** (n = 30)

OBT amount in leaf Cal. & Obs.



	OBT : Cal. / Obs.
9–13 h period	**0.6** (n = 8)
13–120 h period	**1.4** (n = 30)

Fate of OBT generated in leaf



Incorporation of HTO transport into SOLVEG

- Process based HTO transport model to simulate dynamic behavior of HTO in air-soil-plant system
- Explicit calculation of HTO transport in a similar way as water and vapor transport
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- Test using experimental data at Cadarache (Guenot and Belot 1984)

  Calculated results seem to be reasonable.

➔ Submitted to JER:

Masakazu Ota and Haruyasu Nagai, "Development and validation of a dynamical atmosphere–vegetation–soil HTO transport and OBT formation model"