EXCHANGE VELOCITY APPROACH AND OBT FORMATION IN PLANTS DURING THE DAYTIME

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Driving equation for the HTO transfer from atmosphere to leaves:

\[
\frac{dC}{dt} = \frac{V_{\text{exc}}}{M_w} (C_{\text{air}} - 0.91 \rho_s C) + \frac{V_{\text{exc}}}{M_w} (\rho_s - \rho) C_s
\]

- used for all canopy, ignoring the transfer of air HTO to steam, because the exchange velocity is smaller with one order of magnitude;
- ignores the initial diffusion of leaf water to steam.

The tritium dynamics at soil surface:

\[
\frac{dC_{\text{sw,1}}}{dt} = \frac{V_{\text{ex,s}}}{M_{\text{ws}}} (C_{\text{air}} - 0.91 \rho_{\text{sat}}(T_s) C_{\text{sw,1}}) - DF
\]

- depends on soil resistance.

Symbols:
- \(C\) – HTO concentration in plant water (Bq/kg);
- \(C_{\text{air}}\) – HTO concentration in air (Bq/m³);
- \(C_s\) – HTO concentration in the sap water (Bq/kg);
- \(\rho_s\) – saturated air humidity at vegetation temp. (kg/m³);
- \(\rho\) – air humidity at reference level (kg/m³);
- \(M_w\) – water mass in plant on a unit soil surface (kg/m²);
- \(V_{\text{exc}}\) – exchange velocity from atmosphere to canopy (m/s)
- \(M_{\text{ws}}\) – water mass in the surface soil layer;
- \(DF\) – HTO net flux at the bottom interface of the first soil layer.
SIMPLIFIED EQUATION FOR TRITIUM TRANSFER BETWEEN AIR AND PLANTS

If $C_{\text{air}} = ct$ and $V_{\text{exc}} = ct$ and ignoring the soil tritium transfer, a simple equation is obtained:

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

$C_{\text{TFWT}}$ - HTO concentration in plant at the considered time $t$ (Bq L\(^{-1}\));
$C_{\infty}$ - steady-state TFWT concentration (Bq L\(^{-1}\));
$k$ - constant rate for HTO uptake (h\(^{-1}\));
$t$ - time after the beginning of exposure (h);

$$C_{\infty} = \frac{1.1 \cdot \rho_a}{\rho_s C_{\text{ah}}}$$

$\rho_s$ - water vapour density in leaf stomatal pore (g /m\(^3\));
$\rho_a$ - the water vapour density in atmosphere (g /m\(^3\));
$C_{\text{ah}}$ is the air water HTO concentration (Bq/L);

$$k = \frac{\rho_s}{1.1 \cdot W \cdot r}$$

$W$ - water content of leaf (g /m\(^2\));
$r$ - leaf resistance to water transport (h/m);

The above relationships were used to explain the experimental data for various plants and environmental conditions.
Large variability between plants and environmental conditions → Need to consider the variability of exchange velocity

Table 2 Rate constant (k) and steady state concentration ratio ($C_{R_{\text{max}}}$) of D$_2$O uptake from air to vegetation

<table>
<thead>
<tr>
<th></th>
<th>Daytime release</th>
<th>Nighttime release</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$k$ (hr$^{-1}$)</td>
<td>$C_{R_{\text{max}}}$</td>
</tr>
<tr>
<td>Rice plant leaf</td>
<td>2.384±0.965</td>
<td>0.541±0.022</td>
</tr>
<tr>
<td>Unhulled rice</td>
<td>0.636±0.124</td>
<td>0.217±0.010</td>
</tr>
<tr>
<td>Rice plant leaf (flooding)</td>
<td>2.269±0.760</td>
<td>0.440±0.016</td>
</tr>
<tr>
<td>Unhulled rice (flooding)</td>
<td>0.378±0.072</td>
<td>0.216±0.014</td>
</tr>
<tr>
<td>Soybean leaf</td>
<td>2.951±1.668</td>
<td>0.562±0.022</td>
</tr>
<tr>
<td>Soybean pea</td>
<td>0.230±0.375</td>
<td>0.273±0.224</td>
</tr>
<tr>
<td>Soybean hull</td>
<td>0.069±0.083</td>
<td>0.534±0.510</td>
</tr>
</tbody>
</table>

$C_{R_{p}} = C_{R_{\text{max}}}(1-e^{-kt})$

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

<table>
<thead>
<tr>
<th></th>
<th>Daytime release</th>
<th>Nighttime release</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$k$ (hr$^{-1}$)</td>
<td>$t_{1/2}$ (hr)</td>
</tr>
<tr>
<td>Rice plant leaf</td>
<td>1.155±0.204</td>
<td>0.6</td>
</tr>
<tr>
<td>Unhulled rice</td>
<td>0.452±0.087</td>
<td>1.5</td>
</tr>
<tr>
<td>Rice plant leaf (flooding)</td>
<td>1.041±0.212</td>
<td>0.7</td>
</tr>
<tr>
<td>Unhulled rice (flooding)</td>
<td>0.388±0.087</td>
<td>1.8</td>
</tr>
<tr>
<td>Soybean leaf</td>
<td>1.058±0.155</td>
<td>0.7</td>
</tr>
</tbody>
</table>

$^*$, $C_{p} = C_{0}e^{-kt}$

Large variability between plants and environmental conditions → Need to consider the variability of exchange velocity
Resistance Approaches for Deposition and Exchange

- Similitude between water vapour transport and electric circuits → in both cases the transport is due to specific gradients:
  - specific humidity for water
  - electric potential for electricity

- Environmental resistances - analogy with electric resistances → both = the ratio between potential difference and flux

- $R_a$ - turbulence and wind speed

- $R_b$ - turbulence, wind speed and surface properties

- Total surface resistance $R_c$ - split up into canopy and ground related resistance

- Canopy resistance - surface properties, temperature, PAR, humidity, water content in soil

- HT deposition → ground resistance depends on the rates of diffusion and oxidation in soil;
  - much lower than the canopy resistance

\[
V_{ex} = \frac{1}{R_a + R_b + R_c}
\]

exchange velocity at air to plant (soil) interface
Turbulent eddies - responsible for transporting material through the surface boundary layer

Transport processes:
- transfer of heat
- mass
- momentum

modify the atmosphere's properties

Distinct aspect of the boundary layer → turbulent nature

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**

Momentum must be transferred downward.

**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
- **z₀** – **roughness parameter** = 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** = 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.
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.

Turbulent eddies - responsible for transporting material through the surface boundary layer;

\( R_a \) - determines the rate that momentum, and other scalars, are transported between a given level in the atmosphere and the vegetation’s effective surface sink.

\[ R_a = \frac{1}{k u^*} \ln \frac{z - d}{z_o} - \psi_c \]

\( \psi_c \) - adiabatic correction function

Boundary layer = that thin skin of unperturbed air which surrounds the surface of soil or vegetation

\[ R_b = \frac{1}{k u^*} \ln \frac{z_o}{z_c} = \frac{const}{k u^*} (S_c / Pr)^{2/3} \]

\( z_c \) - scalar roughness length;

\( S_c \) - Schmidt number;

\( Pr \) – Prandtl number;

const - often assumed to be 2 over closed canopies, but it can be much larger over rough incomplete canopies.
$R_a$, $R_b$ - affected by wind speed, crop height, leaf size, and atmospheric stability; 
- decrease with the increasing of wind speed and crop height

- Smaller resistances
  - over the tall forests than over short grass;
  - under unstable atmospheric thermal stratification, than under neutral and stable stratification

- For wind speed = 4 m s$^{-1}$ →
  
  $R_b = \begin{cases} 
  60 \text{ s m}^{-1}, & \text{for 0.1 m tall grass} \\
  20 \text{ s m}^{-1}, & \text{for 1.0 m crop} \\
  10 \text{ s m}^{-1}, & \text{for 10 m conifer forest} 
  \end{cases}$

- $R_a, R_b < 20 \text{ s m}^{-1}$ - during the daytime over a temperate deciduous forest (exp. results)
- $R_a \geq 150 \text{ s m}^{-1}$ – during the night time (turbulent mixing is reduced)

$R_a, R_b \div 4 - 18 \text{ s m}^{-1}$
$R_c \div 70 - 160 \text{ s m}^{-1}$
Canopy resistance \((R_C)\)

- \(R_c\) - function of:
  - canopy stomatal resistance \((R_{stom})\)
  - canopy cuticle resistance \((R_{cuticle})\)
  - soil resistance \((R_{soil})\)

- \(R_{stom}\), \(R_{cuticle}\), \(R_{soil}\) act in parallel:

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

- ‘Big-Leaf’ resistance models - 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

affected by:
- leaf area;
- stomatal physiology;
- soil pH;
- presence and chemistry of liquid drops and films
Stomatal cavity → common pathway for water and CO$_2$
Leaf = $\Sigma$ stomata

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

- $E$ – evaporation
- $\rho_a$ – air density
- $q_{in}$ – saturated air vapour at leaf temp.
- $q_{air}$ – air vapour in atmosphere

Scalling from leaf to canopy:
- classic: $R_c = \frac{R_{leaf}}{LAI}$
- big leaf: integral over all canopy as a single leaf
- physiological approach
• Jarvis approach – light, temperature, water vapour deficit, and soil water deficit behave independently as modifying factors (0, 1)
  - minimal leaf resistance $R_{c\text{-}\text{min}}$ is plant characteristic

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

• Physiological approach – link between water and CO$_2$ pathway to photosynthesis ($A_n$), taking into account different diffusion coefficients
Physiological approach (preferred and tested)

- assumes that C conductance is determined by ratio between photosynthetic rate and the concentration difference of CO₂ for leaf surface and leaf interior

\[
g_{l,c} = g_{\text{min},c} + \frac{a_1 A_g}{(C_s - \Gamma)(1 + \frac{D_s}{D_0})}
\]

\[
g_{l,c} = \frac{1}{1.6} \Rightarrow \frac{g_c}{g_{c,c}} = \frac{C_s}{C_i}
\]

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

- \( g_{\text{min},c} \) - the cuticular conductance
- \( A_g \) - the gross assimilation rate of leaf
- \( D_s \) - the vapour pressure deficit at plant level
- \( C_s \) - the CO₂ concentration at the leaf surface
- \( C_i \) - the CO₂ concentration in the plant interior
- \( f_0 \) - the maximum value of \( (C_i - \Gamma)/(C_s - \Gamma) \)
- \( f_{\text{min}} \) - the minimum value of \( (C_i - \Gamma)/(C_s - \Gamma) \)
- \( D_0 \) - the value of \( D_s \) at which the stomata are closed
- \( \Gamma \) - CO₂ compensation point

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

- simplifies Jacobs – Calvet approach:

\[
\frac{C_i - \Gamma}{C_s - \Gamma} = f_0 - a_d D_0,
\]

\[
D_0 = \frac{f_0 - f_{\text{min}}}{a_d}.
\]

\(f_0, a_d\) – empirically found as regression coefficients

\(D_0\) – vapour pressure deficit for which stomata are closed

Water vapour deficit

- light, temperature, VPD, soil water deficit - environmental factors influencing the canopy resistance

<table>
<thead>
<tr>
<th>Vegetation type</th>
<th>(f_0)</th>
<th>(a_d) (kPa(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low vegetation C3</td>
<td>0.89</td>
<td>0.07</td>
</tr>
<tr>
<td>Low vegetation C4</td>
<td>0.85</td>
<td>0.015</td>
</tr>
<tr>
<td>Lobos</td>
<td>0.093</td>
<td>0.12</td>
</tr>
<tr>
<td>Rice and phalaris grass</td>
<td>0.89</td>
<td>0.18</td>
</tr>
<tr>
<td>Forest temperate</td>
<td>0.875</td>
<td>0.06</td>
</tr>
<tr>
<td>Boreal forest</td>
<td>0.4</td>
<td>0.12</td>
</tr>
</tbody>
</table>

Stomatal conductance and humidity deficit - C3 and C4 plants
Soil water deficit

- CO₂ assimilation rate - seriously affected by soil water stress, especially during the summer time → the water supply is low

\[ A_g = A_g^* [2\beta(\theta) - \beta^2(\theta)]. \]

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

correction factor for water stress

\[ \theta = R_1\theta_1 + R_2\theta_2 + R_3\theta_3 + R_4\theta_4. \]

\( A_g \) - the gross assimilation rate of leaf
\( A_g^* \) - the unstressed assimilation (mol m⁻²s⁻¹) rate
\( \theta \) - the average soil water content in root zone
WP - the wilting point
FC - the field capacity
\( \Theta_i \) - mean soil moisture in “i” layer
\( R_i \) - root fraction in “i” layer
Canopy resistance controls the HTO transfer from air to plant – Our model results

\[ g_{c,w} = \frac{g_{\text{min},w}}{1.6} + \frac{a_i A_g}{(C_s - \Gamma)(1 + \frac{D_s}{D_*})} dL = \frac{g_{\text{min},w}}{1.6} LAI + \frac{a_i \int_0^{LAI} A_g dL}{(C_s - \Gamma)(1 + \frac{D_s}{D_*})} \]

Canopy resistance

- Summer wheat
- Maize
- Potato
- Sugar beat
- Winter barley
- Summer barley
- Winter wheat
## Comparison between experimental and theoretical data for maximum stomatal resistance

<table>
<thead>
<tr>
<th>Plant type</th>
<th>Experimental val. (s/m)</th>
<th>Model val. (s/m)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wheat, vegetative stage</td>
<td>41 – 52</td>
<td>56</td>
<td>Baldocchi, 1994</td>
</tr>
<tr>
<td>Wheat, anthesis</td>
<td>62 - 100</td>
<td>60</td>
<td>Baldocchi, 1994</td>
</tr>
<tr>
<td>Maize, vegetative</td>
<td>121 - 131</td>
<td>111</td>
<td>Baldocchi, 1994</td>
</tr>
<tr>
<td>Wheat</td>
<td>17 - 20</td>
<td>18</td>
<td>Choudhury, 1998</td>
</tr>
<tr>
<td>Potato</td>
<td>100 - 130</td>
<td>130</td>
<td>Vos, 1987</td>
</tr>
<tr>
<td>Alpha-alpha</td>
<td>100 - 120</td>
<td>110 – 130 (dep. VPD)</td>
<td>Saugier, 1991</td>
</tr>
<tr>
<td>Soya</td>
<td>66</td>
<td>70</td>
<td>Oliosa, 1996</td>
</tr>
<tr>
<td>Grass C3</td>
<td>74</td>
<td>74 – 120 (dep. VPD)</td>
<td>Knap, 1993</td>
</tr>
<tr>
<td>Grass C4</td>
<td>151</td>
<td>156 – 178 (dep. VPD)</td>
<td>Knap, 1993</td>
</tr>
</tbody>
</table>
The Shuttleworth-Wallace model defines fluxes from the vegetative and soil components with a resistance network.
With the Shuttleworth-Wallace model, there is need to define values of the humidity deficit, temperature and vapour pressure at the canopy source height, $D_0$, $T_0$, $e_0$.

By analogy, for HTO:

\[
F_c (R_{aa} + R_{ab} + R_{ac}) + F_s R_a = C_a - C_c \\
F_c R_a + F_s (R_{aa} + R_{as} + R_{ss}) = C_a - C_s
\]

\(C_a\) – HTO concentration in air; 
\(C_c\) – HTO concentration in vegetation; 
\(C_s\) – HTO concentration in soil; 
\(R_{aa}\) – atmospheric resistance between reference level and canopy source height; 
\(R_{ac}\) – boundary layer resistance; 
\(R_{sc}\) – canopy resistance; 
\(R_{as}\) – atmospheric resistance between canopy source height and soil surface; 
\(R_{ss}\) – soil resistance; 
\(F_c\) – flux atmosphere – vegetation; 
\(F_s\) – flux atmosphere – soil.

\[
F_c = V_{ex} (C_a - C_{va}) - V_{ex2} (C_a - C_{sa}) \\
F_s = V_{ex1} (C_a - C_{sa}) - V_{ex2} (C_a - C_{va})
\]

Details are given elsewhere
HTO concentration in vegetation in the sparse canopy approach

Coupling between soil surface and vegetation layer has a significant influence on canopy HTO concentration at both low and high Leaf Area Index → more studies are justified.
Photosynthesis

Biochemical reactions in the presence of light:

• **Diffusion of CO$_2$ to chloroplasts** - passing through the leaf stomata
• **Photochemical reaction** - light usage to split water producing O$_2$, NADPH and ATP
• **Dark reaction** - NADPH and ATP produced in the light are used to reduce CO$_2$ to carbohydrate and other organic compounds in a chain of reactions mediated by specific enzymes.
• Two biochemical processes important - **C3 and C4 pathways**
  - **C3 pathway (Calvin cycle)** - CO$_2$ is first incorporated into compounds with 3 carbon atoms; most temperate plants are based on the C3 process.
  - **C4 pathway** - CO$_2$ is first fixed in molecules with 4 carbon atoms; C-4 plants (maize, alfalfa, sugarcane) are well adapted to a climate with high temperatures, high light intensities and limited water supply.

Photosynthesis is accompanied by respiration, a process of dry matter oxidation needed to produce energy for the plant growth and maintenance of metabolic processes.

NADPH - reduced nicotinamide adenine dinucleotide phosphate;
ATP - adenosine triphosphate
Photosynthesis approaches

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

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

- Enzyme-limited rate ("RuBisCO")
- Light-limited rate
- Sink-limited rate
- Dark respiration rate

- the most complex biochemical model;
- used in land-atmosphere interaction;
- needs too many parameters for site-specific applications, covering genotype of various species, effect of fertilization and temperature adaptation → great disadvantage
The Romanian photosynthesis approach

- We use the canopy photosynthesis model from the WOFOST;
- Leaf gross photosynthesis rate:

\[ A_{Lg} = A_{gm} \left( 1 - \exp \left( -\frac{\varepsilon \times I_{al}}{A_{gm}} \right) \right) \]

- \( A_{gm} \) - gross assimilation rate at light saturation (kg m\(^{-2}\) d\(^{-1}\))
- \( \varepsilon \) - initial slope or light use efficiency (kg J\(^{-1}\))
- \( I_{al} \) - the absorbed PAR (\(\mu\)mol m\(^{-2}\)s\(^{-1}\))

Many plant specific results given by the biochemical models can be reproduced using the simplified WOFOST model

Comparison between WOFOST model and experimental data for Kansas grass at ambient temperature of 40 °C

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>( A_{max} ) (kg CO(_2) m(^{-2})h(^{-1}))</th>
<th>( \varepsilon ) (kg CO(_2) J(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>19.0</td>
<td>0.33</td>
</tr>
<tr>
<td>20</td>
<td>36.5</td>
<td>0.33</td>
</tr>
<tr>
<td>25</td>
<td>55.5</td>
<td>0.32</td>
</tr>
<tr>
<td>30</td>
<td>74.0</td>
<td>0.32</td>
</tr>
<tr>
<td>35</td>
<td>70.7</td>
<td>0.32</td>
</tr>
</tbody>
</table>
• We distinguish between sunlit and shaded leaves;

• We take into account the difference between air temperature (above the crop) and canopy temperature;

• To explain the experimental data, we recommend to consider the crop development stage effect on photosynthesis and canopy resistance (aging effect);

• We ignore the difference between temperature and stomatal resistance for shaded and sunlit leaves in field conditions.
In the simplest approach, we ignore details on respiration and focus on net photosynthesis rate (net of respiration).

Assume that we know the net assimilation rate of CO₂ as kg CO₂ per unit time and unit surface of crop, Pc.

One mol of CO₂ and one mol of H₂O gives one mol of photosynthate (the initial organic matter produced), with a generic formula CH₂O.

The rate of water assimilation in non-exchangeable matter (bound with C) can be obtained using stoichiometric relations (molar mass of CO₂ is 44, molar mass of H₂O is 18) and is 0.41 Pₐ.

Consider tritium, as tritiated water → due to higher mass, all reactions rates will be slower.

Energy of radioactive disintegration (average 5.8 keV) will be used partially for the activation energy of many biochemical reactions.

Plant varies in their molecular constituent → the balance of slow down and acceleration of biochemical reaction is reflected in a variable fractionation (discrimination) ratio, FD (formation of OBT/formation of OBH), with an average of 0.5 and range between 0.45 and 0.55.
With a known $C_{HTO}$ in leaves, we can assess the formation rate of OBT in light conditions:

$$P_{OBT} = FD \times 0.41 \times P_c \times C_{HTO} \quad (Bq/h/m^2)$$

→ we must use the HTO in leaves, because leaves are the site of photosynthesis

In the same conditions of time and space, the net dry matter production is:

$$P_D = \frac{30}{44} P_c$$

Total organic tritium is higher, because about 22% is non-exchangeable:

$$P_{OBT} = 0.88 \times P_{OT}$$

In practice, the leaf HTO concentration varies in time → $P_c$ varies, also (with zero during the night time)
Consider the start of air contamination with HTO, $t_0$, and a subsequent moment, $t$, later in time; at start, the net dry matter of the crop is $Y_0$ and at time $t$ is:

$$Y = Y_0 + \int_{t_0}^{t} \frac{30}{44} P_c(\tau) d\tau$$

$P_c$- net assimilation rate (net of respiration) (kg dm/m²)
• If we ignore OBT production during the night time, we can derive a similar equation of OBT production for the whole crop.

• The evolution of OBT concentration $C_{OBT}$ (Bq/kg dm) is of interest in food chain modelling.

• First, we consider the concentration in whole crop (including roots); we have:

$$\frac{dC_{OBT}}{dt} = \left(\frac{1}{Y}\right) * P_{OBT} - \left(\frac{C_{OBT}}{Y}\right) * P_D$$

where:

$$A_{OBT} = C_{OBT} * Y$$

$$\frac{dA}{dt} = Y * \frac{dC}{dt} + C * \frac{dY}{dt}$$

$$P_{OBT} = Y * \frac{dC}{dt} + C * \frac{dY}{dt}$$

$$\frac{dC_{OBT}}{dt} = \left(\frac{1}{Y}\right) * 0.41 * FD * P_c * C_{HTO} - \left(\frac{C_{OBT}}{Y}\right) * 0.68 * P_c$$
\[
\frac{dC_{OBT}}{dt} = \left(\frac{1}{Y}\right) \times 0.6 \times FD \times P_D \times C_{HTO} - \left(\frac{C_{OBT}}{Y}\right) \times P_D
\]

Y and \(C_{HTO}\) are function of time.
We demonstrate the close relationship between OBT and C.
\(PD/Y\) is Relative Growth Rate (RGR) - time dependent.

Dynamic equation for OBT production in plants:

\[
\frac{dC_{OBT}}{dt} = \left(\frac{P_D}{Y}\right) \times [0.6 \times FD \times C_{HTO} - C_{OBT}]
\]

\(C_{HTO}\) dynamics depends on air concentration AND canopy resistance and this last one depends on \(Pc\).
• At each stage of plant development, the new formed net dry matter will be differently distributed to various plant parts → initial uptake and time evolution depends on plant part.

• We must know these partition factors in order to assess OBT in the edible plant part.

• Even for leafy vegetables and pasture, we must know the partition to root.

OBT concentration for soybean at harvest for 1 hour air contamination at various plant DVS

Partition fraction of new produced dry matter to roots, leaves, stems and edible grains as function of DVS (0=emergence; 1=flowering; 2=full maturity) for maize cultivar F320 (South Romania)
• PARTITION FACTORS DEPEND ON CULTIVAR (GENOTYPE), not only on PLANT

• $P_c$ depends on:
  - crop type;
  - development stage (DVS);
  - leaf area index (LAI);
  - temperature;
  - light;
  - water stress (air vapour deficit and soil water)

• We must understand the plant growth

• Development stages:

  0 - 1 - emergence to anthesis (flowering) $\rightarrow$ generative stage
  1 - 2 - anthesis to maturity $\rightarrow$ reproductive stage

\{ both can be finer divided \}

• Evolution of plant development depends on Thermal time $=$ sum of air temperature over a basis
OBT concentration in different plant parts

- At least, we must know crop specific accumulated thermal time until anthesis and maturity → we can define the increasing of DVS each day → partition factors → increase in leaf mass → green leaves → LAI

- Knowing the ambient data on temperature, light, vapour pressure and soil water, we can determine $P_C$, $P_D$, $P_{OBT}$

**OBT concentration in plant part $i$**

Partition fraction $PF_i$ (DVS) → $PF_i(t)$

$$P_{D,i} = P_D * PF_i$$

$$P_{OBT,i} = P_{OBT} * PF_i$$

$$\frac{dC_{OBT,i}}{dt} = \left(\frac{1}{Y_i}\right) * P_{OBT,i} - \left(\frac{C_{OBT,i}}{Y_i}\right) * P_{D,i}$$
Comparison between experimental data and model predictions for relative OBT concentration in wheat at harvest

<table>
<thead>
<tr>
<th>Time</th>
<th>Rel. OBT conc. at harvest (%)</th>
<th>Exposure conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exp.</td>
<td>Model</td>
</tr>
<tr>
<td>Dawn</td>
<td>0.18</td>
<td>0.29</td>
</tr>
<tr>
<td>Day</td>
<td>0.25</td>
<td>0.34</td>
</tr>
<tr>
<td>Dusk</td>
<td>0.20</td>
<td>0.34</td>
</tr>
<tr>
<td>Night</td>
<td>0.15</td>
<td>0.31</td>
</tr>
</tbody>
</table>
Model predictions for relative HTO uptake, HTO half-time and relative OBT concentration in potato at harvest

<table>
<thead>
<tr>
<th>Day of year</th>
<th>DVS</th>
<th>LAI</th>
<th>Canopy resistance (s/m)</th>
<th>Rel. HTO uptake (%)</th>
<th>HTO Half time (min)</th>
<th>Rel. OBT (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>162</td>
<td>1.02</td>
<td>2</td>
<td>75</td>
<td>43</td>
<td>44</td>
<td>3.6e-3; 0.03</td>
</tr>
<tr>
<td>177</td>
<td>1.16</td>
<td>3.5</td>
<td>60</td>
<td>51</td>
<td>32</td>
<td>0.026; 0.21</td>
</tr>
<tr>
<td>193</td>
<td>1.31</td>
<td>4</td>
<td>60</td>
<td>49</td>
<td>52</td>
<td>0.051; 0.42</td>
</tr>
<tr>
<td>202</td>
<td>1.4</td>
<td>4</td>
<td>45</td>
<td>50</td>
<td>68</td>
<td>0.075; 0.6</td>
</tr>
<tr>
<td>219</td>
<td>1.55</td>
<td>3.4</td>
<td>95</td>
<td>44</td>
<td>62</td>
<td>0.03; 0.25</td>
</tr>
<tr>
<td>236</td>
<td>1.71</td>
<td>1.9</td>
<td>125</td>
<td>37</td>
<td>90</td>
<td>0.039; 0.33</td>
</tr>
<tr>
<td>177 (night)</td>
<td>1.16</td>
<td>3.5</td>
<td>690</td>
<td>14</td>
<td>600</td>
<td>0.022; 0.23</td>
</tr>
</tbody>
</table>

- DVS is 0 at emergence, 1 at anthesis and 2 at harvest;
- Relative uptake is the concentration of HTO in leaf water at the end of exposure relative to HTO conc. in air moisture;
- Relative OBT is OBT concentration at harvest (per kg fw or per L of combustion water, assuming 0.2 g dm in tuber) relative to HTO conc. in leaf water at the end of exposure.
Having at least one year of data on biomass production (plant part and, total, daily meteo data, soil type), we started with default parameters in the physiological crop growth and adapted them for local conditions.


Sunflower above ground biomass, experimental data (exp), WOFOST result for default cultivar (EC param.) and parameters adapted to Romanian cultivars (rom param)
Role of respiration in OBT formation

- Respiration is often subdivided into:
  - Growth;
  - Maintenance;
  - Transport costs.

**Growth respiration** (a.k.a. “construction respiration”) – a “fixed cost” that depends on the tissues or biochemicals that are synthesized → Often described in terms of “glucose equivalents”

- The conversion of assimilate into dry matter (**growth respiration**) can be counted first converting the CO$_2$ assimilation to assimilate production (30/44) and further considering the conversion from assimilate top dry matter depending also on plant stage

- In vegetative period (only leaves, roots and stems) a value of 0.69 is OK (coefficient of variance less than 5%).

- In reproductive stage the same value can be used, but with a larger variance.

- Storage organs for different plants have:
  - soybean - 0.48;
  - field bean - 0.59;
  - sugar beat - 0.82;
  - potato - 0.85

**It seems that growth respiration ends the next morning!**
**Maintenance respiration** - The cost of maintaining existing tissues and functions  
(Protein turnover is the largest cost of maintenance respiration)  
- is subtracted from the assimilate production and depends on dry mass of plant organs  
\[
W_r = RML \cdot WL + RMS \cdot WS + RMR \cdot WR + RMO \cdot WO
\]
where: L - leaf, S - stem, R - root, O - storage organ; RM – maintenance respiration.

RMX in kg photosynthate per kg dry matter and day (data from Wageningen school)

<table>
<thead>
<tr>
<th></th>
<th>RML=0.026</th>
<th>RMS=0.015</th>
<th>RMO=0.003-0.01</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.03</td>
<td>wheat</td>
<td>maize</td>
<td>barley</td>
</tr>
<tr>
<td>0.02</td>
<td>rice</td>
<td>bean</td>
<td></td>
</tr>
<tr>
<td>0.027</td>
<td>bean</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Sunflower swap

<table>
<thead>
<tr>
<th></th>
<th>RML = 0.0050 ! Rel. maintenance respiration rate of leaves, [0..1 kg CH₂O/kg/d, R]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RMO = 0.0230 ! Rel. maintenance respiration rate of st. org., [0..1 kg CH₂O/kg/d, R]</td>
</tr>
<tr>
<td></td>
<td>RMR = 0.0100 ! Rel. maintenance respiration rate of roots, [0..1 kg CH₂O/kg/d, R]</td>
</tr>
<tr>
<td></td>
<td>RMS = 0.0080 ! Rel. maintenance respiration rate of stems, [0..1 kg CH₂O/kg/d, R]</td>
</tr>
</tbody>
</table>

It seems that maintenance respiration is a long time process (λ~0.2 d⁻¹)

**OPEN QUESTIONS**

OBT formation during the night time
Maintenance respiration dynamics
To re-write the dynamic equation for OBT production taking into account the respiration dynamics
CONCLUSIONS

- Various approaches describing the stomatal (canopy) conductance and photosynthesis rate;

- The goal is to select the best formalism in order to be applied for operational cases in field conditions;

- We developed a research grade model for plants based on process level, pointing out that model inputs can be obtained using Life Science research in connection with National Research on plant physiology and growth, soil physics, and plant atmosphere interaction → Interdisciplinary Research;

- The aim of this work in progress is to develop a robust model for the HTO transfer from atmosphere to plants and the subsequent conversion to OBT.
THANK YOU!