Barreto AA, Abalone R, Gastón A (2016) Computer simulation of gas concentration in the interstitial atmosphere of a soybean (*Glycine max*) silo bag for typical agricultural areas of Argentina. Pp. 291–296. In: Navarro S, Jayas DS, Alagusundaram K, (Eds.) Proceedings of the 10th International Conference on Controlled Atmosphere and Fumigation in Stored Products (CAF2016), CAF Permanent Committee Secretariat, Winnipeg, Canada.

Computer simulation of gas concentration in the interstitial atmosphere of a soybean (*Glycine max*) silo bag for typical agricultural areas of Argentina

ALIEN ARIAS BARRETO, RITA ABALONE[1,2], A GASTÓN[1,2*]

[1]*Fac. de Cs. Exactas Ingeniería y Agrimensura. UNR. IFIR (CONICET/UNR)*

ABSTRACT

A validated mathematical model was used to determine the change in concentration of CO_2 and O_2 in a silo bag holding soybean [*Glycine max* (L.) Merr.] from autumn to summer for a typical agricultural region in the North (Sáenz Peña, Chaco Province), Center (Pergamino, Buenos Aires Province) and South (Balcarce, Buenos Aires Province) of Argentina. Initial moisture content (m.c.) of grain was set to 13, 15 and 17% w.b. and bagging temperatures to 15ºC and 25ºC. In Balcarce and Pergamino, with moderate and intermediate climate, winter CO_2 reference values ranged from 1 to 3% V/V for dry and slightly wet (13 and 15% w.b.) soybean and increased to 2–5% V/V for wet soybean (17% w.b.). In Sáenz Peña, with sub-tropical climate, winter CO_2 reference values ranged from 2.3 to 8% V/V. Values of O_2 concentration below 1% V/V were attained in a soybean silo bag only under sub-tropical climatic conditions (Sáenz Peña). Under temperate and intermediate climate, insect activity would be limited in silo bags as grain mean temperature remained below 15ºC during most of the storage period, while under subtropical climate insect control would mainly depend on the interstitial gas concentration.

Key words: Atmosphere composition, Grain storage, Hermetic storage, Modeling, Soybean, Silo bags

Grain storability in silo bags is based on CO_2 detection according to a protocol developed by The National Institute of Agricultural Technologies of Argentina (INTA), Balcarce Experimental Station (EEA) (Bartosik et al., 2008). This protocol compares the measured CO_2 concentration with a reference value, which represents adequate storage conditions.

Gas concentration in grain bags depends on the respiration of the grain ecosystem (grains + microflora + insects), 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). Experimental field tests and numerical results demonstrated that this reference level is affected by grain temperature and moisture content (m.c.) and permeability of the plastic layer of the silo bag to O_2 and CO_2. Grain temperature change depends on climatic condition of the region, so reference concentration values differ from one agricultural area to another (Bartosik et al., 2008; Cardoso et al., 2008; Abalone et al., 2011a; 2011b; Arias Barreto et al., 2013).

Based on previous works (Gastón et al., 2009, Arias Barreto et al., 2013), Arias Barreto (2016) adapted the model to simulate storage of soybean [*Glycine max* (L.) Merr.] in silo bags. The model was validated by comparison of predicted temperature, m.c. and gas concentration with experimental data (Rodriguez et al., 2001; Cardoso et al., 2008). The rate of O_2 consumption and CO_2 production due to grain respiration were calculated as a function of temperature, grain m.c. and O_2 interstitial concentration (Ochandio, 2014).

In this work, the mathematical model was used to determine the reference levels that corresponds to three typical agricultural regions of Argentina: one

[2]CIC- UNR. Fac. de Cs. Exactas Ingeniería y Agrimensura. UNR, Av. Pellegrini 250. (2000) Rosario. Argentina

[*]Corresponding author email: *analiag@fceia.unr.edu.ar*

with sub-tropical climate in the North (Sáenz Peña, Chaco Province), second with intermediate climate in the Centre (Pergamino, Buenos Aires Province) and third with moderate climate in the South (Balcarce, Buenos Aires Province). The evolution of O_2 and CO_2 concentration during nine months, from April to December, was simulated in the silo bag holding soybean at 13, 15 and 17% w.b. for initial bagging temperatures of 15°C and 25°C.

MATERIALS AND METHODS

Silo bags

Silo bags are 60 m long, 2.70 m diameter and 230-250 microns thick plastic bags. The bags are made of a three-layer plastic, black on the inside and white on the outside with UV stabilizers. The plastic layers are a mixture of high density (HDPE) and low density polyethylene (LDPE). Approximately 200 tonnes of grains (wheat, corn and soybean) can be held in a bag; farmers usually store their production in bags for six to eight months.

Mathematical modelling

A coupled PDE (Partial Differential Equation) system in terms of temperature *T*, grain m.c. *W*, O_2 and CO_2 concentrations is derived from the energy and mass balances for the grain and air phases in a control volume. The balances take into account heat, water vapour, oxygen consumed and carbon dioxide released by respiration of the grain ecosystem. A detailed description of the model is presented elsewhere (Gastón et al., 2009; Abalone et al., 2011a; b; Arias Barreto et al., 2013). Gas transfer through the plastic layer was modeled by defining an equivalent permeability of the plastic to O_2 and CO_2. Equivalent permeability of the plastic layer to O_2 was set equal to $9.75\ 10^{-8} m^3 md^{-1} m^{-2} at^{-1}$ and to CO_2 equal to $3.22\ 10^{-7} m^3 md^{-1} m^{-2} at^{-1}$, average plastic thickness L to 240 μm, effective diffusivity to CO_2 and O_2 to $3.97\ 10^{-6}\ m^2 s^{-1}$ and $5.22\ 10^{-6}\ m^2 s^{-1}$, respectively, soybean porosity to 0.34 and tortuosity to 1.53. The mathematical model was implemented in *COMSOL Multiphysics 4.3a* and solved by the finite element method. Fig. 1 shows the calculation domain, which represents a cross section of the silo bag.

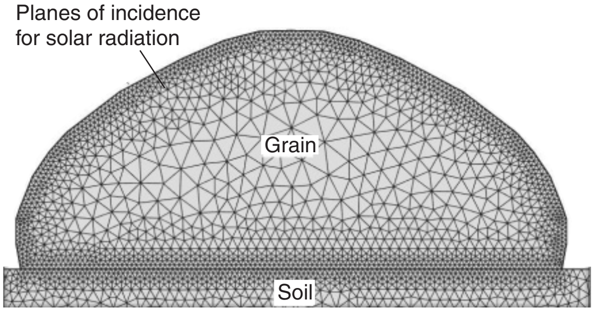

Fig. 1. Cross section of the silo bag and discretization domain

Heat and water vapour released during respiration was modeled by the complete combustion of a typical carbohydrate. Soybean respiration was modelled according to correlations developed by Ochandio (2014).

For 13% w.b. moisture content

$$Y_{CO_2} = -1.020 - 0.0878\ O_2 + 0.0512 T_c + 0.00676 T_c\ O_2 \quad R = 0.914 \qquad ...(1)$$

$$Y_{O_2} = 0.972 + 0.124\ O_2 - 0.0437 T_c - 0.0105 T_c\ O_2 \quad R = 0.962 \qquad ...(2)$$

For 15% w.b. moisture content

$$Y_{CO_2} = 0.595 - 0.492\ O_2 + 0.00925 T_c + 0.0258 T_c\ O_2 \quad R = 0.959 \qquad ...(3)$$

$$Y_{O_2} = 0.468 + 0.229\ O_2 - 0.0454 T_c - 0.0200 T_c\ O_2 \quad R = 0.984 \qquad ...(4)$$

For 17% w.b. moisture content

$$Y_{CO_2} = -5.813 - 0.577\ O_2 + 0.379 T_c + 0.0420 T_c\ O_2 \quad R = 0.918 \qquad ...(5)$$

$$Y_{O_2} = 0.617 + 0.888\ O_2 - 0.0687 T_c - 0.0712 T_c\ O_2 \quad R = 0.976 \qquad ...(6)$$

Compared to wheat (White et al., 1982), at 15°C and medium O_2 concentration (10% v/v), the rate of respiration of soybean is 1 to 3 orders of magnitude, lower than that of wheat. For the other combinations of moisture content (13–17% w.b.) and temperature (25–35°C), on average, it is about 4-fold lower.

Definition of initial bagging conditions and weather data for simulation

The model was applied to analyze the storage of soybean in a silo bag from April to December (nine months). Initial grain m.c. was set to 13, 15 and 17% w.b. and initial bagging temperatures to 15ºC and 25ºC. Climatic data corresponding to 1999–2004 years were considered for Balcarce (37.84S; 58.26W), in the Southwest of Buenos Aires Province; to 2001–2006 years for Pergamino (33.85S; 60.93W), in the North of Buenos Aires Province and to 2001–2006 years for Sáenz Peña (26.78S; 60.45 W), in Chaco Province.

RESULTS AND DISCUSSION

Annual mean temperature and solar radiation were compared at the three locations (Fig. 2). Usually, soybean is stored in silo bags during autumn (90th day). In this period, mean ambient temperature in Sáenz Peña is about 5ºC higher than in Pergamino and 7ºC

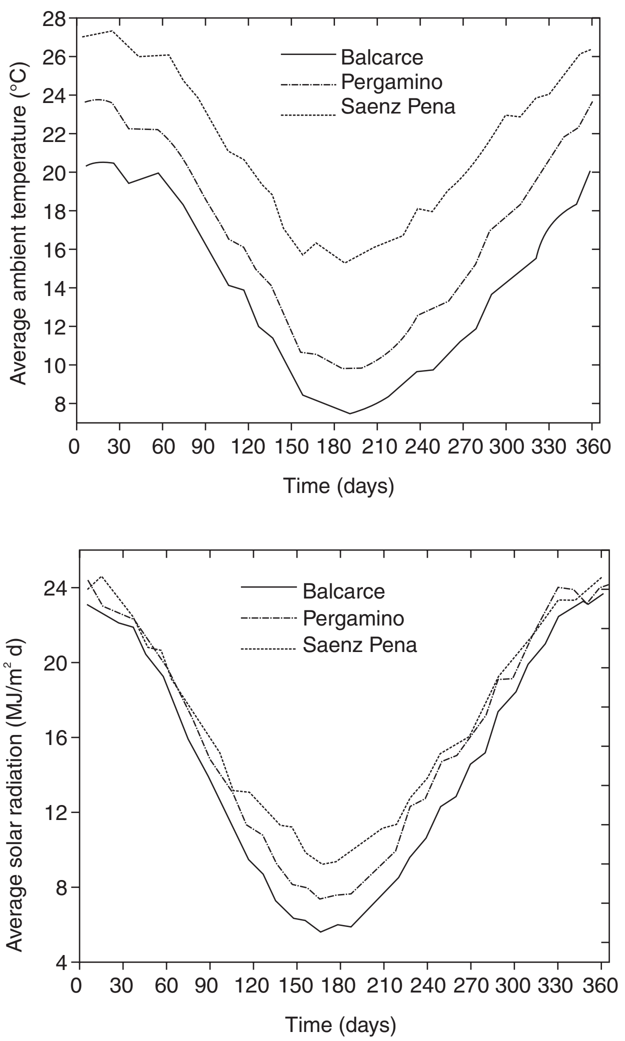

Fig. 2. Comparison of mean ambient temperature and solar radiation of agricultural areas

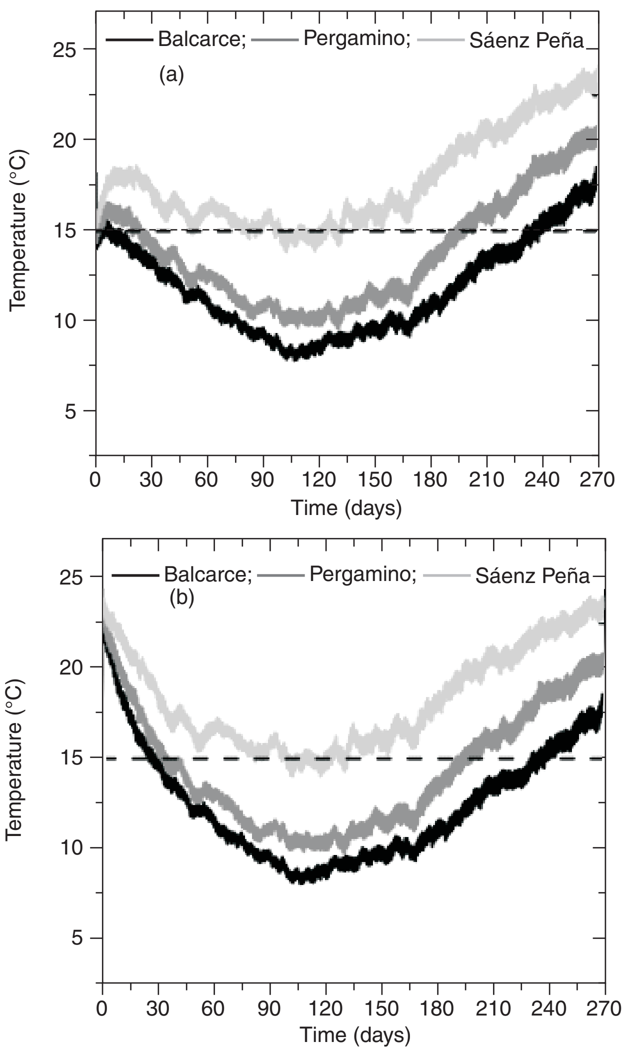

Fig. 3. Grain mean temperature evolution at Balcarce, Pergamino and Sáenz Peña. Initial temperature: (a) 15ºC ; (b) 25ºC . Initial moisture content: 17% w.b.

higher than in Balcarce, while in winter is about 7ºC and 10ºC higher respectively. Solar radiation in Sáenz Peña during autumn and winter was about 13 and 30% higher than in Pergamino and Balcarce, respectively.

The evolution of the mean temperature of the silo bags for 15°C (a) and 25°C (b) initial bagging temperature and 17% w.b. initial m.c. is illustrated in Fig. 3. Simulation results for 13 and 15% w.b. were almost identical. It can be observed that in Balcarce and Pergamino after 30–45 days of storage, grain mean temperature decreased and remained below 15°C until the beginning of the warm season. In contrast, in Sáenz Peña grain mean temperature was above 15°C during the whole storage period. Fig. 4 compares mean grain temperature and average ambient temperature at each location. Regardless of the initial bagging temperature, during winter mean grain temperature was very similar to average ambient temperature. During the warm season, grain temperatures increased following the ambient pattern but remained always below average ambient temperature.

According to Ochandio (2014), respiration of soybean is very low below 15°C and increased by 3 to 10-fold at 25°C, depending on m.c. Therefore, as will be shown, the effect of climatic conditions produced significant changes in the reference levels of O_2 and CO_2.

Results for each bagging condition and location were averaged over the six years. Figs. 5 and 6 show the change of mean gas concentration for 15ºC and 25°C initial bagging temperature respectively. As a general trend, in Balcarce and Pergamino, with moderate and intermediate climate, CO_2 concentration was very low during autumn and winter and increased during the last two months, as respiration was activated with the warming up of the silo bag. The effect of initial grain temperature is reflected on the fast initial accumulation

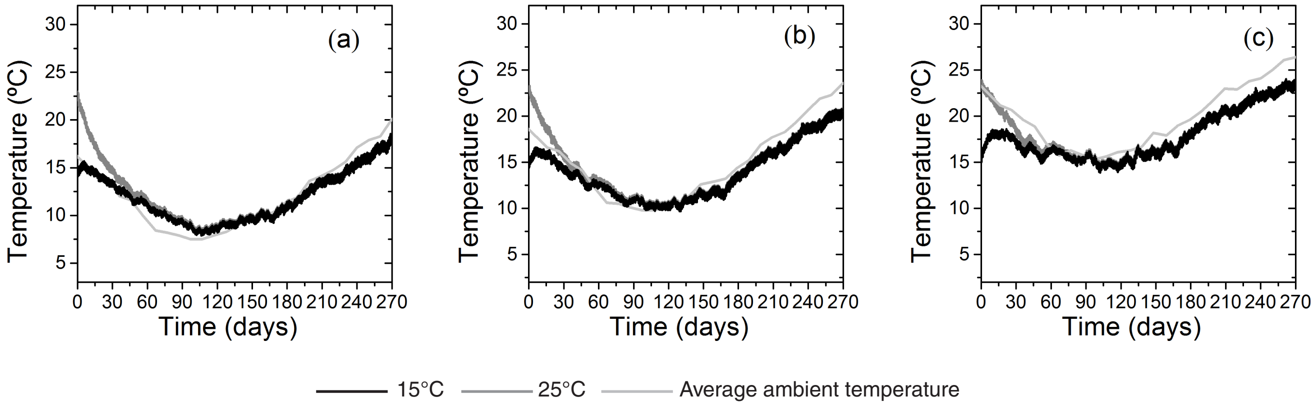

Fig. 4. Comparison between grain mean temperature evolution and average ambient temperature (a) Balcarce; (b) Pergamino; (c) Sáenz Peña.

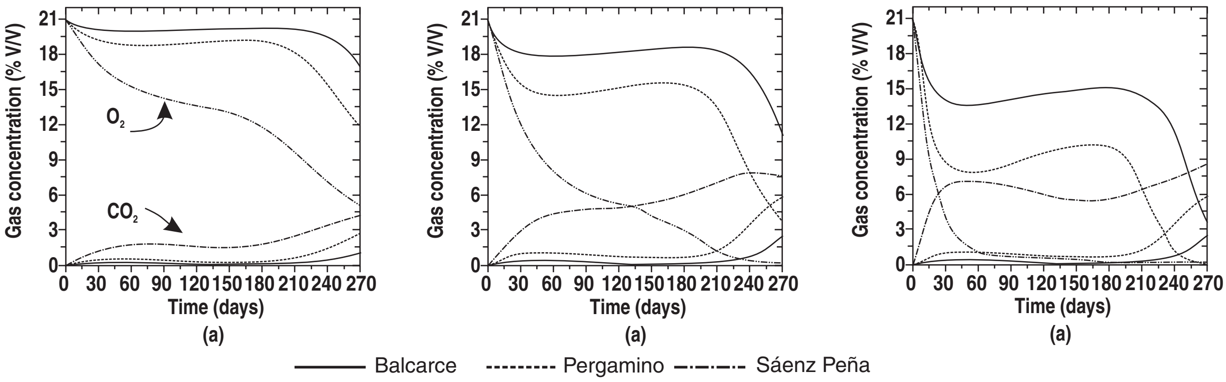

Fig. 5. Gas concentration evolution at Balcarce, Pergamino and Sáenz Peña. Initial temperature 15ºC (a) 13% w.b. (b) 15% w.b. (c) 17% w.b.

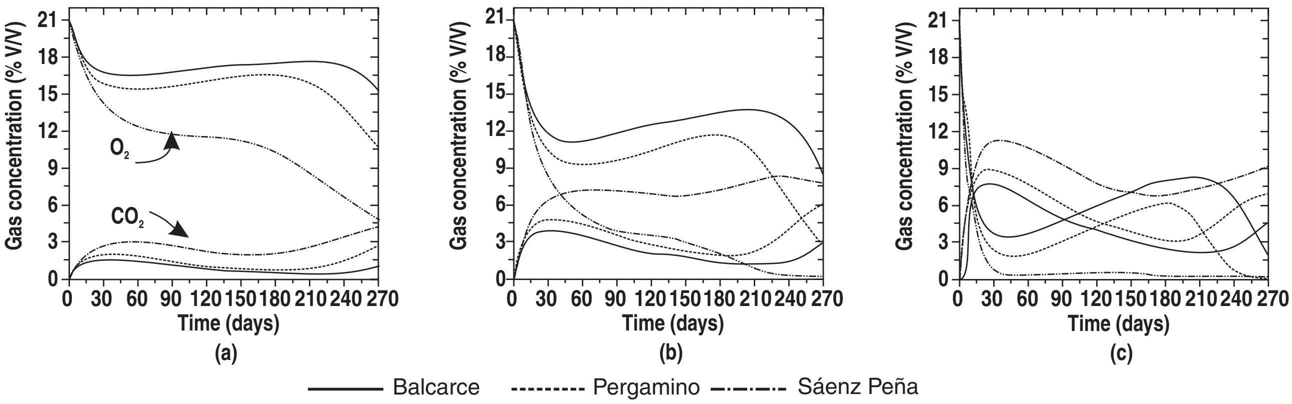

Fig. 6. Gas concentration evolution at Balcarce, Pergamino and Sáenz Peña. Initial temperature 25ºC (a) 13% w.b. (b) 15% w.b. (c) 17% w.b.

of CO_2 and consumption of O_2 during the first month (Fig. 6), followed by a decay of CO_2 and a recovery of O_2 due to gas transfer with the ambient. It can also be observed, that for slightly wet and wet soybean, the rate of increase of CO_2 was higher by the end of spring in Balcarce and Pergamino than in Sáenz Peña. This is because of the lower O_2 level achieved in this location, which slows down the rate of respiration. On an average, O_2 level remained above 6% V/V. Only in Sáenz Peña, with sub-tropical climate, O_2 was almost consumed after two months of storage in the wet silo bag (17% w.b.).

Reference values of CO_2 for winter and spring were selected from Figs. 5, 6 and summarized in Tables 1, 2. An increase of 10ºC in ambient temperature and 30% in solar radiation between the northern (Sáenz Peña) and southern location (Balcarce), produced on average an increase of 5% V/V points in the concentration of CO_2 for slightly wet and wet soybean. The difference between the winter and spring reference values ranged from 3 to 5% V/V points, depending on the grain initial condition.

Table 1 Estimated reference level of CO_2 for winter and end of spring in a soybean silo bag. Initial grain temperature 15°C

	Winter reference value (around 120th day)			Spring reference value (end of storage)		
m.c.	13% w.b.	15% w.b.	17% w.b.	13% w.b.	15% w.b.	17% w.b.
Balcarce	<0.3	<0.3	1.0	1.1	2.5	4.6
Pergamino	<0.3	0.6	2.0	2.7	5.7	6.7
Sáenz Peña	1.6	4.9	6.0	4.5	7.5	8.5

Table 2 Estimated referential level of CO_2 for winter and end of spring in a soybean silo bag. Initial grain temperature 25°C

	Winter reference value (around 120th day)			Spring reference value (end of storage)		
m.c.	13% w.b.	15% w.b.	17% w.b.	13% w.b.	15% w.b.	17% w.b.
Balcarce	0.8	2.1	3.8	1.2	2.9	4.6
Pergamino	1.0	2.8	4.9	2.6	6.0	6.8
Sáenz Peña	2.3	7.0	7.9	4.2	7.9	9.0

It is important to remark that the simulations carried out assumed a silo bag without structural damage. Abalone et al. (2011b) demonstrated by computer simulation that the presence of small perforations altered considerably the transfer of O_2 and CO_2 through the plastic layer. Also, as perforations are not selective, changes in the reference values of O_2 were more pronounced than those of CO_2. It is highly probable that a silo bag in the field may have such perforations (Cardoso et al., 2012) and therefore the O_2 concentration be higher than the predicted one. Also, although storage was simulated from April to December (270 days), soybean is not usually stored in silo bags for such a long period.

Though in Argentina soybean does not have frequent insect infestations, some speculations regarding the effect of typical temperature and modified atmosphere conditions in silo bags could be derived. Fig. 3 showed that the mean temperature of the silo bags, remained below 15ºC most of the storage period under temperate and intermediate climate. These results indicate that for these climatic conditions of Argentina, insect activity would be limited for dry and moist grain because mean grain temperature decreases below 17ºC, preventing insect infestation. CO_2 level (>20%V/V) that can be toxic to insects were not achieved. Oxygen concentration to arrest insect development would only be attained for moist soybean under sub-tropical climate conditions.

In a previous work (Arias Barreto et al., 2013),

Table 3 Comparison of estimated reference level of CO_2 for winter in a soybean and wheat silo bag

Grain type	Soybean			Wheat		
m.c.	13% w.b.	15% w.b.	17% w.b.	12% w.b.	14% w.b.	16% w.b.
Gas	CO_2%V/V	CO_2%V/V	CO_2%V/V	CO_2%V/V	CO_2%V/V	CO_2%V/V
Balcarce	0.8	2.1	3.8	4	11.7	> 14
Pergamino	1.0	2.8	4.9	4.6	13	> 14
Sáenz Peña	2.3	7.0	7.9	6	> 14	> 14

Table 4 Comparison of estimated reference level of O_2 for winter in a soybean and wheat silo bag

Grain type	Soybean			Wheat		
m.c.	13% w.b.	15% w.b.	17% w.b.	12% w.b.	14% w.b.	16% w.b.
Gas	O_2 %V/V	O_2 %V/V	O_2 %V/V	O_2 %V/V	O_2 %V/V	O_2 %V/V
Balcarce	18	12	6	15.5	5	~ 0 (Ac)
Pergamino	17.5	10	4.5	15	3	~ 0 (Ac)
Sáenz Peña	10.5	4	~ 0.5	13	~ 0 (Ac)	~ 0 (Ac)

Ac: Anaerobic conditions attained

the reference level for a silo bag holding wheat from summer to winter (January–July, 180 days of storage) were obtained for the same agricultural areas. Initial bagging conditions were 12, 14 and 16% w.b. initial m.c. and 25 and 40°C initial grain temperature. For comparison, Table 3 and Table 4 show the reference winter values of CO_2 and O_2 for wheat and soybean for 25°C initial bagging temperature. Reference values for wet and slightly wet wheat are considerably higher than those for soybean. The higher respiration rate of wheat compared to soybean and the higher average temperature of the wheat silo bag during summer (which ranged from 20 to 25°C) favoured the accumulation of CO_2. Table 4 shows that anaerobic conditions, which are beneficial for conservation of wet grain, were attained in a soybean silo bag only under sub-tropical climatic conditions (Sáenz Peña).

CONCLUSION

Results showed that reference levels of O_2 and CO_2 depend on initial moisture content and bagging grain temperature. In Balcarce and Pergamino, with moderate and intermediate climate, CO_2 concentration was very low during autumn and winter, in the range 1–3% V/V for dry and slightly wet soybean, but increased to 2–5% V/V for wet soybean. In Sáenz Peña, with sub-tropical climate, winter CO_2 reference values ranged from 2.3 to 8% V/V, for an initial bagging temperature of 25°C. Low O_2 concentration values, which are beneficial for conservation of wet grain, were attained in a soybean silo bag only under sub-tropical climatic conditions (Sáenz Peña).

As grain mean temperature remained below 15ºC during most of the storage period under temperate and intermediate climate, insect activity would be limited in silo bags. Under subtropical climate conditions, the effect of temperature would be limited, and insect control would mainly depend on the interstitial gas concentration, a lethal atmosphere would only be achieved during storage of wet soybean.

ACKNOWLEDGEMENT

The authors like to acknowledge National University of Rosario (PID ING295 and 526), AVE PROGRAM (Programa Ayuda para Viajes al Exterior) and Convenio De Asistencia Tecnica Inta–Empresas Fabricantes De Bolsas Plásticas for support.

REFERENCES

Abalone R, Gastón A, Bartosik R, Cardoso L, Rodríguez J (2011a) Gas concentration in the interstitial atmosphere of a wheat silobag. Part I. Model development and validation. Journal of Stored Products Research **47(4)**: 268–275.

Abalone R, Gastón A, Bartosik R, Cardoso L, Rodríguez J (2011b) Gas concentration in the interstitial atmosphere of a wheat silobag. Part II. Model sensitivity and effect of grain storage conditions. Journal of Stored Products Research **47(4)**: 268–275.

Arias Barreto A, Abalone R, Gastón A (2013) Analysis of storage conditions of a wheat silobag for different weather conditions by computer simulation. Biosystems Engineering **116(4)**: 497–508.

Arias Barreto A (2016) Modelización de fenómenos de transporte en el almacenamiento hermético de granos. Predicción de condiciones de almacenamiento seguro para silos bolsa [Modelling transport phenomea in hermetic storage of grains. Prediction of safe storage conditions for silobags]. Dissertation. Universidad Nacional de Rosario.

Bartosik RE, Cardoso ML, Rodríguez JC (2008) Early detection of spoiled grain stored in hermetic plastic bags (silobags) using CO_2 monitoring. In: Proc 8th Int Conf on Controlled Atmosphere and Fumigation in Stored Products, China, pp 550–554.

Cardoso L, Bartosik R, Campabadal C, de la Torre, D (2012) Air-tightness level in hermetic plastic bags (Silo-Bags) for different storage conditions. Proc 9th Int Conf on Controlled Atmosphere and Fumigation in Stored Products, Turkey, pp 583–589.

Cardoso ML, Bartosik RE, Rodríguez JC, Ochandio D (2008) Factors affecting carbon dioxide concentration in interstitial air of soybean stored in hermetic plastic bags (silobag). In: Proc 8th Int Conf on Controlled Atmosphere and Fumigation in Stored Products, China, pp 565–568.

Gastón A, Abalone R, Bartosik R, Rodríguez J (2009) Mathematical modelling of heat and moisture transfer of wheat stored in plastic bags (silobags). *Biosystems Engineering* **(104)**: 72–85.

Ochandio D (2014) Tasa respiratoria de granos de soja (*Glicyne max*) almacenada herméticamente [Respiration rate of soybean grains (*Glicyne max*) hermetically stored]. Master Dissertation, Universidad Nacional de Mar del Plata.

Rodríguez JC, Bartosik RE, Malinarich HD, Exilart JP, Nolasco ME (2001) Almacenaje de granos en bolsas plásticas: Sistema silobag. Informe final de soja. [Grain storage in plastic bags. Silobag System. Soybean Final Report]. EEA INTA Balcarce. http://www.inta.gov.ar/balcarce/info/documentos/agric/posco/granos/silobag.htm

White N, Sinha R, Muir W (1982) Intergranular carbon dioxide as an indicator of biological activity associated with the spoilage of stored wheat. Canadian Journal of Agricultural Engineering **24(1)**: 35–42.