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Research Paper

Validation of a heat, moisture and gas concentration transfer model for soybean (*Glycine max*) grains stored in plastic bags (silo bags)

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A two dimensional finite element model that predicts temperature distribution and moisture content of soybean stored in silo bags due to seasonal variation of climatic conditions is described. The model includes grain respiration and calculates carbon dioxide and oxygen concentrations during storage.

The model validation was carried out by comparing predicted temperature, moisture content and gas concentration with measured data in field tests. Overall, the model underpredicted grain temperatures. Mean absolute difference was 0.5–1 °C for the bottom and middle layers and about 1.5 °C for the top layer. A slight moisture increase (0.4% w.b. at most) was predicted for the top grain layer while moisture for the middle and bottom layers remained almost unchanged during the storage period.

A model of respiration rate of soybean as a function of temperature, moisture content and O_2 level was used to predicted gas concentrations in the interstitial air. Average CO_2 and O_2 concentrations were compared with measured data. As mean grain temperature was below 15 °C for most of the storage period, O_2 consumption and CO_2 production were low. O_2 level was about 19–20% V/V for dry soybean (13% w.b.) and about 16–17% V/V for wet soybean (15% w.b.). Predicted CO_2 concentration varied from 1% V/V for dry soybean (13% w.b.) to 2% V/V points for wet soybean (15% w.b.). Though CO_2 relative differences were high, the general trends of measured gas evolution were compatible with the simulated ones, indicating that the changes in CO_2 and O_2 concentrations during storage were satisfactorily predicted by use of the proposed correlations.

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Notation

x, y	Cartesian coordinates, m
c	specific heat capacity of grain bulk, J kg^{-1} K^{-1}
C_H, K_H, N	parameters of the modified Henderson equation, °C, °C^{-1}, dimensionless, respectively
CO_2	carbon dioxide concentration, % V/V
D_i	diffusivity of component i through air, m^2 s^{-1} (with i = w, CO_2 and O_2)
D_i^*	effective diffusivity of component i through intergranular air, m^2 s^{-1}
G	incident solar radiation on the silo bag surface, W m^{-2}
h_c	convective heat transfer coefficient, W m^{-2} K^{-1}
k	thermal conductivity, W m^{-1} K^{-1}
L	silo bag characteristic length, m
L_g	latent heat of vaporisation of moisture in the grain, J kg^{-1}
M	grain moisture content, % w.b.
M_i	molecular weight of component i, grams mol^{-1} (with i = CO_2 and O_2)
n	normal direction
O_2	oxygen concentration, % V/V
p_s	saturation pressure of water vapour, Pa
p_v	partial pressure of water vapour, Pa
p_{atm}	atmospheric pressure, 101,325 Pa
P_{CO_2}	equivalent permeability of CO_2 through plastic layer, m^3 m s^{-1} m^{-2} Pa^{-1}
P_{O_2}	equivalent permeability of O_2 through plastic layer, m^3 m s^{-1} m^{-2} Pa^{-1}
q_H	heat released in respiration, 14.766 J mg^{-1} [O_2]
q_w	water vapour produced in respiration, 5.62×10^{-7} kg [H_2O] mg^{-1} [O_2]
R_w	water vapour gas constant, 461.52 J kg^{-1} K^{-1}
R_g	universal gas constant, 8.314 J mol^{-1} K^{-1}
R	correlation coefficient
t	time, s
T_C	temperature, °C
T	absolute temperature, K
T_{Ci}	daily or annual soil temperature parameters, °C, i = 1, 2
V	bed of grain volume, m^3
W	grain moisture content, d.b.
Y_{CO_2}	rate of carbon dioxide production, mg [CO_2] kg^{-1} [dry matter] d^{-1}
Y_{O_2}	rate of oxygen consumption, mg [O_2] kg^{-1} [dry matter] d^{-1}
Y_{H_2O}	rate of water vapour production, mg [H_2O] kg^{-1} [dry matter] d^{-1}

Greek symbols

α	silo bag surface absorptivity
ε	porosity, fractional
φ	daily or annual phase angle
Γ	domain boundary
η	change in the partial pressure due to change in the moisture content at constant temperature, Pa
ρ	density, kg m^{-3}
ρ_{bs}	dry bulk density, kg [dry matter] m^{-3}
σ	Stefan–Boltzmann's constant, 5.6697×10^{-8} W m^{-2} K^{-4}
τ	tortuosity factor
ω	change in the partial pressure due to change in the temperature at constant moisture content, Pa K^{-1}
Ω	domain
ξ	emissivity
ψ	daily or annual angular frequency, s^{-1}

Subscripts

amb	ambient
b	bulk grain
g	grain
0	initial
sky	sky
soil	soil
w	water vapour

1. Introduction

During the last 10 years the overall grain production in Argentina increased by 50 Mt and soybean was the greatest contributor to this increase. Soybean has a major impact on the Argentina economy. Argentina is the third world producer (after the USA and Brazil) and exporter of soybean, the fourth world producer of soybean meal (after China, the USA and Brazil) and the largest exporter of soybean meal and soybean oil. The Argentine soybean chain is the most integrated in world trade: more than 90% of total production is destined for international markets (Ciani, 2016; Regunaga, 2010).

In Argentina during year 2014, around 200,000 "silo bags" were used to store more than 40% of the total grain production (107 Mt) (INTA Informa, 2014). Because of its economic implications (grain identity preservation, variety segregation, farm logistics, storage cost reduction, marketing benefits, etc.) and successful experience of this technology during the last 15 years in Argentina, the silo bag system is now being adopted in more than 40 countries worldwide with a wide range of weather conditions, from hot (e.g. Sudan and Brazil) to cold (e.g., Russia and Canada) (Bartosik, 2012).

This storage technique was originally used for grain silage, and is now used for storing dry grain in sealed plastic bags. The respiration process of the biological agents in the grain ecosystem (grain, insects, mites and microorganisms) increases carbon dioxide (CO_2) and reduces oxygen (O_2) concentrations. This modified atmosphere inhibits biotic activity, promoting a suitable environment for grain conservation (Navarro, Noyes, & Jayas, 2002, chap. 2).

Gas concentration depends on the balance between respiration of the ecosystem, the entrance of external O_2 to the system, and the loss of CO_2 to the ambient air. The transfer of gases depends on the gas partial pressure differential and the effective permeability of the plastic cover (openings and natural permeability of the plastic layer to gases). Grain type and condition, moisture content (MC), temperature, storage time and O_2 and CO_2 concentrations affect the biotic respiration rate (Abalone, Gastón, Bartosik, Cardoso, & Rodríguez, 2011a, 2011b; Arias Barreto, Abalone, & Gastón, 2013; Gastón, Abalone, Bartosik, & Rodríguez, 2009; Navarro et al., 2002).

The research carried out so far in Argentina to analyse the effect of grain MC and storage time on the quality of several commodities (wheat, corn, sunflower, soybean, barley) was summarised by Bartosik (2012). Based on previous work (Abalone et al., 2011a, 2011b; Gastón et al., 2009), Arias Barreto et al. (2013) applied a validated mathematical model to analyse grain storage condition and determine the change in concentration of CO_2 and O_2 in a silo bag holding wheat from summer to winter for typical productive regions with three distinctive weather conditions of Argentina: sub-tropical, intermediate and temperate.

Among the work related to silo bag storage in other countries, Darby and Caddick (2007) published an exhaustive analysis and field evaluation of silo bag technology for storing mainly wheat under typical Australian conditions. Chelladurai, Jian, Jayas, and White (2011) analysed the feasibility of storing canola in silo bags under western Canadian prairie conditions. Canola of 8, 10, 14% w.b. MC was loaded into the bags and temperature, seed germination, free fatty acid value (FAV), and intergranular CO_2 concentration were measured. There was no significant change in quality of dry seeds stored in the silo bags. Recently, Jian, Challadurai, Jayas, and White (2015a, 2015b) presented a three-dimensional transient heat, mass, and momentum transfer model to predict conditions of canola stored inside silo bags under Canadian prairie conditions. The developed model calculated the condensation and production of water and heat generated by the respiration of microorganisms inside silo bag and was validated by comparing predicted temperature and MC with measured data. Although momentum transfer was taken into account, no information was provided regarding the magnitude of convection currents developed under Canadian climatic conditions.

Due to the economic importance that soybean production has for Argentina and the need to preserve its quality during storage prior to processing, the aims of the present work were:

(1) to adapt the heat and mass transfer model presented by Arias Barreto et al. (2013) to analyse the storage of soybean in silo bags. Correlations developed by Ochandio (2014) for soybean CO_2 production and O_2 consumption were used to model soybean respiration.
(2) to validate the heat, moisture and gas transfer model by comparing the predictions of temperature, moisture content and CO_2 and O_2 gas concentrations with field measured data.

2. Materials and method

2.1. *Silo bags*

The silo bags considered in this study are 60 m long, 2.70 m diameter and 235 μm thick. The bags are made with a three-layer plastic, black on the inner side and white on the outer side with UV stabilisers. The plastic layers are a mixture of high density (HDPE) and low density polyethylene (LDPE). Permeability at 25 °C of HDPE to O_2 is 7.43×10^{-18} m^3 m s^{-1} m^{-2} Pa^{-1} and of LDPE is 2.22×10^{-17} m^3 m s^{-1} m^{-2} Pa^{-1}. Permeability at 25 °C of HDPE to CO_2 is 2.16×10^{-17} m^3 m s^{-1} m^{-2} Pa^{-1} and of LDPE is 1.20×10^{-16} m^3 m s^{-1} m^{-2} Pa^{-1} (Osborn & Jenkins, 1992).

Approximately 200 t of wheat and 180 t of soybean can be held in the bag and usually farmers store their grain for six to eight months.

2.2. *Mathematical modelling*

2.2.1. *Model assumptions*

The following assumptions were made to simplify the mathematical model:

(1) the bed of grain is assumed to be a continuum where the grain phase and intergranular air phase are evenly distributed through the porous media;
(2) in a control volume, grain and intergranular air are in local thermodynamic equilibrium;
(3) a planar 2D model is adopted;
(4) convection transport is not considered;
(5) grain bed shrinkage is negligible;
(6) moisture diffusion by grain to grain contact (Pixton & Griffiths, 1971) and accumulation of moisture in the intergranular air are negligible and the air–vapour mixture behaves as an ideal gas (Khankari, Morey, & Patankar, 1994).

The Method of Volume Average (Slattery, 1972; Whitaker, 1977) is applied to obtain the average transport equations of energy and mass transfer in porous media such as grain bulks. Non-equilibrium models consider four independent variables in time and space, the temperatures and moisture contents of intergranular air and grain kernels, while equilibrium models have two independent variables, the temperature of intergranular air and grain kernels and moisture content of grain or air, with these latter two variables related by a sorption isotherm. Non-equilibrium models are usually applied to model high temperature and high flow rate drying of grain (Aregba, Sebastian, & Nadeau, 2006; Aregba & Nadeau, 2007; Brooker, Bakker-Arkema, & Hall, 1992; Giner, Mascheroni, & Nellist, 1996; Zare & Chen, 2009) while equilibrium models have been shown to be adequate to model low temperature and low flow rate drying or aeration (Sharp, 1982; Sutherland, Banks, & Griffiths, 1971; Thompson, Peart, & Foster, 1968). Natural convection currents are several orders of magnitude smaller than those involved in drying or aeration of bulks of grain. Therefore, the grain kernels and intergranular air have enough time to be in contact and attain equilibrium. To model non-aerated grain bulks, equilibrium models have been successfully applied to predict temperature and moisture content changes as result of weather conditions (Gastón et al., 2009; Jian et al., 2015b; Khankari, Morey, & Patankar, 1995; Khankari, Patankar, & Morey, 1995; Khankari et al., 1994; Lawrence, Maier, & Stroshine, 2013a, 2013b; Montross, Maier, & Haghighi, 2002a, 2002b; Smith & Sokhansanj, 1990).

Silo bags are 60 m long and, after loading, the initial and final portion of the bag may roughly represent 5–10% of its total length. On the one hand, regardless of the N–S or E–W orientation of a silo bag in the field, ambient conditions and solar radiation are uniform for a cross section along the longitudinal axis, except at the ends of the bag. Therefore, in most of the silo bag, heat and mass transfer in the longitudinal direction will be negligible compared to that across the cross section of the silo bag. On the other hand, as will be explained later, the data used for model validation was recorded at the middle of the bag, far from the influence of the ends. Because, in the present study, initial temperature and MC are assumed to be constant, the use of a 2D model is justified. A 3D model is mandatory when a non-uniform initial MC distribution is considered as a result of the loading process (Arias Barreto, 2016). When the initial and final portion of the bag are comparable to the total length of the silo bag, a 3D model would be necessary. Recently, Chelladurai (2016) analysed the feasibility of storing canola in silo bags. The study reported measured data in a silo bag 21.34 m long. The head and tail of the bag were 4.57 m each (43% of total length). It was found that the grain layer (top, middle and bottom) had significant effect on moisture content changes but not the sample location along the bag (head, centre, and tail). These results show that even in a silo bag that is one third of the standard length (60 m), the experimental moisture data did not show a significant influence of the head or tail of the bag.

Arias Barreto (2016) analysed the effect of natural convection currents on temperature distribution and moisture migration in a silo bag holding wheat and soybean with N–S and E–W orientation for typical agricultural areas of Argentina with moderate, intermediate and subtropical weather conditions. The inclusion of convective transport did not produce significant changes with respect to considering only diffusive transport in the energy and mass equations. Therefore natural convection was not included to keep the model as simple as possible.

For conservation, grains are usually stored with low moisture content. Measured moisture changes during storage due to migration are in the order 1% w.b. As a result, grain bed shrinkage will be very small. Generally, shrinkage must be taken into account when modelling drying of high moisture content products like vegetables and fruits (Katekawa & Silva, 2006) as well as deep beds of grains (Bartosik, 2005).

2.2.2. *Energy and mass transfer balances*

Stating the energy and mass balances for the grain and air phases in a control volume, a coupled system in terms of temperature T, grain moisture content W_g, oxygen O_2 and carbon dioxide CO_2 concentrations is derived:

$$c_b \rho_{bs} \frac{\partial T}{\partial t} = \left[\frac{\partial}{\partial x}\left[k_b \frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[k_b \frac{\partial T}{\partial y}\right]\right] + \rho_{bs} L_g \frac{\partial W_g}{\partial t} + \rho_{bs} q_H Y^*_{O_2} \quad \text{in } \Omega_1 \tag{1}$$

$$\rho_{bs} \frac{\partial W_g}{\partial t} = \frac{\partial}{\partial x}\left[D_w \left(\eta \frac{\partial W_g}{\partial x} + \omega \frac{\partial T}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D_w \left(\eta \frac{\partial W_g}{\partial y} + \omega \frac{\partial T}{\partial y}\right)\right] + \rho_{bs} q_w Y^*_{O_2} \quad \text{in } \Omega_1 \tag{2}$$

$$\varepsilon \frac{\partial CO_2}{\partial t} = \frac{\partial}{\partial x}\left[D^*_{CO_2}\left(\frac{\partial CO_2}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D^*_{CO_2}\left(\frac{\partial CO_2}{\partial y}\right)\right] + \rho_{bs} r_{CO_2} \quad \text{in } \Omega_1 \tag{3}$$

$$\varepsilon \frac{\partial O_2}{\partial t} = \frac{\partial}{\partial x}\left[D^*_{O_2}\left(\frac{\partial O_2}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[D^*_{O_2}\left(\frac{\partial O_2}{\partial y}\right)\right] + \rho_{bs} r_{O_2} \quad \text{in } \Omega_1 \tag{4}$$

where T in K is temperature, W_g in d.b. is grain moisture content, O_2 and CO_2 (% V/V) are oxygen and carbon dioxide concentrations, ε porosity, ρ_{bs} in kg m^{-3} is dry bulk density, c_b in J kg^{-1} K^{-1} is bulk specific heat, k_b in W m^{-1} K^{-1} is bulk thermal conductivity, L_g in J kg^{-1} is the latent heat of vaporisation of moisture in the grain, η in Pa is the change in the partial pressure due to change in the MC at constant temperature, ω in Pa K^{-1} is the change in the partial pressure due to change in the temperature at constant MC, R_w in J kg^{-1} K^{-1} is water vapour gas constant, D^*_i in m^2 s^{-1} (with i = w, CO_2 and O_2) is the effective diffusivity through the intergranular air of water vapour, carbon dioxide and oxygen, calculated according to Thorpe (1981) and Geankoplis (1998), where D_i in m^2 s^{-1}, is the diffusivity of component i through air, and τ is grain tortuosity:

$$D^*_i = \frac{\varepsilon D_i}{\tau}; \quad i = w; O_2; CO_2 \tag{5}$$

In Eqs. (1)–(4), the last term represents heat, water vapour and carbon dioxide released and oxygen consumed, respectively, due to respiration of the grain ecosystem. To account for heat and moisture released, respiration is modelled as complete combustion of a typical carbohydrate. $Y^*_{CO_2}$ is the rate of CO_2 production, in mg [CO_2] kg^{-1} [dry matter] s^{-1}, $Y^*_{O_2}$ is the rate of O_2 consumption, in mg [O_2] kg^{-1} [dry matter] s^{-1}, q_H is 14.766 J mg^{-1} [CO_2], q_w is 5.62 × 10^{-7} kg [H_2O] mg^{-1} [O_2]; $Y^*_i = Y_i/86,400$. The rate of CO_2 production r_{CO_2} and O_2 consumption r_{O_2} in m^3 s^{-1} kg^{-1} [dry matter] are given by:

$$r_i = \frac{Y^*_i R_g T}{1,000 M_i p_{atm}}; \quad i = O_2; CO_2 \tag{6}$$

Boundary conditions associated with Eqs. (1)–(4) are given by:

$$-k_b \frac{\partial T}{\partial n} = h_c(T - T_{amb}) - \alpha G + \xi\sigma\left(T^4 - T^4_{sky}\right) \quad \text{on } \Gamma_1 \tag{7}$$

$$\sigma T^4_{sky} = \xi_{sky} \sigma T^4_{amb} \tag{8}$$

$$\frac{\partial p_v}{\partial n} = 0 \;\Rightarrow\; \eta D_w \frac{\partial W_g}{\partial n} = -\omega D_w \frac{\partial T}{\partial n} \quad \text{on } \Gamma_1 + \Gamma_2 \tag{9}$$

$$-D^*_{CO_2} \frac{\partial CO_2}{\partial n} = \frac{P_{CO_2} P_{atm}}{L}(CO_2 - CO_{2out}) \quad \text{on } \Gamma_1 \tag{10}$$

$$-D^*_{O_2} \frac{\partial O_2}{\partial n} = \frac{P_{O_2} P_{atm}}{L}(O_2 - O_{2out}) \quad \text{on } \Gamma_1 \tag{11}$$

and initial conditions by:

$$T(x, y, t = 0) = T_0 \quad \text{on } \Omega_1 \tag{12}$$

$$W(x, y, t = 0) = W_0 \quad \text{on } \Omega_1 \tag{13}$$

$$O_2(x, y, t = 0) = 21\% \quad \text{on } \Omega_1 \tag{14}$$

$$CO_2(x, y, t = 0) = 0.03\% \quad \text{on } \Omega_1 \tag{15}$$

To account for the interaction between the soil and the bottom layer of the silo bag, a subdomain Ω_2 was incorporated into the heat transfer model. Convection and radiation loss to the ambient and incident solar radiation were taken into account on the soil surface Γ_3. At 2 m depth (Γ_5), the mean annual local soil temperature was imposed, with the other boundaries isolated (Γ_4). The initial soil temperature T_{soil} in K was calculated with the following expression (Carslaw & Jaeger, 1959) where t_1 is the bagging date:

$$T = T_{soil}(y, t_1) = 273.15 + T_{C1}(y) + T_{C2} \exp\left(-y\sqrt{\frac{2\Psi}{D_{soil}}}\right) \left[\cos\left(\Psi t_1 - y\sqrt{\frac{2\Psi}{D_{soil}}} - \varphi\right)\right] \quad \text{on } \Gamma_3 \tag{16}$$

2.3. Input model parameters

The Modified Henderson equation was used to model soybean sorption equilibrium (Brooker et al., 1992):

$$p_v = p_s\left\{1 - \exp\left[-K_H(C_H + T_c)(100W_g)^N\right]\right\} \tag{17}$$

where p_s in Pa is the saturation vapour pressure. Model parameters L_g, η, ω, were calculated applying Eq. (17) as described in detail in Gastón et al. (2009). Parameters of Eq. (17) are listed in Table 1 as well as bulk density, porosity of the bed and thermal properties of soybean grain. Water vapour properties are listed in Table 2.

The equivalent permeability of the silo bag to O_2 and CO_2 was calculated by use of a resistance series model (Abalone et al., 2011b, 2011a). Estimated equivalent permeability to O_2 was 1.11×10^{-17} m^3 m s^{-1} m^{-2} Pa^{-1} and to CO_2 was 3.67×10^{-17} m^3 m s^{-1} m^{-2} Pa^{-1}. The radiometric properties of the plastic bag are listed in Table 3 (Gastón et al., 2009).

Table 3 – Input parameters of the thermal model.

Reference	Parameter
Sky emissivity (Mills, 1995)	$\xi_{sky} = 0.82$
Silo bag emissivity	$\xi = 0.6$
Silo bag absorptivity	$\alpha = 0.26$

2.4. Soybean rate of respiration

Ochandio (2014) measured CO_2 and O_2 concentration of soybean stored in hermetic flasks at 15, 25 and 35 °C under laboratory conditions. Rate of O_2 consumption and CO_2 production were obtained from experimental data and correlations depending on O_2 concentration and temperature were developed for 13%, 15% and 17% w.b. soybean moisture content.

For 13% w.b. moisture content:

$$Y_{CO_2} = -1.020 - 0.0878 O_2 + 0.0512 T_c + 0.00676 T_c O_2, \quad R = 0.914 \tag{18}$$

$$Y_{O_2} = 0.972 + 0.124 O_2 - 0.0437 T_c - 0.0105 T_c O_2, \quad R = 0.962 \tag{19}$$

For 15% w.b. moisture content:

$$Y_{CO_2} = 0.595 - 0.492 O_2 + 0.00925 T_c + 0.0258 T_c O_2, \quad R = 0.959 \tag{20}$$

$$Y_{O_2} = 0.468 + 0.229 O_2 - 0.0454 T_c - 0.0200 T_c O_2, \quad R = 0.984 \tag{21}$$

For 17% w.b. moisture content:

$$Y_{CO_2} = -5.813 - 0.577 O_2 + 0.379 T_c + 0.0420 T_c O_2, \quad R = 0.918 \tag{22}$$

$$Y_{O_2} = 0.617 + 0.888 O_2 - 0.0687 T_c - 0.0712 T_c O_2, \quad R = 0.976 \tag{23}$$

Figures 1 and 2 plot the rate of O_2 and CO_2 respiration for the 15–35 °C temperature range, 21% V/V and 10% V/V O_2 concentration, 13, 15 and 17% w.b., applying the correlation listed above (negative values mean consumption and positive ones production). It can be observed that at 15 °C respiration is very low.

Table 1 – Input parameters of bed of soybean.

Reference	Property
Henderson equation parameters (Brooker et al., 1992)	$K_H = 30.053 \times 10^{-5}$; $C_H = 1.216$; $N = 134.136$
Bulk density, kg m^{-3} (ASABE, 2003a)	$\rho_b = 734.5 - 219M + 70M^2$
Grain thermal conductivity, W m^{-1} K^{-1} (ASABE, 2003b)	$k = 0.139 + 0.00123M$
Bulk specific heat, kJ kg^{-1} K^{-1} (ASABE, 2003b)	$c_b = 1.699 + 0.0172M$
Porosity (ASABE, 2003a)	$\varepsilon = 0.34$
Tortuosity (Keey, 1975)	$\tau = 1.53$

Table 2 – Water vapour properties.

Reference	Property
Water vapour diffusivity in air, m^2 s^{-1} (Thorpe, 1981)	$D_V = \frac{9.1 \times 10^{-9} (T)^{2.5}}{(T + 245.18)}$
Saturation vapour pressure, Pa (Giner et al., 1996)	$p_s = \exp\left\{54.12 - \frac{6547.1}{T} - 4.230 \ln T\right\}$

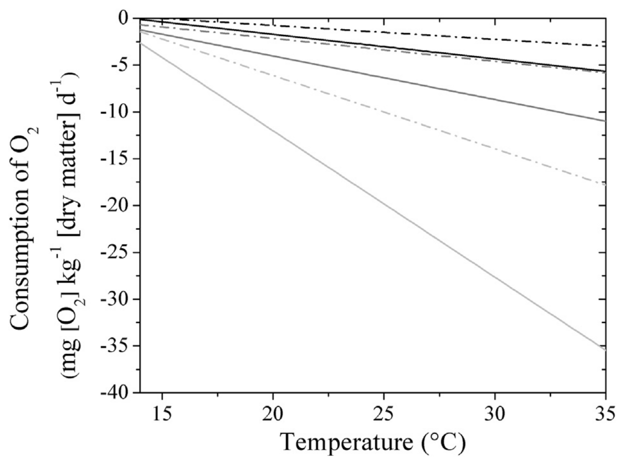

Fig. 1 – Soybean rate of O_2 consumption as function of temperature. O_2 21% V/V: ——, 13% w.b.; ——, 15% w.b.; ——, 17% w.b.; O_2 10% V/V: – · –, 13% w.b.; – · –, 15% w.b.; – · –, 17% w.b.

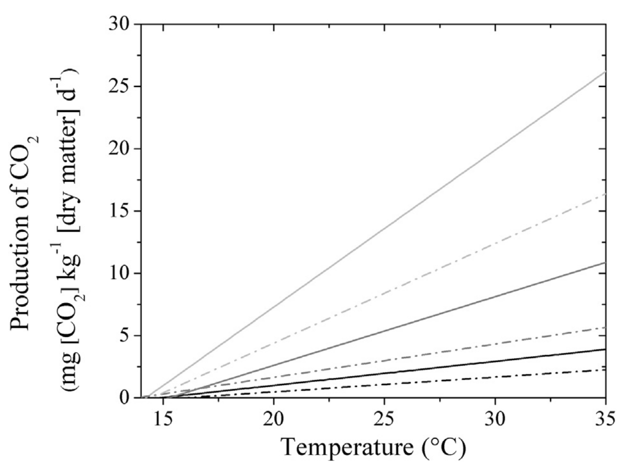

Fig. 2 – Soybean rate of CO_2 production as function of temperature. O_2 21% V/V: ——, 13% w.b.; ——, 15% w.b.; ——, 17% w.b.; O_2 10% V/V: – · –, 13% w.b.; – · –, 15% w.b.; – · –, 17% w.b.

As these correlations were obtained for the 15–35 °C range, according to the trend of behaviour shown by the curves in Figs. 1 and 2, it was assumed that respiration below 15 °C was negligible. This assumption is supported by the experimental data reported by Ochandio, Bartosik, Yommi, and Cardoso (2012). When soybean was incubated at 11% and 13% w.b. and 5 °C, almost no increase in CO_2 was observed after 1 year (less than 1%) and at 17% w.b., the CO_2 concentration increased to 5.5–7% V/V after 1 year.

Besides, since the correlations depend linearly on O_2, around 15 °C, the application of Eqs. (18)–(23) is limited to give a negative value for O_2 rate of respiration (consumption) and a positive one for CO_2 rate of respiration (production), in other words to avoid a result without physical meaning.

2.5. *Numerical solution*

The mathematical model was implemented using COMSOL Multiphysics 4.3 and solved numerically by the finite element method (AB COMSOL, 2013). Figure 3a shows the calculation domain, which represents a cross section of the silo bag and the soil. A refined mesh was generated at the boundaries of the silo bag (Fig. 3b), where the highest temperature and moisture gradients are expected. Quadratic Lagrangian elements and a fourth order numerical quadrature were applied. A total of 23,596 elements were used to discretise the silo bag domain Ω_1 and 9,067 elements for the soil domain Ω_2. A further mesh refinement of the silo bag did not produce significant changes in numerical results. An implicit scheme algorithm (BDF, Backward Difference Formula of order 2) was used to discretise the temporal variable. UMFPACK solver was selected to solve the PDE system (unsymmetrical multifrontal method and direct sparse LU factorisation). The calculation time corresponding to the simulation of 240 days of grain storage was approximately 20 min on an Intel Core i7 computer with 16 GB of RAM.

The step change in respiration rate below 15 °C was handled by use of a smoothed Heaviside Function available in COMSOL Multiphysics 4.3. Also, to avoid unrealistic values of the respiration rates, the sign of the calculated values is checked. If the change in sign occurs slightly above 15 °C, the respiration rate is set to zero.

2.6. *Experimental field tests used to validate soybean temperature and moisture content predictions*

Two tests were carried out for soybean (*Glycine max, Nidera 4100, cultivar*) on a farm (Estancia San Lorenzo de Zubiaurre S.A) close to Tandil (37.317 South, 59.150 West) in the south east of the Buenos Aires province, Argentina (Rodríguez, Bartosik, Malinarich, Exilart, & Nolasco, 2001). The objective

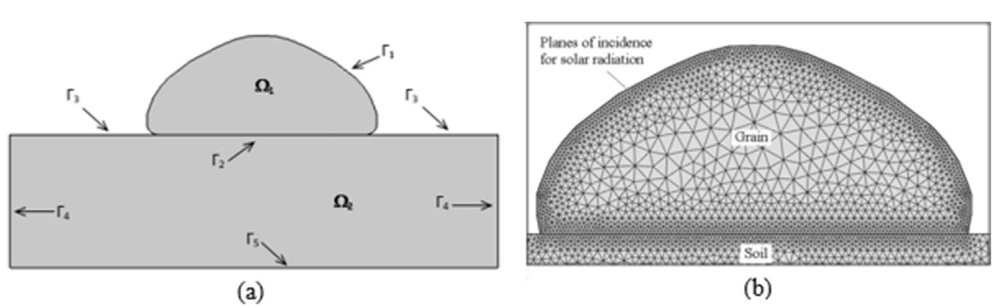

Fig. 3 – Discretisation of the calculation domain.

was to investigate the effect of silo bag storage conditions (temperature and MC) on the evolution of grain quality parameters during a storage period of 160 days. After harvest, one bag was filled with wet soybean (15.6% w.b.; 18.48% d.b.) and the other with dry soybean (12.5% w.b.; 14.28% d.b.). Grain temperatures at three levels in the bags (top = 1.45 m; middle = 0.8 m; bottom = 0.10 m; total height of the bag = 1.5 m) were recorded along with the ambient temperature (HOBO temperature datalogger) with an accuracy of ±0.5 °C.

The grain was sampled after 49, 92 and 160 days. Samples were taken with a simple truck probe at three levels in three locations along the length of the bag, with three replicates per location. Grain samples from each of the three sampling locations were segregated by level (top, middle, bottom). Moisture content was determined according to ASABE Standards S352.1 (1984). Experimental error in MC determination was ±0.5% w.b. After ANOVA of experimental data it was concluded that the grain layer (top, middle and bottom) had a significant effect on measured data (temperature or moisture content) but the sample location along the bag did not. Soybean from each level at each sampling location (at the centre of the bag and at 5 m from head and tail) was blended together for a composite sample per level. Several quality analyses (germination, test weight, damage test, composition, oil acidity index) were performed on each of the sub-samples. A detailed discussion of these tests was presented by Rodríguez et al. (2001).

2.7. Experimental field tests used to validate intergranular gas concentration predictions

The National Institute of Agricultural Technologies (INTA) of Argentina conducted a series of field experiments at Balcarce Experimental Station (EEA) in order to identify the main factors affecting carbon dioxide (CO_2) and oxygen (O_2) concentration as indicators of biological activity and appropriated soybean storability. The experiments consisted of monitoring the gas composition of the interstitial air, grain commercial quality, MC and grain temperature in silo bags. The tests were carried out at grain elevators and on farms in the south east of Buenos Aires province, Argentina. Most of the soybean silo bags were filled in April–May and stored until October or November, from autumn to spring during 2007. Initial moisture content was in the range 11–15% w.b. The silo bags were sampled every 20 days during the entire storage period. For each silo bag, two sampling locations were established. The procedure consisted of first measuring the gas concentration (O_2 and CO_2) with a portable gas analyser (PBI Dan Sensor, CheckPoint, Denmark), perforating the plastic cover with a needle. The gas composition was analysed for three levels in each sampling location, close to the top of the bag, at the middle and close to the bottom. Experimental error in gas concentration was ±0.5% V/V. The ANOVA showed that neither the grain layer (top, middle and bottom) nor the sample location along the bag had a significant effect on gas concentration. Therefore, average values for the silo bag were presented. The same behaviour was reported by Chelladurai (2016). A detailed discussion of the results of these tests was presented by Cardoso, Bartosik, Rodríguez, and Ochandio (2008) and Bartosik, Cardoso, and Rodríguez (2008).

2.8. Model accuracy

To determine the model accuracy, the criteria used by Jian, Jayas, and White (2014) and Jian et al. (2015a, 2015b) were applied. Mean relative difference (MRD), maximum relative difference (RD_{max}), mean absolute difference (MAD) and maximum absolute difference (AD_{max}) were calculated to evaluate the agreement between the predicted and measured variables ($X = T_c$, M, O_2, CO_2).

$$MRD = \frac{1}{n_s}\sum_{i=1}^{n_s}\frac{|(X_m - X)|}{X_m} \tag{24}$$

$$MAD = \frac{1}{n_s}\sum_{i=1}^{n_s}|(X_m - X)| \tag{25}$$

$$RD_{max} = \max\left(\frac{|(X_m - X)|}{X_m}\right) \tag{26}$$

$$AD_{max} = \max(|X_m - X|) \tag{27}$$

Linear regressions with zero intercept were calculated, and the slope was compared with a hypothetical slope of 1 using Student's t-test. A slope significantly <1 or >1 ($p < 0.05$) indicated that the predicted temperature respectively underestimated or overestimated the measured temperature. Data analysis was carried out with STATGRAPHICS® software (Statgraphics Centurion XVI, 2010).

3. Results and discussion

3.1. Heat and mass transfer model validation

To validate the model, temperature and MC evolution were simulated and the numerical results were compared with the experimental data. The field test started on June 5th, 2001. The initial bagging conditions of dry soybean were 12.5% w.b. (14.28% d.b.) and 6 °C while for wet soybean 15.6% w.b. (18.48% d.b.) and 10 °C, respectively.

A contribution to heat and water vapour by insect respiration was not included in the study since no insect infestation was detected (Rodríguez et al., 2001). Besides, this assumption has been widely justified in previous works (Abalone et al., 2011a; Arias Barreto et al., 2013; Gastón et al., 2009).

The horizontal global solar irradiance was calculated for the climatic conditions of Buenos Aires province with variable cloudiness. In the field, the silo bag had a N–S orientation. Incident solar radiation on silo bag boundary Γ_1 and soil surface Γ_3 was determined according to the orientation of each surface element.

Figure 4 compares the predicted and measured temperatures at the three levels (top = 1.45 m; middle = 0.80 m; bottom = 0.10 m) in the silo bag filled with dry soybean (12.5% w.b.) during 160 days. Computed temperatures at the top were compared only in the first 110 days because, as a result of thermocouple damage, no data was recorded thereafter at that level. Figure 5 compares the results for the silo bag with wet soybean (15.6% w.b.).

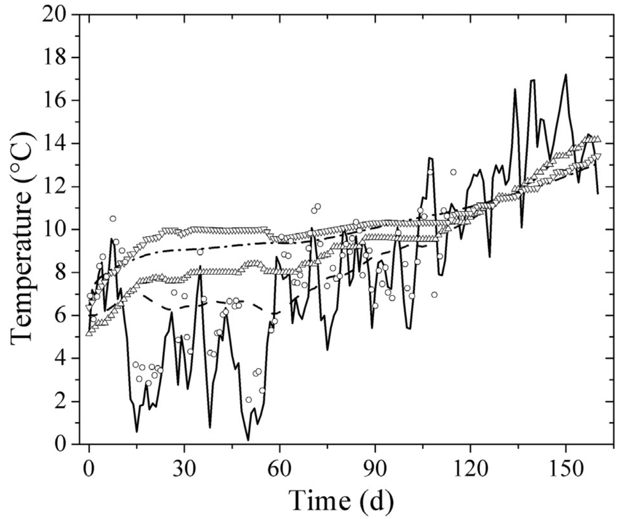

Fig. 4 – Comparison between measured (symbol) and predicted temperatures (line) at three levels in the silo bag during 160 days of storage (June–November 2001). ○, top; △, middle; ▽, bottom. ——, top; – – -, middle; – · –, bottom. M_0, initial moisture content 12.5% w.b.; T_0, initial temperature 6 °C.

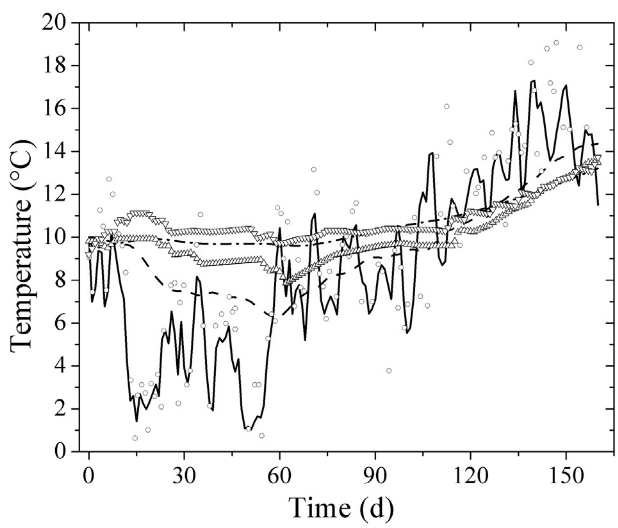

Fig. 5 – Comparison between measured (symbol) and predicted temperatures (line) at three levels in the silo bag during 160 days of storage (June–November 2001). ○, top; △, middle; ▽, bottom. ——, top; – – -, middle; – · –, bottom. M_0, initial moisture content 15.6% w.b.; T_0, initial temperature 10 °C.

Values of MRD, RD_{max}, MAD, AD_{max}, slope and Student's t-test values are summarised in Table 4. AD_{max} occurred at the top layer and was about 7 °C for the wet soybean bag and 5.4 °C for the dry one, while for the middle and bottom it was about 2 °C and 1 °C, respectively. Greater errors for the top layer may be explained by taking into account, on the one hand, the experimental error of thermocouple location inside the silo bag, and on the other hand, the variation of temperature associated with the point domain selected for comparison. Gastón et al. (2009) revealed that high temperature and moisture gradients developed below the silo bag surface within a layer of 0.1–0.20 m thick. However, the MAD was about 1.5 °C for the upper layer and from 0.5 to 1 °C for the middle and bottom layers. In all cases (expect the middle layer of the wet bag) the slope was significantly <1, implying that the model underpredicted the temperature.

Figures 4 and 5 presented the temperatures at the three levels in the silo bag during the 160 days of storage (June–November). Though the transfer area/grain volume ratio (~1.43 m^2 m^{-3} for a 200 tonnes silo bag) is favourable for natural cooling during fall and winter, with the advent of spring and summer an adverse warming effect took place.

Figure 6 compares experimental values for the middle layer of dry and wet soybean bags and Fig. 7 the temperatures for the bottom layer. The difference between grain temperatures at the beginning is mainly due to different bagging conditions (6 and 10 °C, for dry and wet grain, respectively) and tends to disappear with the progress of storage. This shows that the heat released due to respiration by the wet grain was not significant. For the climatic conditions prevailing during the field test, grain temperature was below 15 °C (see Figs. 4 and 5) and it is very likely that the heat released by respiration had been negligible for most of the storage period.

Predicted temperatures for the middle and bottom are also plotted in Figs. 6 and 7. To carry out the simulation, it was assumed that below 15 °C respiration was suppressed. Therefore, the difference of at most 1 °C between the temperature of dry and wet grain has to be attributed to different initial grain temperatures and the dependency of grain properties on MC. Soybean at 15% w.b. and 15 °C liberates 0.18 W m^{-3}. When an energy release of 0.18 W m^{-3} and even one four fold higher (0.72 W m^{-3}) were considered below 15 °C in the simulation, the temperature change of wet soybean was between 0.5 °C and 1 °C greater compared to the results shown in Figs. 6 and 7. This result is in accordance with Gastón et al. (2009), who showed that for a silo bag holding wheat (16.4% w.b. MC), the effect of heat released by respiration was weak. The energy release by respiration could not compensate for the heat losses to the surroundings and the temperature of wet wheat decreased from summer to winter, with the temperature of wet grain and dry grain very similar.

Finally, Fig. 8 shows that the average temperature of the silo bags, either simulated or measured, followed the daily average ambient temperature pattern. The measured average was calculated as the arithmetic average of temperature data, while the computed as the average over the silo bag domain. Grain temperature remained below ambient temperature during the whole storage period as a consequence of the low initial bagging temperature but the difference tended to decrease during spring.

Measured MC for the top, middle and bottom levels after 49, 92 and 160 days are compared with the computed change of MC in Figs. 9 and 10 for dry and wet soybean, respectively. The overall behaviour predicted by the model was an increase in MC in the peripheral grain layer (0.4% w.b., at most for wet soybean) while moisture at the middle and bottom of the bag remained almost unchanged. Measured values

Table 4 – Mean relative difference (MRD) and Mean absolute difference (MAD) between measured (T_m) and predicted temperatures (T).

MC (% w.b.)	Layer	MRD		MAD (°C)		Slope	Slope statistic	
		Mean ± SE	RD_{max}	Mean ± SE	AD_{max}		t	p
12.50	Top	0.23 ± 0.02	0.93	1.43 ± 0.11	5.39	0.87 ± 0.02	−6.32	<0.001
	Middle	0.08 ± 0.01	0.24	0.63 ± 0.07	2.03	0.95 ± 0.01	−4.68	<0.001
	Bottom	0.04 ± 0.00	0.10	0.37 ± 0.04	0.97	0.98 ± 0.01	−3.79	<0.001
15.60	Top	0.23 ± 0.03	1.70	1.69 ± 0.13	7.01	0.89 ± 0.02	−5.96	<0.001
	Middle	0.10 ± 0.01	0.26	0.99 ± 0.11	2.34	0.98 ± 0.02	−1.01	0.052
	Bottom	0.04 ± 0.00	0.12	0.41 ± 0.05	1.31	0.97 ± 0.01	−8.63	<0.001

Slope of the regression between measured and predicted soybean temperatures. Student's t-test 0.05 level.

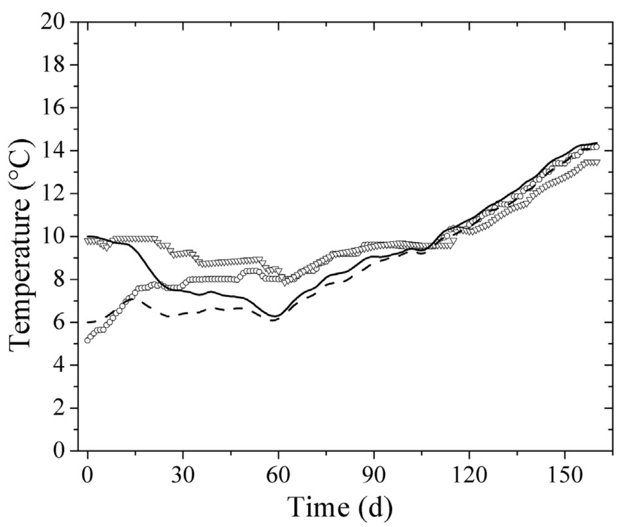

Fig. 6 – Comparison of temperature at the middle layer of the dry and wet soybean silo bag during 160 days of storage (June–November 2001). Measured (symbol); predicted temperatures (line); ○, dry soybean; ▽, wet soybean. – – -, dry soybean; ——, wet soybean.

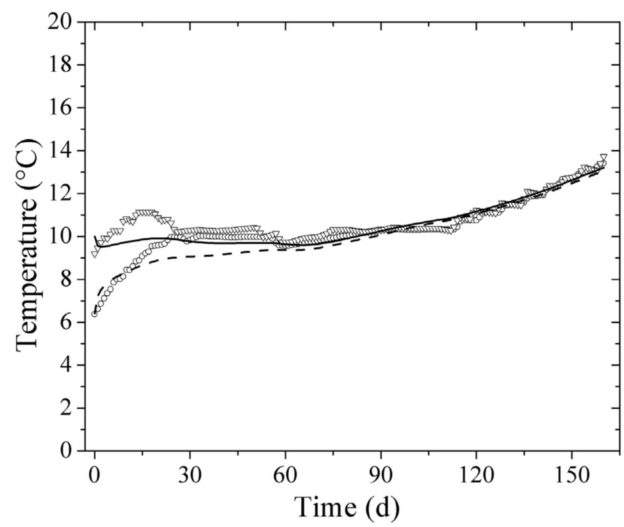

Fig. 7 – Comparison of temperature at the bottom layer of the dry and wet soybean silo bag during 160 days of storage (June–November 2001). Measured (symbol); predicted temperatures (line); ○, dry soybean; ▽, wet soybean. – – -, dry soybean; ——, wet soybean.

showed a random behaviour in both silo bags. Rodríguez et al. (2001) concluded that the average MC did not significantly change during the storage experiment and no moisture stratification was observed in the soybean silo bags. However, further experimental tests conducted to study moisture content change in individual soybean kernels stored in silo bags (Cardoso, Bartosik, & Rodríguez, 2007) showed a slight but significant increase in soybean MC in the top layer of about 0.9% w.b. in 60 days. This behaviour is in accordance with the trend predicted by the model. Differences between the magnitude of measured and predicted moisture migration may be explained by the fact that measured values were the result of a sampling, blending and averaging procedure as described previously, while numerical results are point values. MRD and MAD between measured and predicted MC were of about 2% and less than 0.3% w.b., respectively (see Table 5); they are of the same order of magnitude of experimental errors in MC determination (about 0.5% w.b.).

Other researchers have reported moisture migration in silo bags. Darby and Caddick (2007) measured changes between 0.7 and 1.1% w.b. in the upper layer of silo bags holding dry and wet wheat. Jian et al. (2015b), in accordance with this work, predicted moisture migration to the top layer of canola and negligible moisture changes in the middle and bottom of the silo bag. Jian et al. (2015b) also pointed out that the experimental MC at the top, middle and bottom of the bag used for his model validation showed significant dispersion, as a consequence of the difficulty of the sampling procedure during probing of the silo bag.

3.2. CO_2 and O_2 concentrations model validation

3.2.1. Measured CO_2 concentrations

The data collected by Cardoso et al. (2008) correspond to silo bags with a wide range of initial storage conditions (bag filling April–May, initial MC range 11–15% w.b.) and, in many cases, gas concentration values sampled during the warm and the

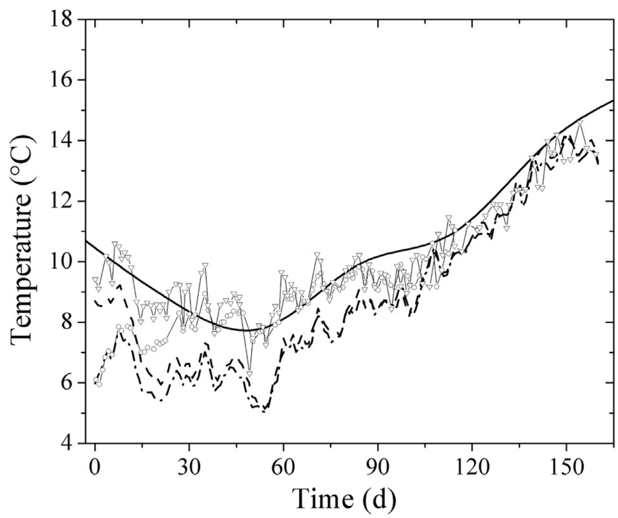

Fig. 8 – Comparison between daily average ambient temperature and average grain temperature during 160 days of storage (June–November 2001). Measured (symbol); predicted temperatures (line); ○, dry soybean; ▽, wet soybean. ——, ambient temperature; – · –, dry soybean; – – -, wet soybean.

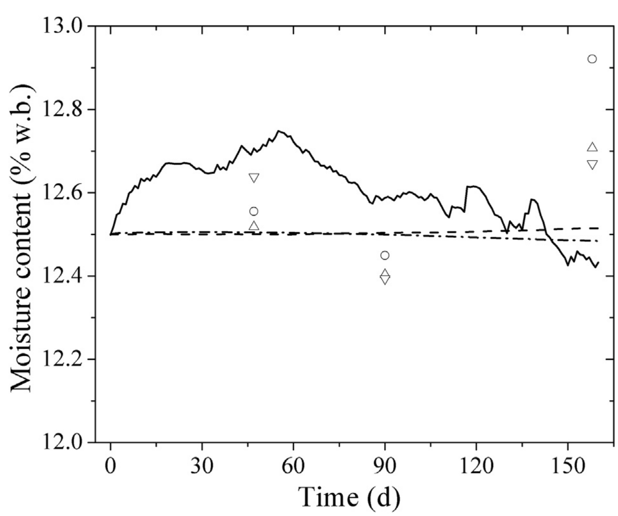

Fig. 9 – Comparison between measured (symbol) and predicted moisture content (line) at three levels in the silo bag during 160 days of storage (June–November 2001). ○, top; △, middle; ▽, bottom. ——, top; – – -, middle; – · –, bottom. M_0, initial moisture content 12.5% w.b.; T_0, initial temperature 6 °C.

cold storage seasons did not belong to the same set of silo bags. These data are shown in Fig. 11 as a function of moisture content, grouped according to the sampling season. They correspond to silo bags without visible plastic layer damage, although some silo bags could have had perforations in the bottom that were not noticed during sampling. A large variability can be observed in the measured data, as a result of many factors that cannot be controlled in field tests. While, at

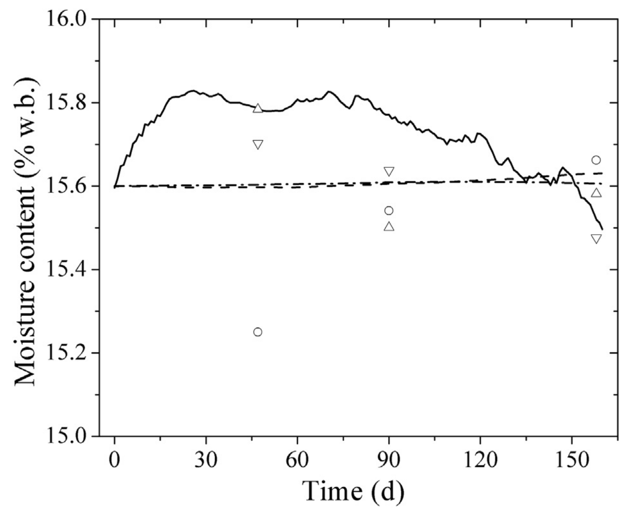

Fig. 10 – Comparison between measured (symbol) and predicted moisture content (line) at three levels in the silo bag during 160 days of storage (June–November 2001). ○, top; △, middle; ▽, bottom. ——, top; – – -, middle; – · –, bottom. M_0, initial moisture content 15.5% w.b.; T_0, initial temperature 10 °C.

Table 5 – Mean relative difference (MRD) and Mean absolute difference (MAD) between measured and predicted moisture content.

MC (% w.b.)	Layer	MRD Mean ± SE	MAD (% w.b.) Mean ± SE
12.50	Top	0.02 ± 0.02	0.26 ± 0.20
	Middle	0.01 ± 0.01	0.10 ± 0.09
	Bottom	0.01 ± 0.00	0.14 ± 0.04
15.60	Top	0.02 ± 0.01	0.30 ± 0.21
	Middle	0.01 ± 0.00	0.11 ± 0.07
	Bottom	0.01 ± 0.00	0.09 ± 0.05

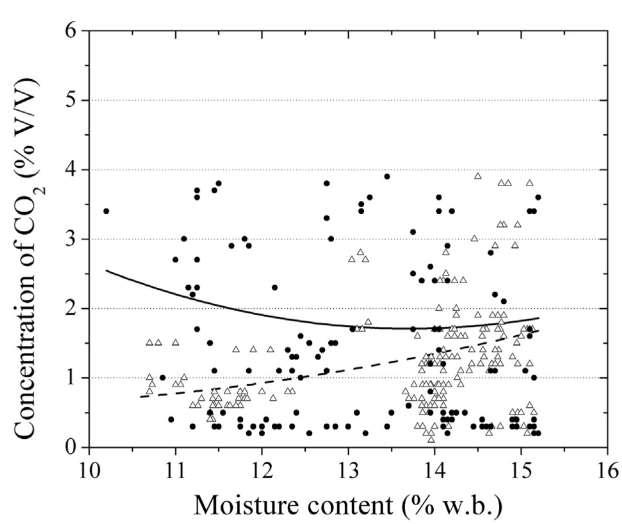

Fig. 11 – CO_2 concentration at different grain moisture content for silo bags sampled during the winter △ (– – - cold season) and spring ● (—— warm season). Source: Cardoso et al. (2008).

laboratory scale, the effect of soybean moisture content on gas concentration has been clearly observed (Ochandio, 2014), the tests showed that the relationship between grain MC and CO_2 concentration was less clear for soybean silo bags in the field compared to data from wheat silo bags under similar climatic conditions (Bartosik et al., 2008).

3.2.2. *Definition of initial bagging conditions and weather data for simulation*

Since only monthly average ambient temperature data were reported, to reproduce average weather condition, hourly ambient temperature and solar radiation from May to December were averaged over six years (1999–2004) and used as input data for the south east of Buenos Aires province. Figure 12 shows measured monthly average ambient temperature values during the field tests, hourly weather input data used in the simulation and the corresponding daily average ambient temperature. Maximum absolute difference between average values was 3 °C. Initial grain temperature was set to 25 °C, initial moisture content to 13, 15 and 17% w.b. and bagging date to May 1st. The computed mean temperature of soybean bags is also plotted in Fig. 12. Compared to Fig. 8, as the initial bagging temperature now was rather high, the average grain temperature first remained above daily ambient temperature and then during spring evolved in similar way.

3.2.3. *Comparison between measured and predicted gas concentrations*

The analysis of gas distribution in the silo bag shows that, although the rate of respiration may have a strong variation in the domain as result of temperature and moisture content gradients, the gas concentration gradients within the bag are small because the diffusion of gases in the silo-bag flattens

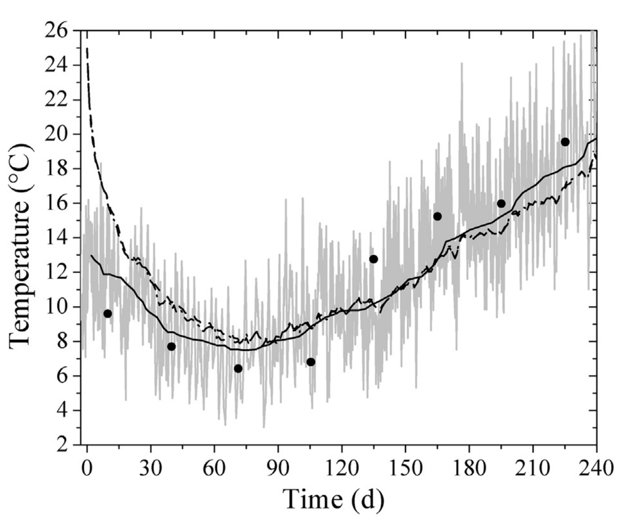

Fig. 12 – Comparison between monthly average ambient temperature and average grain temperature during storage (May–December). ——, hourly averaged ambient temperature used as input data (1999–2004); ——, daily averaged ambient temperature (1999–2004); •, monthly averaged ambient temperature (measured during filed test); – · –, dry soybean; – – -, wet soybean.

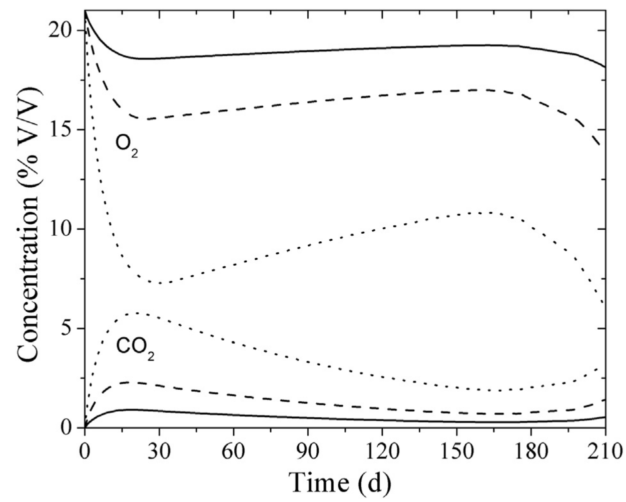

Fig. 13 – Comparison between predicted gas concentration during storage (May–December) for different initial moisture content. ——, 13% w.b.; – – -, 15% w.b.; ----, 17% w.b. T_0, initial temperature 25 °C.

the gas concentration profiles. These results are similar to those obtained in a silo bag holding wheat (Arias Barreto, 2016) and are in accordance with the reported experimental result that the layer (top, middle, bottom) did not have a significant effect on measured gas concentration in silo bags (Bartosik et al., 2008; Cardoso et al., 2008). Therefore, the mean measured value was compared to the mean predicted gas concentration.

Figure 13 shows predicted mean O_2 and CO_2 concentration for 13, 15 and 17% w.b. MC for a storage period of 240 days. The effect of moisture content as well as temperature (storage started in late fall and early winter and was prolonged into spring and early summer) on soybean respiration can be clearly observed in the predicted curves. The initial accumulation of CO_2 and fast consumption of O_2 were due to the initial high temperature of soybean (25 °C). Once the temperature fell below 15 °C respiration was negligible, CO_2 concentrations decreased because of gas permeation through the plastic layer and O_2 concentration increased for the same reason. By the end of the storage period, the model predicted a sharp decrease in O_2 as respiration was reactivated with the rise of grain temperature, though CO_2 did not increase in the same proportion. It can be observed that between 13 and 15% w.b., a difference of 2% w.b. in MC resulted in a maximum difference of about 3% V/V in O_2 concentration and of 1.5% V/V in CO_2 after one month. The difference remained nearly constant for O_2 and decreased for CO_2 until respiration was reactivated after five months of storage. Between 15 and 17% w.b. the difference increased to 7.5% V/V in O_2 concentration and to 3% V/V in CO_2.

Among the data shown in Fig. 11 (range 11–15% w.b. MC), three bags were selected to validate the model. As the experimental accuracy in moisture content determination was ±0.5% w.b., CO_2 and O_2 measured values (two replicates) corresponding to a bag with 12.7% w.b. were plotted according to the sampling date and compared to the predicted 13% w.b. curve in Fig. 14, values belonging to a bag with 14.3% w.b.

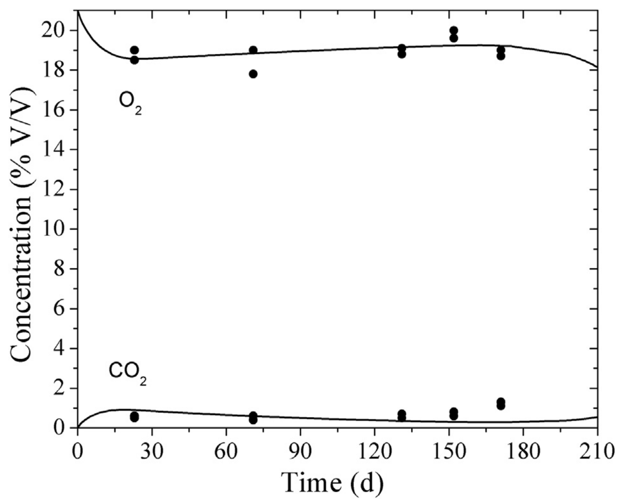

Fig. 14 – Comparison between measured (——) and predicted (•) gas concentration during storage (May–December). Initial temperature 25 °C, initial moisture content 13% w.b.

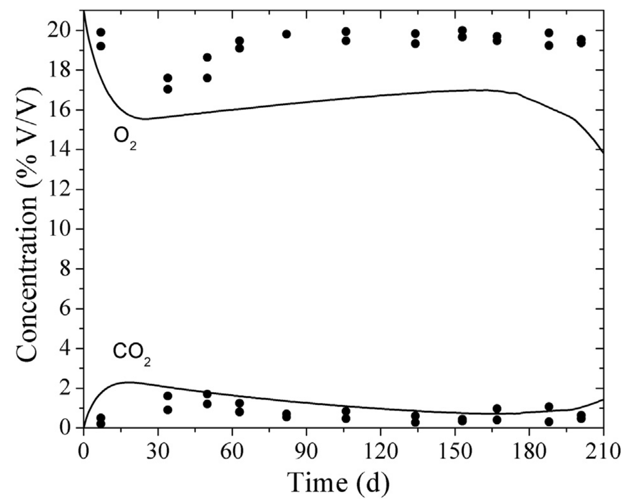

Fig. 16 – Comparison between measured (——) and predicted (•) gas concentration during storage (May–December). Initial temperature 25 °C, initial moisture content 15% w.b.

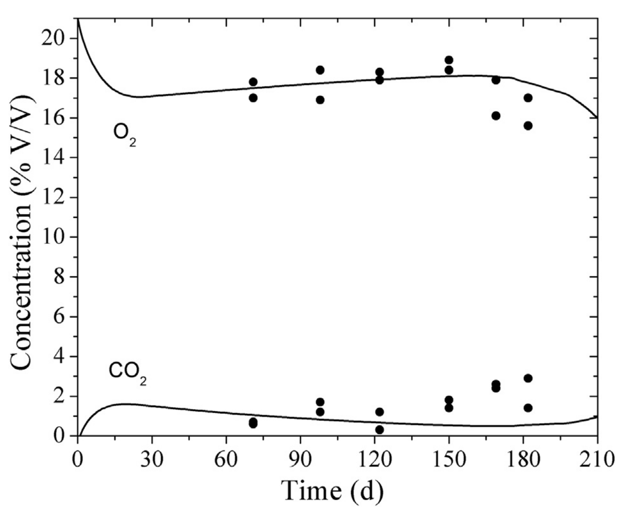

Fig. 15 – Comparison between measured (——) and predicted (•) gas concentration during storage (May–December). Initial temperature 25 °C, initial moisture content 14% w.b.

compared to the predicted 14% w.b. curve in Fig. 15 and those from a bag with 14.9% w.b. with the 15% w.b. curve in Fig. 16. No data from a silo bag with 17% w.b. was available (farmers typically do not store soybean at such high (unsafe) MC). To predict the evolution of gas concentration for 14% w.b. moisture content, interpolation was applied between 13 and 15% w.b.

Values of MRD and MAD are summarised in Table 6. It can be observed that the general trends of the measured concentrations both for dry and wet soybean silo bags were satisfactorily reproduced by the correlations developed by Ochandio (2014). MAD ranged from 0.48 %V/V to 0.97% V/V for CO_2 and from 0.43% V/V to 2.63% V/V for O_2. MRD or MAD values shown by present model were of the same order of magnitude as those reported by Lawrence et al. (2013b), Rennie and Tavoularis (2009) and recently by Chelladurai (2016). The latter developed a model to predict CO_2 concentration in a silo bag holding canola and reported errors of around 1.3% V/V and 1.7% V/V of CO_2 for low (dry) and high moisture canola, respectively. Also, the measured evolution of CO_2 and O_2 concentration up to 280 days of storage showed the same trend as the one illustrated in Fig. 13.

The model assumed that below 15 °C respiration was negligible (suppressed) and that the silo bag had no structural damage. To test the effect on model predictions both constraints were removed, one at a time.

A simulation was carried out for wet soybean (15% w.b.) setting the O_2 consumption to 30% and to 10% of that at 15 °C. The deviation from measured data was considerably higher when the negligible respiration assumption was removed. O_2 concentration decayed to 10% V/V and 14% V/V respectively, after 180 days (not shown) while CO_2 level increased less than

Table 6 – Mean relative difference (MRD) and Mean absolute difference (MAD) between measured and predicted mean CO_2 and O_2 concentrations.

MC (% w.b.)	Gas	MRD Mean ± SE	MAD (% V/V) Mean ± SE
13	CO_2	0.52 ± 0.24	0.41 ± 0.30
	O_2	0.023 ± 0.016	0.43 ± 0.29
14	CO_2	0.69 ± 0.28	0.97 ± 0.67
	O_2	0.046 ± 0.03	0.78 ± 0.55
15	CO_2	1.26 ± 0.59	0.59 ± 0.34
	O_2	0.14 ± 0.03	2.64 ± 0.66

1% V/V point. This result confirms that suppressing respiration below 15 °C was an adequate assumption.

The discrepancies observed between measured and predicted values are likely to occur when comparing model results with experimental data obtained from commercial scale tests (i.e., 200 tonnes silo bag) and may originate from different sources as discussed in Abalone et al. (2011a). Abalone et al. (2011b) demonstrated by computer simulation that the presence of small perforations considerably altered the effective permeance of gases through the plastic layer. Gas concentration values shown in Figs. 14–16 belong to different silo bags in the field. For the wet silo bag without damage, the model underestimated O_2 concentration (Fig. 16). It can be observed that after 45 days, measured O_2 started to rise and remained around 19–20% V/V. It can be speculated that the plastic layer might have been damaged so the model was run assuming the silo bag had perforations (1 perforation of 10 mm diameter per metre of silo bag, Abalone et al., 2011b). With such an increase in the effective permeance of the silo bag, the predicted evolution of O_2 and CO_2 were improved (MAD was 0.65% V/V for O_2 and 0.43% V/V for CO_2). New predictions are presented in Fig. 17. This example illustrates that the degree of airtightness is a key factor for gas concentration predictions, but unfortunately it is very complex to characterise in silo bags in the field.

If the experimental data collected in Fig. 11 are plotted together as a function of storage time, it can be observed that on average 50% of measured values during the warm and cold seasons fall within the bands defined by the 13 and 15% w.b. curves. For practical purposes, the O_2 and CO_2 gas evolution predicted for 14% w.b. could be considered as an average or reference value for bags in the field with the 11–15% w.b. range and different levels of airtightness of the silo bags as shown in Fig. 18. Any concentration above 3% V/V would imply that there is a certain mass of grain with a respiration rate significantly higher than that of soybean at 14% w.b. In the field, this is typically observed when water enters in the bag through some perforation and results in grain spoilage (Taher, Bartosik, Cardoso, & Urcola, 2014).

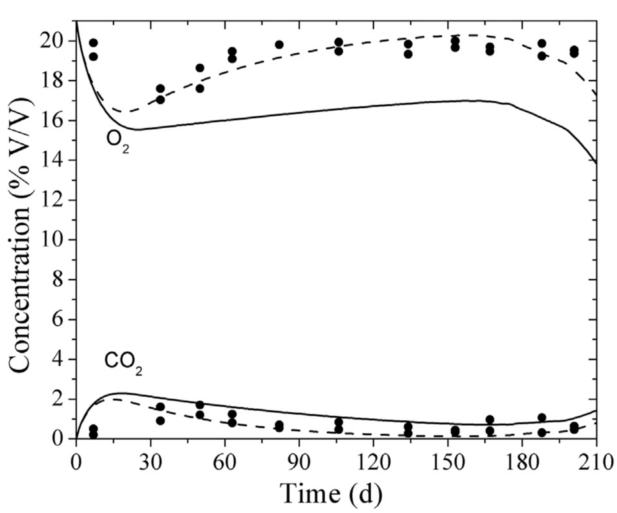

Fig. 17 – Comparison between measured (•) and predicted gas concentration (line) during storage (May–December) for a damaged silo bag. ——, without damage; – – -, with damage; initial temperature 25 °C, initial moisture content 15% w.b.

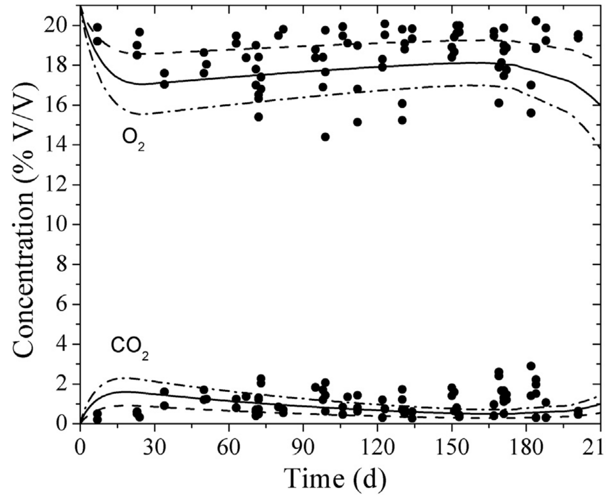

Fig. 18 – Comparison between measured data in silo bags with moisture content in the range (11–15% w.b.) (•) and predicted gas concentration (line) during storage (May–December). – – -, 13% w.b.; ——, 14% w.b.; – · –, 15% w.b.; Initial temperature 25 °C.

Table 7 – Absolute difference (AD) between CO_2 predicted with the correlation developed by Cardoso et al. (2008) (CO_{2corr}) and mean CO_2 ($CO_{2average}$) predicted by the model for the cold and warm season.

Absolute difference, $AD = \lvert CO_{2corr} - CO_{2average} \rvert$	Cold season CO_2 (% V/V)	Warm season CO_2 (% V/V)
Dry soybean (13% w.b)	0.0.5	0.01
Wet Soybean (15% w.b)	0.1	0.01

$CO_{2corr} = 0.067M^2 - 1.856M + 14.43$ (warm season).
$CO_{2corr} = 0.02M^2 - 0.137M + 1.807$ (cold season).

Finally, CO_2 concentration estimated by use of the correlation proposed by Cardoso et al. (2008) for the cold and warm season (CO_{2corr}) (Fig. 11) was compared with the value derived with present model ($CO_{2average}$) for soybean with 13 and 15% w.b. A representative value for the cold season was calculated by averaging mean CO_2 concentration from July to September (60–150 simulation days) and for the warm season from October to December (151–250 simulation days). Mean absolute differences between models are summarised in Table 7. Despite the dispersion in the experimental data, both predictions are in good accordance.

4. Conclusions

In this work, a two dimensional coupled heat and mass transfer model was described to predict the temperature distribution, moisture distribution and interstitial gas concentrations associated with seasonal variation of climatic conditions of soybean stored in hermetic plastic bags (silo bag). The numerical solution was carried out applying the finite element method.

Predicted values of temperature were compared with field test data at three levels in the silo bag. The model showed good agreement with the experimental data. Mean absolute difference was 0.5–1 °C for the bottom and middle layers and about 1.5 °C for the top layer. Mean relative difference was 4% at bottom, 10% at the middle and 23% at the top layer. A slight moisture increase (0.4% w.b. at most) was predicted for the top grain layer while moisture for the middle and bottom layers remained almost unchanged during the storage period.

CO_2 and O_2 concentrations in the silo bag were predicted applying the correlations developed by Ochandio (2014). When predicted and measured values were compared at a given monitored date, MAD ranged from 0.48% V/V to 0.97% V/V for CO_2 and from 0.43% V/V to 2.63% V/V for O_2, for 13, 14 and 15% w.b. as data collected in field test usually presented high variability. Therefore, the overall trend of gas evolution was satisfactorily represented.

For typical storage conditions, the correlations can be applied to assist in the design of a monitoring protocol for these variables as a tool for predicting grain storability for the silo bag system.

As practical recommendations for silo bag monitoring based on CO_2 concentration, a reference value of 3% V/V should be considered as a threshold for safe storage condition of 13–15% w.b. soybean. Additionally, since the outer layer of grain is influenced by daily temperature oscillation and a MC increase should be expected, a differential sampling from the surface of the silo bag is recommended for early detection of grain quality deterioration.

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