Crop growth modeling and OBT

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OBT production in the daytime

- 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 photosinthate (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 P_C.
- 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 reflects 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 HTO concentration in leaves C_{HTO}, we can assess the formation rate of OBT in light conditions:

 P_{OBT} =FD*0.41* P_c * C_{HTO} (Bq/h/m²) \rightarrow 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} = 30/44 P_{c}

- Total organic tritium is higher, because about 22 % is non-exchangeable: $P_{OBT}=0.88*P_{OT}$
- In practice, the leaf HTO concentration varies in time → Pc varies, also (with zero in the night time);
- Consider the start of air contamination with HTO, t₀, and a subsequent moment, t, later in time; at start, the net dry matter of the crop isY₀ and at time t is:

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

 $(kg dm/m^2)$

P_c-net assimilation rate (net of respiration)



- If we ignore night OBT production we can derive a similar equation of OBT 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:

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

where: $A_{OBT} = C_{OBT} * Y$, dA/dt = Y * dC/dt + C * dY/dt, $P_{OBT} = Y * dC/dt + C * P_D$

$$\frac{dC_{OBT}}{dt} = (\frac{1}{Y}) * 0.41 * FD * P_c * C_{HTO} - (\frac{C_{OBT}}{Y}) * 0.68 * P_c$$

$$\frac{dC_{OBT}}{dt} = (\frac{1}{Y}) * 0.6 * FD * P_D * C_{HTO} - (\frac{C_{OBT}}{Y}) * P_D$$

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

$$\frac{dC_{OBT}}{dt} = \left(\frac{P_D}{Y}\right) * \left[0.6 * FD * C_{HTO} - C_{OBT}\right] \qquad \qquad \frac{dOBT_{plant}(t)}{dt} = -g_r OBT_{plant}(t) + g_r TFWT(t)$$

- $C_{\rm HTO}$ dynamics depends on air concentration AND canopy resistance and this last one depends on ${\rm P_c}$

OBT production in night time

- The formation of OBT in the dark is only partly understood because the plant physiological processes implied cannot be quantitatively assessed.
- Possible processes:
 - oxidative respiratory pathways;
 - tricarboxilic acid cycle;
 - isomerisation and hydrolytic splitting reactions
- Various organic molecules are formed in the plant basal metabolism (Thornley, 1990) with addition of water and without the need of light. For example the following organic acids:

glucose +H₂O+NADPH => <u>citrate</u> + 4 NADH+2 ATP

glucose +H₂O+NADPH => <u>succinate</u> +2CO₂+6 NADH+2 ATP+GTP

glucose +H₂O+NADPH => $\underline{fumarate}$ +2 CO₂ +7 NADH+2 ATP

0.5 glucose + H₂O => malonate +2 NADH+ATP

0.6 glucose +0.5 O2 +2 H_2O => <u>oxalate</u> +2 CO₂ +4 NADH +ATP and aminoacids:

0.5 glucose +NH₃ +H₂O => glycine +CO₂+2 NADDH + NADPH

- Organic acids and glycine add up to 4-8 % of the plant dry mass and we expect that 4-8 % of the new dry matter produced in photosynthesis enters in reactions producing OBT.
- Between anthesis and maturity about 9 g of dry matter is produced per day. Thus about 0.03 g/h is treated by the above mentioned reactions.
- OBT production in night recycles previously day produced photosinthate
- Night OBT production is given by:

P_{OBT}=FD*0.41*K*[average prev day P_c]* C_{HTO}

where K – coefficient for OBT night production (still unclear → the need for more experimental work and biochemical understanding)

For cereals

 $P_{OBT} = FD^*0.41^*0.012^* (lai/maxlai)^*C_{HTO}$

- night production, assumption ;: 2 weeks after anthesis the rate is 5 times less full sun it decreases after as LAI (becoase is linked with basal metabolism) preliminary rate 0.2 * 0.012 kg CO2/m2h
- cdandec2000 decrease 2 times

OBT concentration in edible plant parts (net of respiration)

- At each stage of plant development, the newly formatted 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.





Partition fraction of newly produced dry matter to roots, leaves, stems and edible grains as function of development stage (0=emergency; 1= flowering; 2= full maturity) for maize cultivar F320 (South Romania)

1

DVS

0.5

Roots

— leaves

---steams

- grain

2

1.5

- 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

J both can be finer divided

- Evolution of plant development depends on Thermal time = sum of air temperature over a basis
- At least, we must know crop specific accumulated thermal time until anthesis and maturity → we can define the increasing of development stage 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 $PF_i(DVS) \rightarrow PF_i(t)$ $P_{D_i}=P_D^*PF_i$

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

$$\frac{dC_{OBT,i}}{dt} = (\frac{1}{Y_i}) * P_{OBT,i} - (\frac{C_{OBT,i}}{Y_{i_i}}) * P_{D,i}$$

