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# Mathematical modelling of oxygen and carbon dioxide concentration profiles in the interstitial atmosphere of silo-bags

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# Silobags in the field

In Argentina, the use of silbags to store grains in the field has undergone an important increase.

In 2010, around 1/3 of the total grain production (45 millions tones) was stored in “silobags”.

The “silobag” is a modified atmosphere storage system.
The grain is loaded in sealed plastic bags.
As result of the respiration of the grain ecosystem, a modified atmosphere is achieved, poor in $O_2$ and rich in $CO_2$, suitable for grain conservation.

National Institute of Agricultural Technologies of Argentina

## Guidelines for grain handling based on experimental results

A novel technology for monitoring grain storability in silobags based on $CO_2$ detection was implemented at the Balcarce Experimental Station ((INTA -EEA) by (Bartosik et al., 2008; Cardoso et al., 2008)

The procedure consists of comparing the measured $CO_2$ concentration with a referential value which corresponds to adequate storage conditions.

To improve the technology based on $CO_2$ detection it is relevant to understand the dynamics of gas concentration in silobags

Aim of this study: Model the difussion process of $O_2$ and $CO_2$ in the interstitial air of silo-bags

" Validated computer model" = "virtual bagging" without any risk

¿What - if ? studies – Analysis of a wide range of storage conditions that could hardly be covered by experimental tests , which are expensive and time consuming

## Mathematical models → Energy and mass balances

$$c_b \rho_b \frac{\partial T}{\partial t} = \left[ \frac{\partial}{\partial x}\left[ k_b \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y}\left[ k_b \frac{\partial T}{\partial y} \right] \right] + \rho_{bs} L_g \frac{\partial W_g}{\partial t} + \rho_{bs} q_H Y_{CO2} \quad in\ \Omega_1$$

$$\rho_{bs} \frac{\partial W_g}{\partial t} = \frac{\partial}{\partial x}\left[ D_w \left( \eta \frac{\partial W_g}{\partial x} + \omega \frac{\partial T}{\partial x} \right) \right] + \frac{\partial}{\partial y}\left[ D_w \left( \eta \frac{\partial W_g}{\partial y} + \omega \frac{\partial T}{\partial y} \right) \right] + \rho_{bs} q_w Y_{CO2} \quad in\ \Omega_1$$

## Diffusion Model

$$\varepsilon \frac{\partial CO_2}{\partial t} = \frac{\partial}{\partial x}\left[ D^*_{CO2} \left( \frac{\partial CO_2}{\partial x} \right) \right] + \frac{\partial}{\partial y}\left[ D^*_{CO2} \left( \frac{\partial CO_2}{\partial y} \right) \right] + \rho_{bs} r_{CO2} \quad in\ \Omega_1$$

$$\varepsilon \frac{\partial O_2}{\partial t} = \frac{\partial}{\partial x}\left[ D^*_{O2} \left( \frac{\partial O_2}{\partial x} \right) \right] + \frac{\partial}{\partial y}\left[ D^*_{O2} \left( \frac{\partial O_2}{\partial y} \right) \right] + \rho_{bs} r_{O2} \quad in\ \Omega_1$$

$$r_{CO2} = \frac{Y_{CO2}}{1000 M_{CO2}} \frac{R\,T}{P_{at}} \quad ; \quad r_{O2} = r_{CO2}$$

- Boundary conditions for energy balance

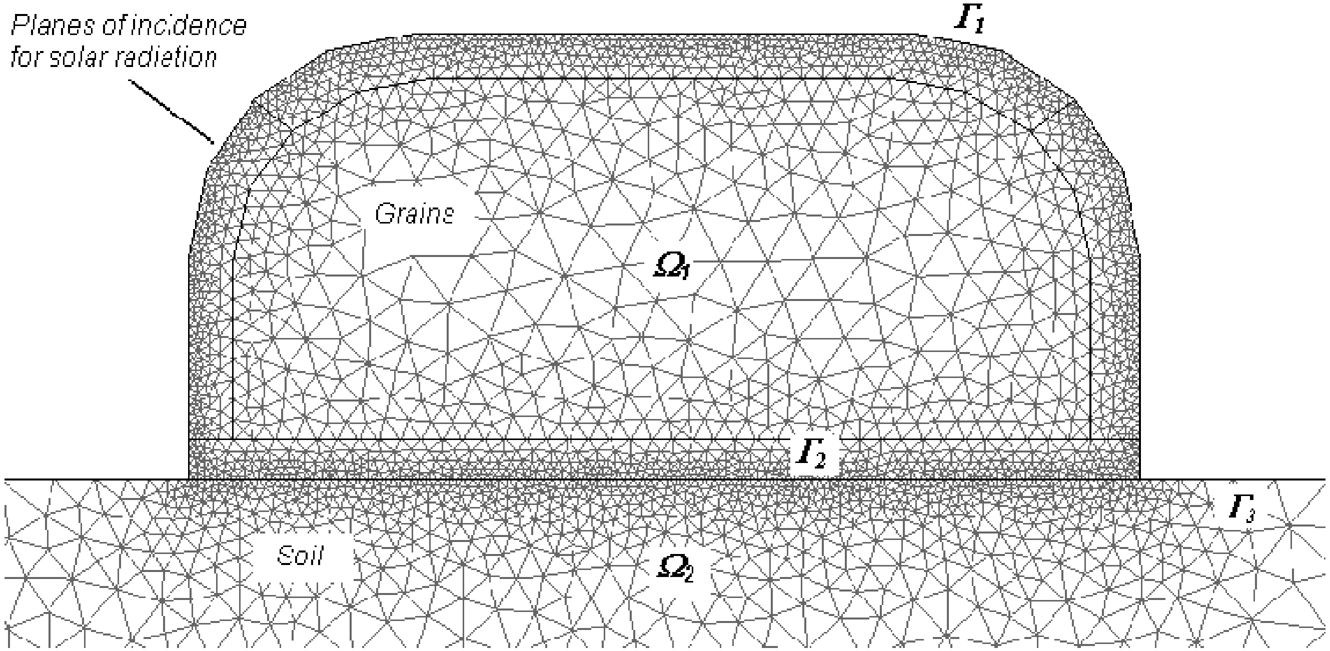
(Convection + radiation) to ambient air + incidence of solar radiation on the silobag surface

Bottom of the silbag: Conduction to soil

- Boundary conditions for mass balances

Silobag is impermeable to water vapour transfer

Gas transfer through the plastic layer is a function of the equivalent permeability of the plastic layer- (Series resistance model)




## Comsol Multiphysics 3.5a Version

## Finite Element Method

## The model was applied to:

- Predict gas distribution in the silo-bag

- Compare mean concentration evolutions predicted by Diffusion Model and Lumped Model (validated model)
(Quantify the effect of averaging local temperature variations and moisture migration)

- Study how local effects affect the evolution of gas concentration
non uniform initial MC distribution
damage of the plastic layer (perforations)

# Numerical Simulation

Storage of wheat in a silo-bag from summer (January) to winter (June), (six months).

Climatic conditions of the South East of Buenos Aires province (Argentina)

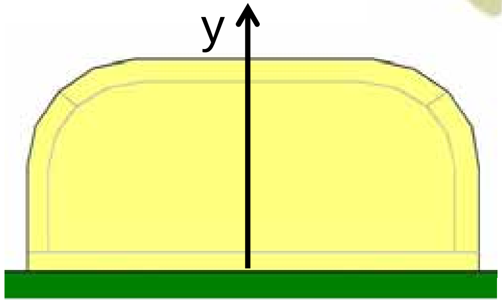
Initial grain temperatures: 20, 25, 30 and 40C.
Initial grain MC range: 12 to 16 % w.b.

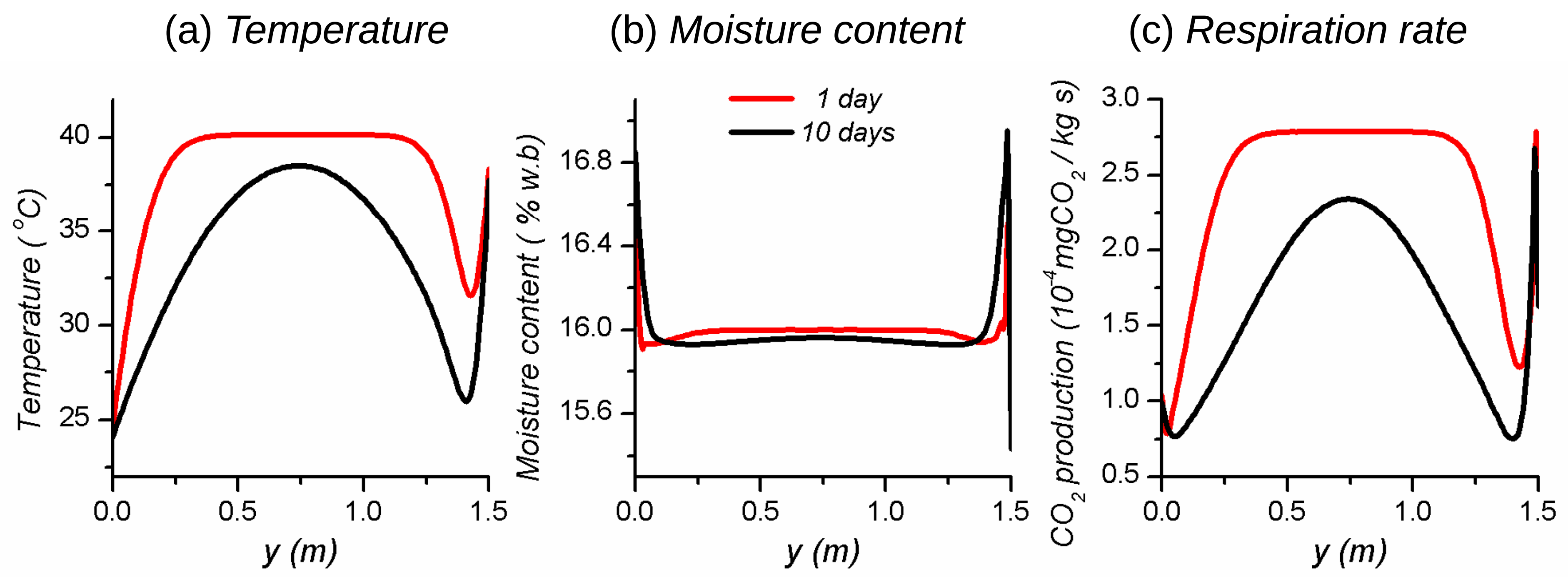
Dependence of the rate of $CO_2$ production $Y_{CO2}$ was evaluated by use of the correlation developed by White et al. (1982)

$$\log Y_{CO2} = -4.054 + 0.0406\,T - 0.0165\,\theta + 0.0001\,\theta^2 + 0.2389\,M$$

Initial storage conditions 40C and 16%w.b

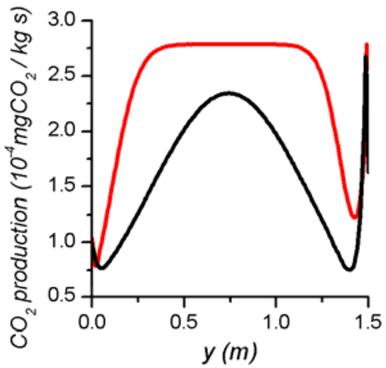
Profiles of T, W, $Y_{CO2}$, along the vertical section of the silo-bag

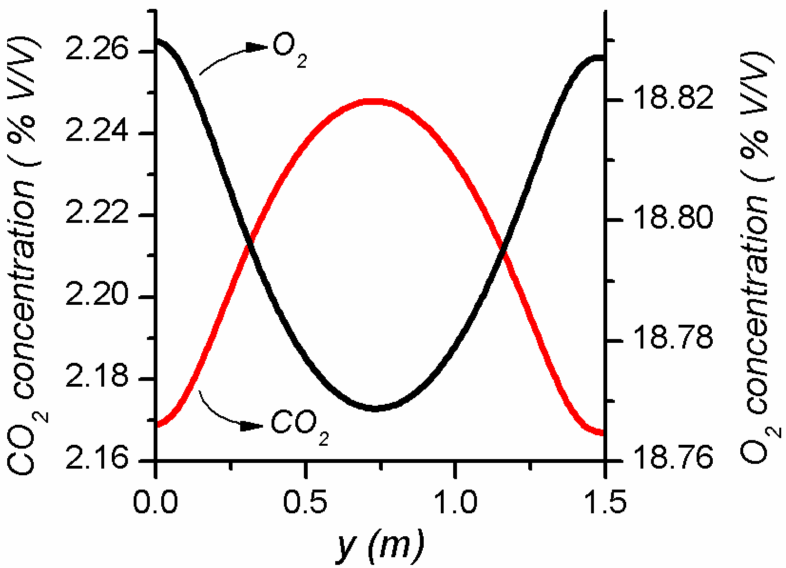


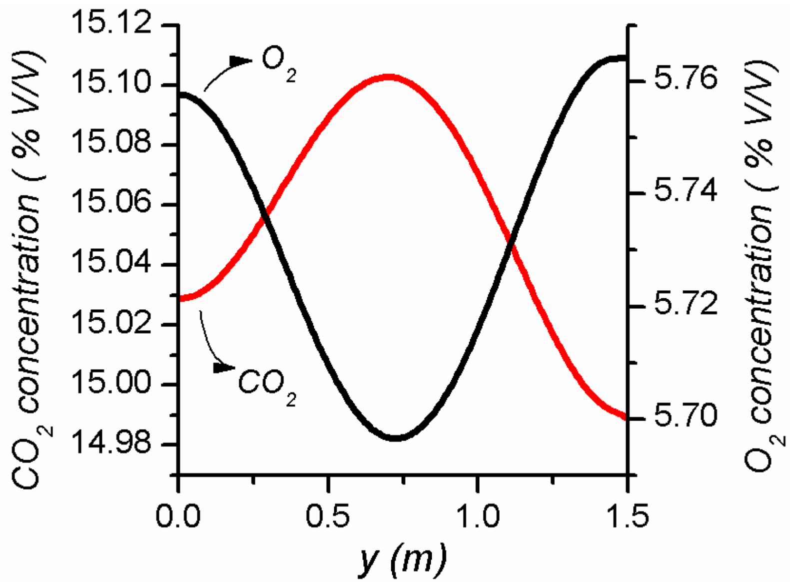
## Initial storage conditions 40C and 16%w.b

## Profiles of $CO_2$ and $O_2$ along the vertical section of the silo-bag




(a) First day of storage

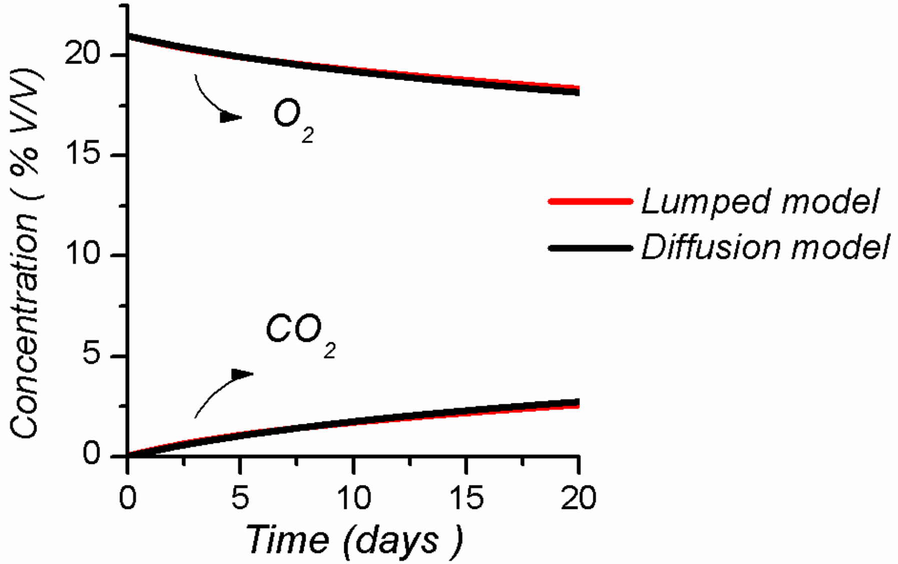



(b) Tenth day of storage

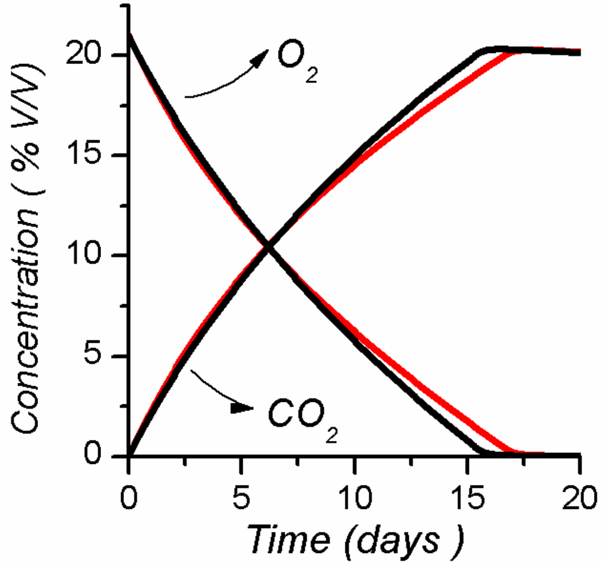
Initial grain temperature 40C

Comparison between $O_2$ and $CO_2$ mean concentration evolutions predicted by use of the diffusion and lumped models.

(a) *MC 12%w.b*




(b) *MC 16%w.b*

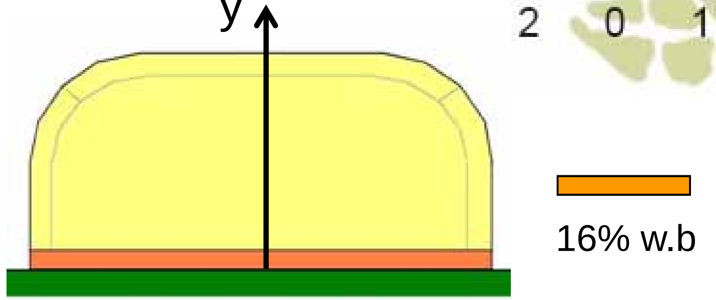


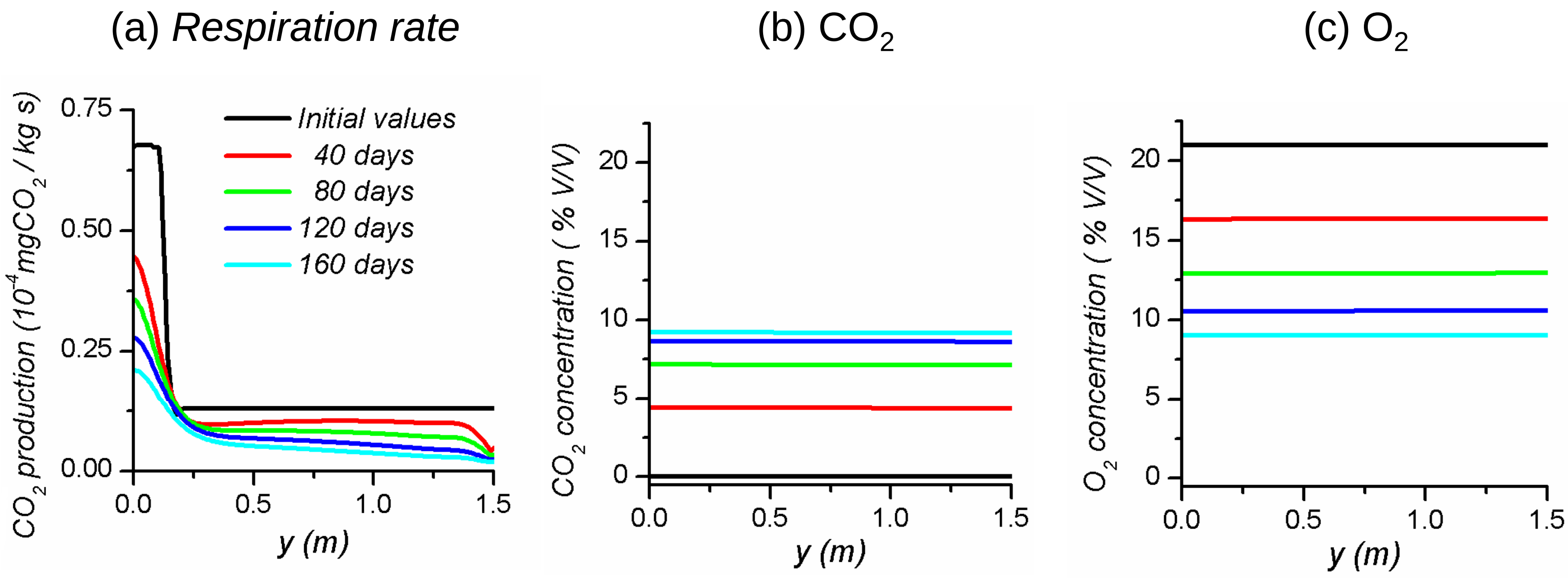

Differences are negligible

Difference less than 1 point %

## Non uniform initial MC (13-16% w.b)
## Initial grain temperature 25C

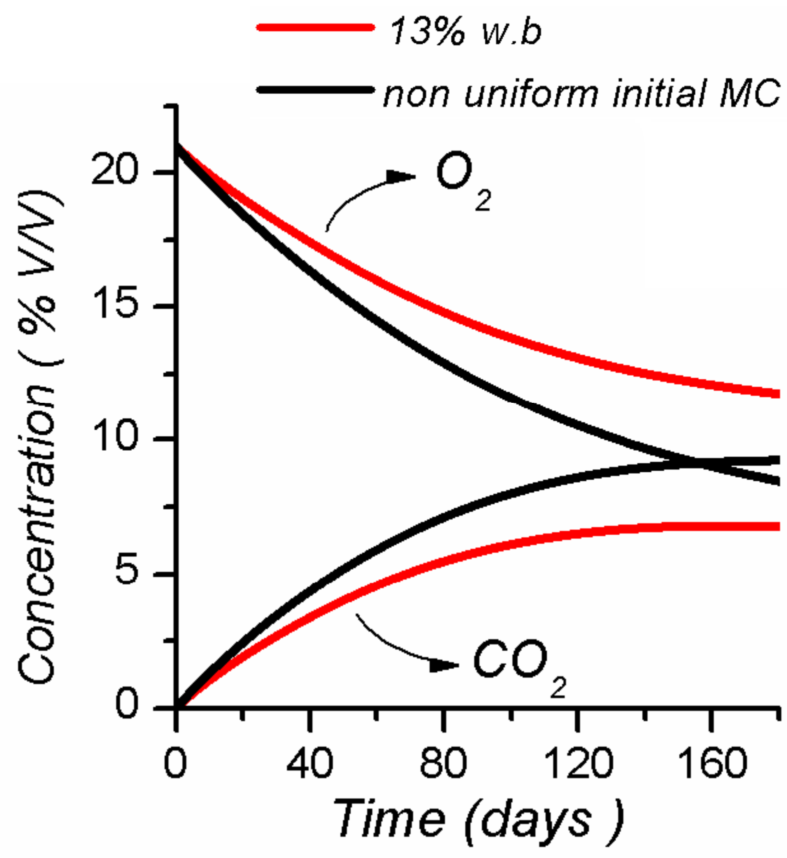
10% of the grain stored per unit length



Base case: 13%w.b, $T_i$= 25C

Comparison between the evolution of the mean gas concentrations for the base case with the non uniform MC distribution case




During the first month, measured and referential values are within experimental errors.

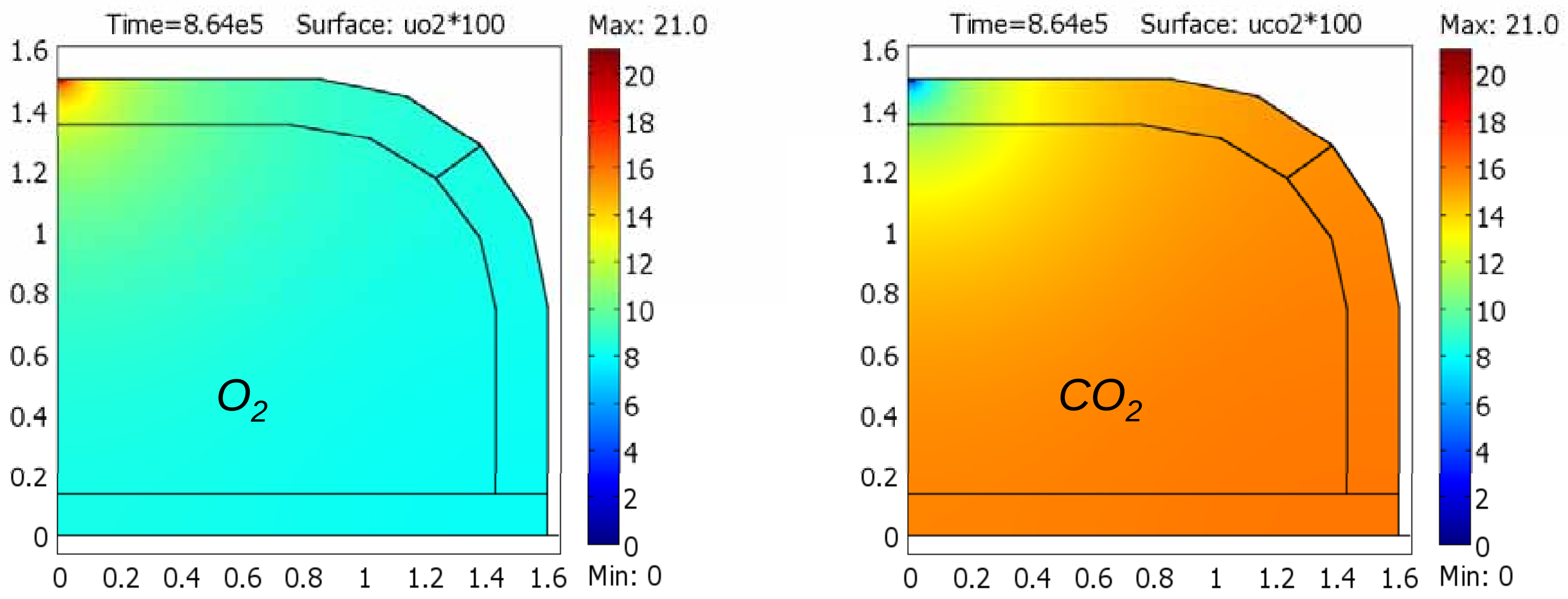
Wet spot not detected.

After two months, measured $CO_2$ is 3 or 4 points above the referential value

Clear warning of possible grain spoilage in the silo-bag

# **Effect of a perforation on the silobag** (1cm long)
## MC (16% w.b) – Ti=40 C ; $O_2$ = 0%V/V; $CO_2$ = 21 %V/V

After 10 day O2 is above 9% everywhere.
Risk of grain spoilage because biological activity may be posible




*Gas concentration (%V/V) after 10 days of storage*

## Conclusions

- Differences in mean gas concentrations predicted by Lumped and Diffusion models were less than 1point %.

- Lumped model is adequate for generating referential values of $CO_2$ concentrations for different storage conditions.

- A wet spot at 16% w.b affecting 10% of the grain loaded at 13% w.b increases 3 to 4 points $CO_2$ levels with respect to the referential curve.

- Significant penetration of $O_2$ through a 1cm diameter hole. A silobag initially in anaerobiosis, may attain $O_2$ levels of 10% V/V in ten days

## Future work and model improvements

- Respiration rate $Y_{CO2}$= f(W, T, $CO_2$,$O_2$)
- 3D model : analysis of local effects along the longitudinal direction on the silobag

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ANPCYT/FONCYT (PICT 2008 0460)

National University of Rosario (PID ING295)

INTA-PRECOP Proyect: Postharvest Efficiency

# Thank you very much for your attention…..

## Input parameters of Difussion model (CO2 and O2)

$$\log Y_{CO2} = -4.054 + 0.0406\,T - 0.0165\,\theta + 0.0001\,\theta^{2} + 0.2389\,M$$ White et al. (1982)

Wheat porosity = 0.38; Wheat tortuosity = 1.5

Equivalent permeability of the plastic layer
$P_{O2}$ = 9.75 10-$^{8}$ $m^3 md^{-1} m^{-2} at^{-1}$
$P_{CO2}$= 3.22 $10^{-7}$ $m^3 md^{-1} m^{-2} at^{-1}$

$$h_i = \frac{P_i P_{at}}{L}$$

Effective diffusivity of the plastic layer
$D^*_{CO2}$ = 3.97 $10^{-6}$ $m^2 s^{-1}$
$D^*_{O2}$ = 5.22 $10^{-6}$ $m^2 s^{-1}$

$$Bi = \frac{V h_i}{A D_i^*} \cong 10^{-4}$$

For one meter long of silobag,
transfer area *A*= 5.54 $m^2$; volume *V* = 4.54 $m^3$
Plastic thickness *L* is 240 $\mu$m

## Silobags Characteristic Dimensions

Length: 60 m ; Diameter 2.70 m ; Thickness : 230 - 250 microns (U$D 400)

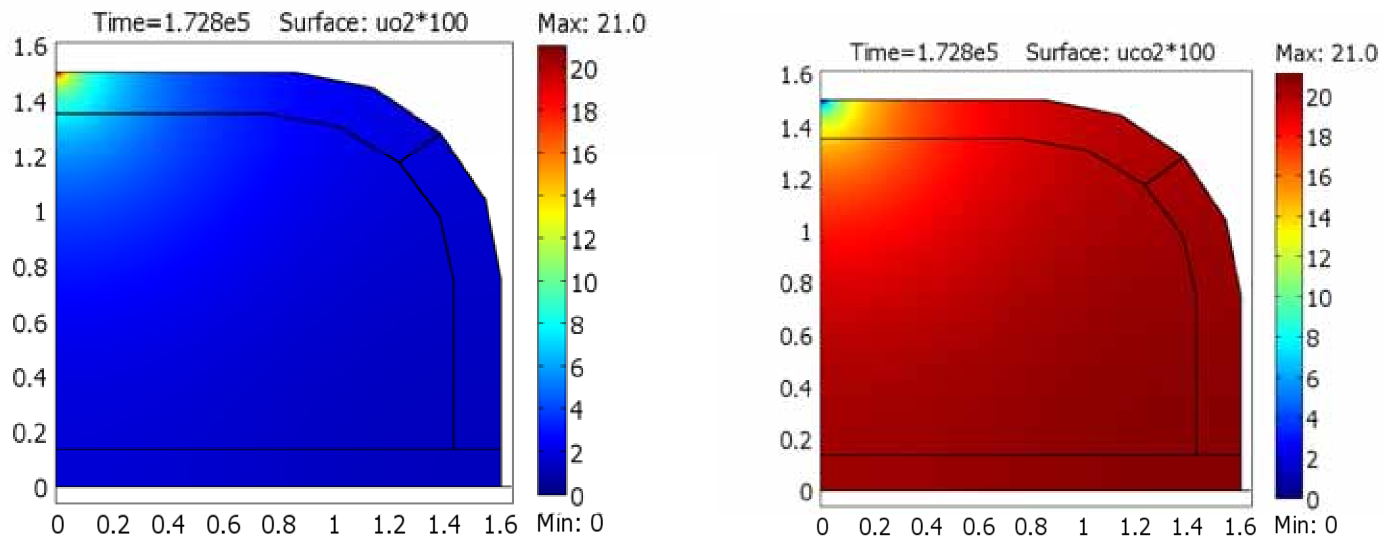
Made of a three-layer plastic, (HDPE and LDPE)

Black in the inner side and white in the outer side with UV stabilizers.

Storage capacity : 200 tones of wheat , soybean and corn; 120 tones of sunflower

Storage time: six to eight months

*Distribution of O2 (a) and CO2 (b) concentration (%V/V) after two days of storage*



## Diffusion Model

$$\varepsilon \frac{\partial CO_2}{\partial t} = \frac{\partial}{\partial x}\left[D^*_{CO2}\left(\frac{\partial CO_2}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D^*_{CO2}\left(\frac{\partial CO_2}{\partial y}\right)\right] + \rho_{bs}\, r_{CO2} \text{ in } \Omega_1$$

$$\varepsilon \frac{\partial O_2}{\partial t} = \frac{\partial}{\partial x}\left[D^*_{O2}\left(\frac{\partial O_2}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D^*_{O2}\left(\frac{\partial O_2}{\partial y}\right)\right] + \rho_{bs} r_{O2} \quad \text{in } \Omega_1$$

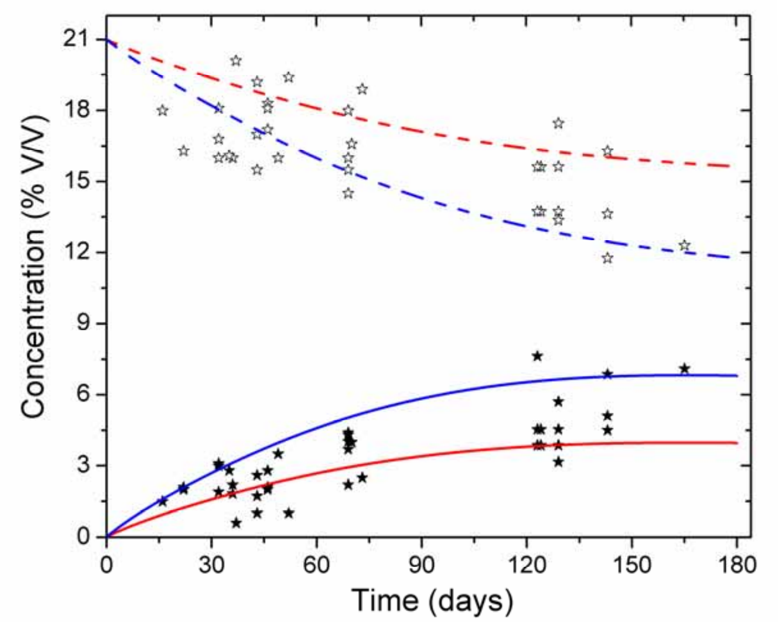
$$r_{CO2} = \frac{Y_{CO2}}{1000 M_{CO2}} \frac{RT}{P_{at}} \quad ; \quad r_{O2} = r_{CO2}$$

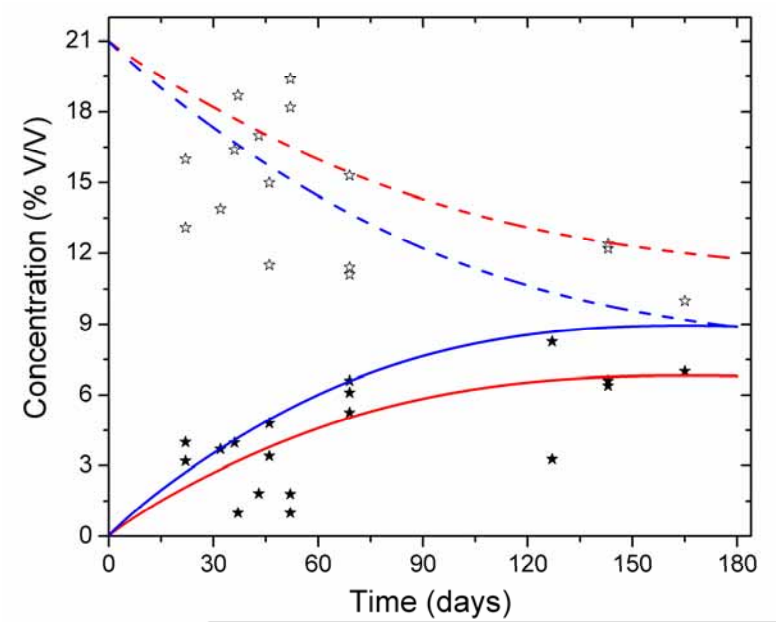
## Lumped Model

$$\frac{d\overline{O}_2}{dt} = K_{O_2}\frac{\left(O_{2out} - \overline{O}_2\right)}{\varepsilon V} - \frac{\rho_{bs}}{\varepsilon}\bar{r}_{O2}\left(\overline{T}, W_0\right) \qquad in\ \Omega_1$$

$$\frac{d\overline{CO}_2}{dt} = K_{CO_2}\frac{\left(CO_{2out} - \overline{CO}_2\right)}{\varepsilon V} + \frac{\rho_{bs}}{\varepsilon}\bar{r}_{CO2}\left(\overline{T}, W_0\right) \qquad in\ \Omega_1$$

$$r_{CO2} = \frac{Y_{CO2}\left(\overline{T}, W_0\right)}{1000 M_{CO2}}\frac{R\overline{T}}{P_{at}} \quad ; \quad r_{O2} = r_{CO2}$$


Concentration (% V/V)
Time (days)
0
3
6
9
12
15
18
21
0
30
60
90
120
150
180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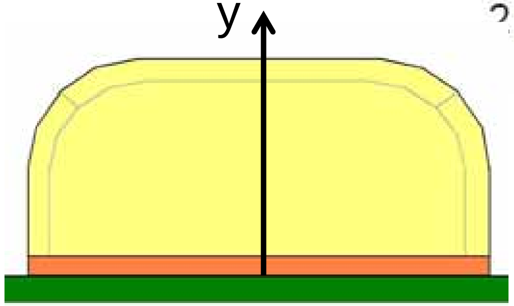


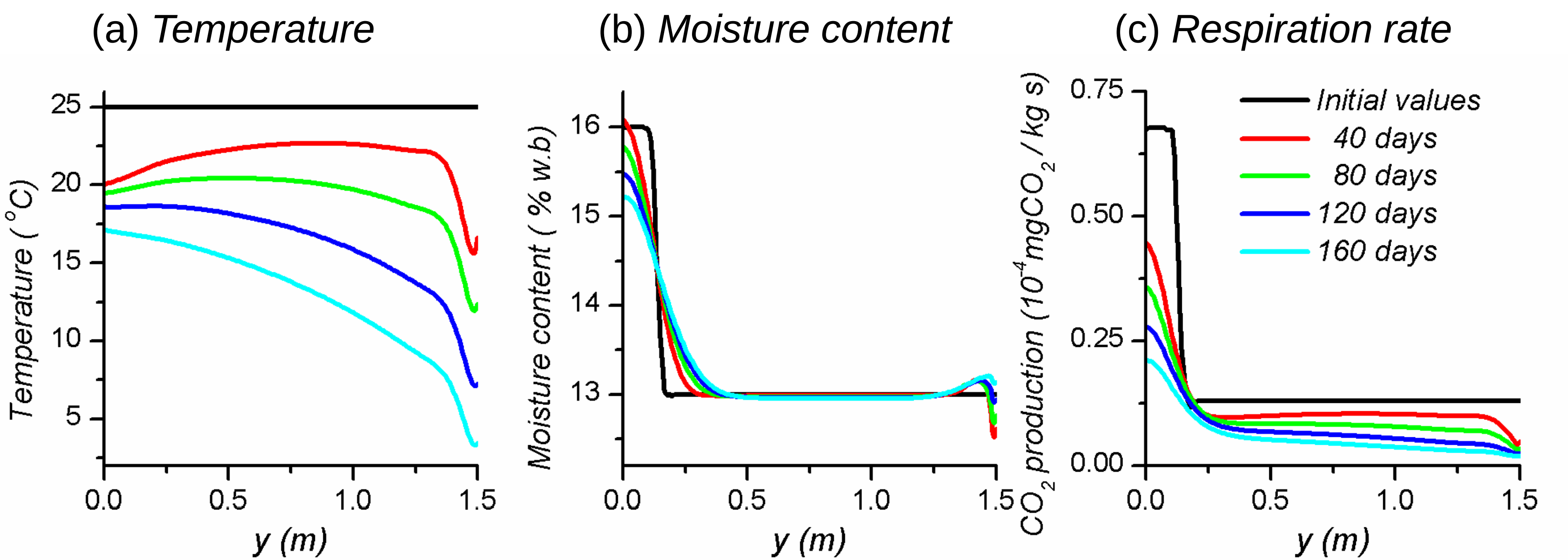

$$-k\frac{\partial T}{\partial n} = h_c\left(T - T_a\right) - \alpha G + \xi\sigma\left(T^4 - T_{sky}^4\right) \quad on \quad \Gamma_1$$

$$T = T_{soil}(y,t) \quad on \quad \Gamma_3$$

$$\frac{\partial p_v}{\partial n} = 0 \Rightarrow \eta D_{ef}\frac{\partial W_g}{\partial n} = -\omega D_{ef}\frac{\partial T}{\partial n} \quad \Gamma_1 + \Gamma_2$$

$$-D^*_{CO_2}\frac{\partial CO_2}{\partial n} = \frac{P_{CO_2}P_{atm}}{L}\left(CO_2 - CO_{2out}\right) = h_{CO_2}\left(CO_2 - CO_{2out}\right) \quad on \quad \Gamma_1$$

$$-D^*_{O_2}\frac{\partial O_2}{\partial n} = \frac{P_{O_2}P_{atm}}{L}\left(O_2 - O_{2out}\right) = h_{O_2}\left(O_2 - O_{2out}\right) \quad on \quad \Gamma_1$$