# APPLICATION OF MODIFIED ATMOSPHERES IN GRAIN STORAGE: RETENTION OF CARBON DIOXIDE WITHIN TREATED ENCLOSURES[*]

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**Abstract** - A numerical model to simulate the influence of the different factors that affect gas behavior within a treated enclosure was outlined. The model was compared with experimental results obtained on concentration changes measured in two silos treated with carbon dioxide. The silos were of the same dimensions: one contained 52 tons and the other 28 tons of wheat. Changes in carbon dioxide concentrations, grain and ambient temperatures were recorded periodically throughout the trials. Results of the measured gas concentrations in the trials were compared with the calculated gas concentrations obtained from the numerical model and found to fit satisfactorily. Several numerical experiments were run to simulate the influence of different head space/total volume ratios, pressure relief valve settings, and degrees of gas tightness. The model may be used as a tool in grain storage management to estimate the most important factors which influence gas loss, and to assess the need for improvements in the gas tightness of the treated structure.

## INTRODUCTION

Modified atmosphere (MA) is an alternative method that retains the special capacity of fumigation for in-situ treatment of stored commodities as well as offering a diversity of application technologies (Banks and Ripp, 1984; Fleurat Lessard and Le Torc'h, 1987; Jay and d'Orazio, 1984; Navarro and Donahaye, 1990; Shejbal, 1980).

The application of MAs and fumigants is most appropriate for bulk storage of grain either on-farm, or at central storage installations which are gas-tight according to accepted standards. The fundamental requirement that the structure in which the gaseous treatment is carried out be gas-tight, is rarely met in practice. The major factors which determine the level of gas tightness are permeation through the structural material or fabric, and structural defects which cause leakage. Even when large structures are rendered virtually gas-tight, external factors - including diurnal ambient temperature fluctuations, changes in barometric pressure, and wind velocities - have been recognized as influencing gas loss after application (Winks, 1979).

A choice of two basic approaches can be made to the application of gaseous treatments including MAs, namely: a) high application rates at the purge and maintenance phase of the treatment in leaky containers or b) a high standard of gas

tightness (Winks, 1987). The importance of retaining the gas concentration during the application of MAs should be considered from at least two different aspects: a) the costs involved in an unsuccessful treatment and thereby leaving the commodity subject to insect damage; and b) the risks of increasing selection of a resistant population to the gaseous treatment (Navarro et al., 1985; Winks, 1986, 1987).

This study was undertaken to simulate the different factors which influence gas loss during and after the application of carbon dioxide for stored-product pest control in storage facilities.

## MATERIALS AND METHODS

The metal structures:

These structures consisted of two circular silos each of 68 m$^3$ capacity. They were made of welded rings of sheet steel 8.75 m high and 3.0 m in diameter, with conical lower section of 2.5 m to facilitate unloading. After loading was completed, the lower opening of the same pipe was attached to the pressure release valve designed to hold a positive pressure of 20 cm and a negative pressure of 14 cm water.

In loading of grain:

Wheat of 11% moisture content at an average temperature of 29°C was in-loaded into the metal silos. One silo was filled with 52 tons, and the other with 28 tons of wheat.

Application of carbon dioxide:

Carbon dioxide (CO$_2$) was supplied from pressurized cylinders equipped with a siphon. By this means CO$_2$ was released in a liquid state in order to introduce a large volume of it into the silos over a relatively short time (10 min at a rate of 7 kg CO$_2$/min).

Gas concentrations were monitored periodically using a GowMac thermal-conductivity gas analyzer.

Temperature measurements:

Grain and head space of the silo temperatures were monitored using thermocouples, while ambient air temperature fluctuations were recorded by a thermohygrograph.

Description of the model:

The model used in this study was aimed at running numerical experiments to investigate how changes in the external and internal factors influence the behavior of CO$_2$ within the treated enclosure containing grain. A personal computer (Macintosh IIci) was used to run the simulation model written in STELLA language (Pytte and Doyle, 1984). The independent variables chosen to drive the model were the temperature of the storage environment, the grain mass, head space volume of the treated structure, weight of carbon dioxide used, sorption rate of the gas by the grain (Banks, 1986), degree of gas-tightness of the structure and the pressure-relief valve setting.

This model assumes that:

a) Carbon dioxide is distributed uniformly throughout the grain mass and no gas stratification occurs.

b) After an initial adsorption has taken place, desorption from the grain will not influence the gas concentration.

c) Approximate experimental values based on a pressure decay test were used to determine the rate of gas loss due to leakage.

d) Temperature of the grain mass is uniform, and therefore a chimney effect due to temperature gradients was ignored.

e) Influence of wind on the structure is negligible.

f) Influence of changes in barometric pressure was ignored.

A schematic presentation of the simulation model showing the interrelated variables which influence loss of CO$_2$ from a treated structure are shown in Figure 1. Explanations to the symbols used in the model and the different parameters and values of the constants are given in Table 1.
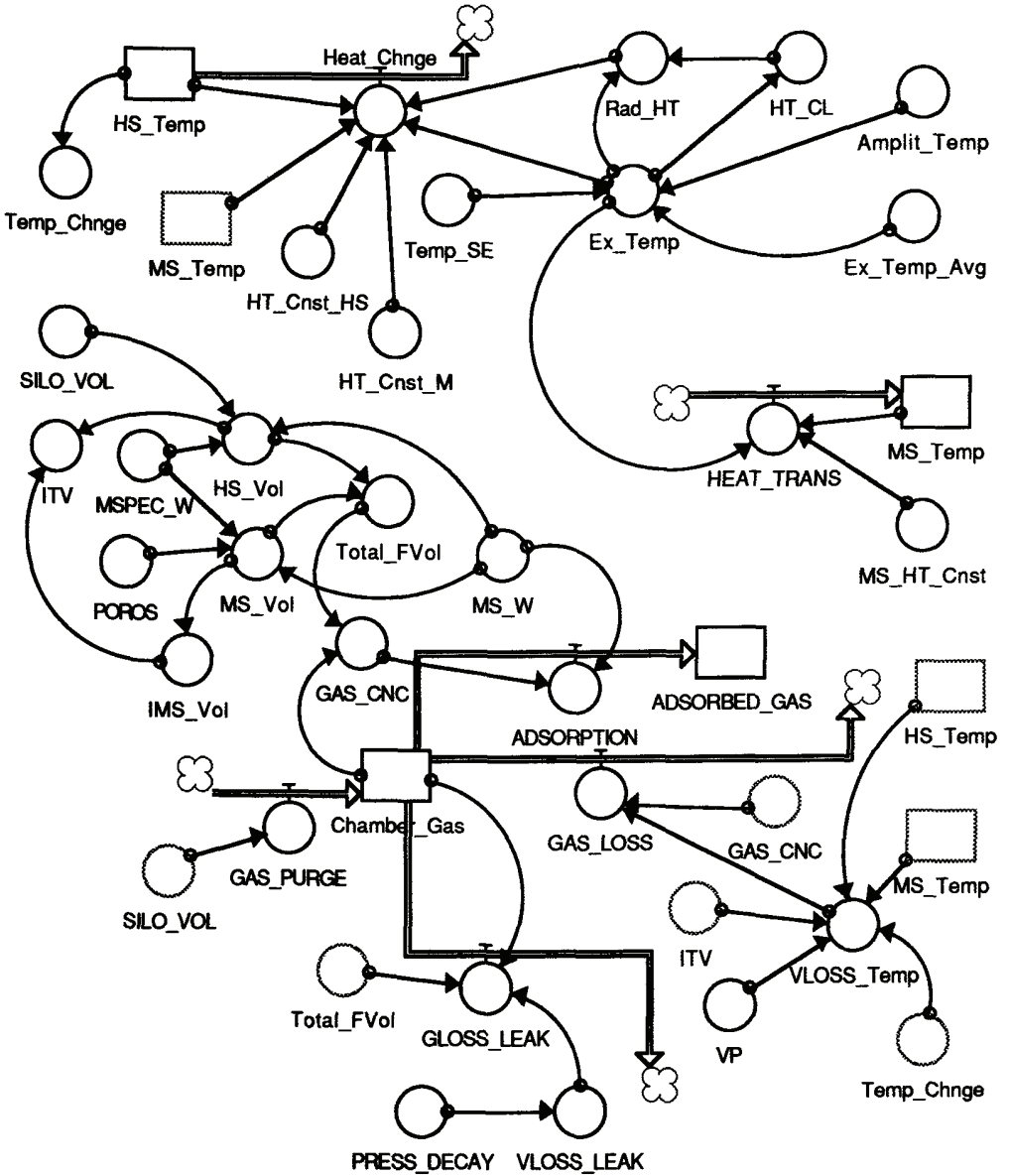
Fig. 1- Schematic presentation of the simulation model showing the interaction of different variables which influence loss of carbon dioxide from a treated structure. Symbols used in Table 1 refer to the variables used in the model.

Table 1- Nomenclature of symbols used in the schematic flow chart presented in Figure 1, the different parameters, values of constants, and the model equations used to simulate retention of carbon dioxide within treated enclosures.

**ADSORBED_GAS** = ADSORBED_GAS + dt * ( ADSORPTION )
INIT(ADSORBED_GAS) = 0
{Amount of $CO_2$ adsorbed at start of purge}
**Chamber_Gas**=Chamber_Gas+dt*(GAS_PURGE-GAS_LOSS- ADSORPTION - GLOSS_LEAK )
INIT(Chamber_Gas)  = 0
{Amount of $CO_2$ initially found in the silo in kg}
**HS_Temp** = HS_Temp + dt * ( -Heat_Chnge )
INIT(HS_Temp) = 30
{Initial head space temperature ($^{\circ}$C)}
**MS_Temp** = MS_Temp + dt * ( HEAT_TRANS )
INIT(MS_Temp) = 30
{Initial grain mass temperature ($^{\circ}$C}
**ADSORPTION** =(GAS_CNC/100)*0.29*MS_W*0.067*EXP(-0.067*TIME)
{Amount of $CO_2$ adsorbed in kg}
**Amplit_Temp** = 10
{Amplitude of temperature change between night and day ($^{\circ}$C}}
**Ex_Temp**=Ex_Temp_Avg+NORMAL(7)*Temp_SE+ Amplit_Temp/2*COS(2*PI/24*(TIME-0))
{Ambient temperature ($^{\circ}$C}}
**Ex_Temp_Avg** = 18 + 7*COS(6.2831853*(TIME-5280)/8760)
{Annual average ambient temperature ($^{\circ}$C}}
**GAS_CNC** = ((Chamber_Gas/2)/Total_FVol)*100
{$CO_2$ gas concentration within the silo in %}
**GAS_LOSS** = if VLOSS_Temp>0 then 2*VLOSS_Temp*(GAS_CNC/100) else 0
{$CO_2$ loss in kg due to influence of ambient temperature on silo interstitial air space, head space and pressure relief valve setting}
**GAS_PURGE** = if TIME <= 5280.1 then (.895*SILO_VOL)/DT else 0
{Gas injection kg $CO_2$/m$^3$  silo total volume}
**GLOSS_LEAK** = (VLOSS_LEAK/24)*DT*Chamber_Gas*Total_FVol*2     {Amount of $CO_2$ loss in kg due to leaks}
**Heat_Chnge** =  -(Ex_Temp-MS_Temp)*HT_Cnst_M - Rad_HT -(Ex_Temp-HS_Temp)*HT_Cnst_HS
{Heat exchange which influence the head space air temperature fluctuations}
**HEAT_TRANS** = MS_HT_Cnst*(Ex_Temp-MS_Temp)
{Heat transfer from the grain mass}
**HS_Vol** = SILO_VOL-(MS_W/MSPEC_W)
{Head space volume in m$^3$}
**HT_CL** = Ex_Temp-DELAY(Ex_Temp,DT)
{Time elapsed to influence head space air to cool or to heat}
**HT_Cnst_HS** = .6*DT
{Constant of heat exchange between external to head space temperatures}
**HT_Cnst_M** = 1*DT
{Constant of heat exchange between ambient and grain mass temperatures}
**IMS_Vol** =0.05*MS_Vol
{Intergranular space influenced by daily temperature fluctuations in m$^3$ (it was estimated as an approximate value of 5% of the grain mass volume)}
**ITV** = HS_Vol+IMS_Vol
{Volume (m3) of air-$CO_2$ mixture influenced due to temperature changes}
**MSPEC_W** = .83
{Bulk density of grain mass (ton/m$^3$)}
**MS_HT_Cnst** = 0.002
{Constant of grain mass heat exchange rate}
**MS_Vol** = (MS_W/MSPEC_W)*POROS

{Intergranular air space volume {m$^3$} of the grain mass}
**MS_W** = 50
{Weight {ton} of grain mass in the silo}
**POROS** = .40
{porosity of the grain mass in % {40% estimated for wheat}
**PRESS_DECAY** = 22
{Pressure decay rate expressed as time {min} needed for pressure drop from 1500 to 750 Pa   }
**Rad_HT** = if HT_CL > 0 then 0.1*Ex_Temp else 0
{Influence of ambient temperature and solar irradiation on head space air temperature {it was estimated as an approximate value 10% of the ambient temperature}}
**SILO_VOL** = 68.21
{Total silo volume in m$^3$}
**Temp_Chnge** = HS_Temp-delay(HS_Temp,DT)
{Time delay to influence head space temperature change}
**Temp_SE** = 0.2
{Ambient temperature standard deviation}
**Total_FVol** = HS_Vol+MS_Vol
{Head space and intergranular air space total volume {m$^3$}}
**VLOSS_LEAK** = IF PRESS_DECAY<21.38 THEN  -( (PRESS_DECAY-21.38)/ 1.798)/100 ELSE 0
{CO$_2$ decay rate in %/day as a measure of gas loss}
**VLOSS_Temp** = if Temp_Chnge>0  then
ITV-(ITV*(HS_Temp+273)*(101308+10*VP)/((MS_Temp+273)*101308))  else  0
{Volume of air-CO$_2$ mixture lost due to temperature fluctuations in each expansion}
**VP** =50
{Valve presure set in mm water}

## RESULTS AND DISCUSSION

Values obtained from numerical experiments were compared with those obtained from field trials. Figures 2 and 3 show the measured and calculated changes of CO$_2$ concentrations during and after the treatment. The similarity between the measured and the calculated values corroborates the validity of the model.

Based on this model, numerical experiments on gas concentration decay were run for 20 days using the main features shown in Table 2. A model silo of a capacity similar to that used in the field experiments containing 52 tons of wheat grain, was used to run the simulation model. Since the head space volume was considered important, head space/total volume ratios of 0.1, 0.3, 0.5 and 0.7 were investigated. For silos with a very high degree of gas tightness, the pressure-relief valve appears to play an important role in maintaining the gas within the treated structure. Therefore, pressure-relief valve settings of 10, 500, 1000, 1500 and 2000 Pa were compared. To study the importance of gas tightness, a completely gas-tight structure was compared with a structure which maintains a pressure decay from 1500 to 750 Pa in 10, 15, and 20 min (Banks et al., 1980).

Figures 4, 5 and 6  show the results of the numerical experiments on the retention of CO$_2$ within the silo under the different simulation conditions given in Table 2. Fig. 4 shows that increasing the head space/total volume ratio has a significant influence on the gas concentration decay rate (runs 1 to 4 in Table 2). Pressure-relief valve settings influenced slightly the gas decay rate (Fig. 5, runs 5 to 9 in Table 2). Fig. 6 (runs 10 to 13 in Table 2) of the numerical experiment enabled assessment of the gas retention time in a leaky container, and the results   differ significantly from those of the other runs in Figures 4 and 5. This indicates the extreme importance of a gas-tight enclosure to control insects. This information may be used to determine the relative importance of the variables which influence gas loss, the necessity to increase the gas tightness of a structure, and the need to predict the effectiveness of the planned treatment in controlling insects.
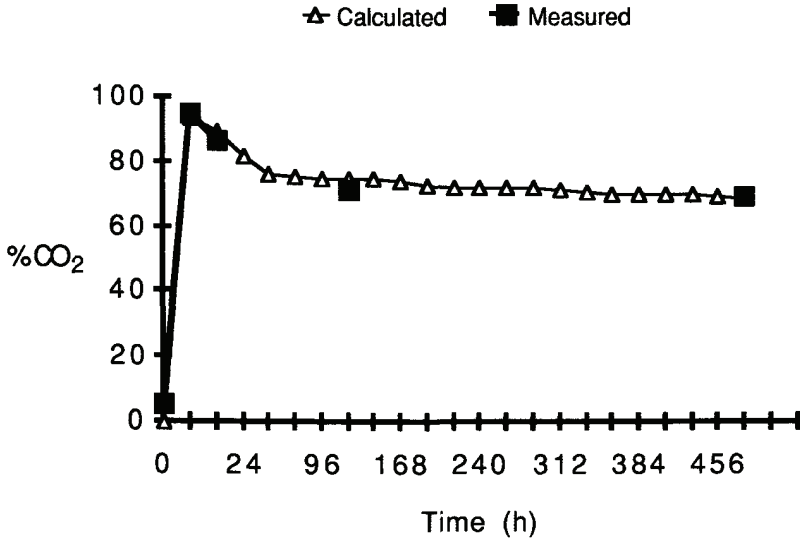
Fig. 2- Calculated and measured average carbon dioxide concentrations in a silo containing 52 tons of wheat at $29^{\circ}C$ with a head space/total volume ratio of 0.1. Calculated gas concentrations were obtained from the numerical experiment.
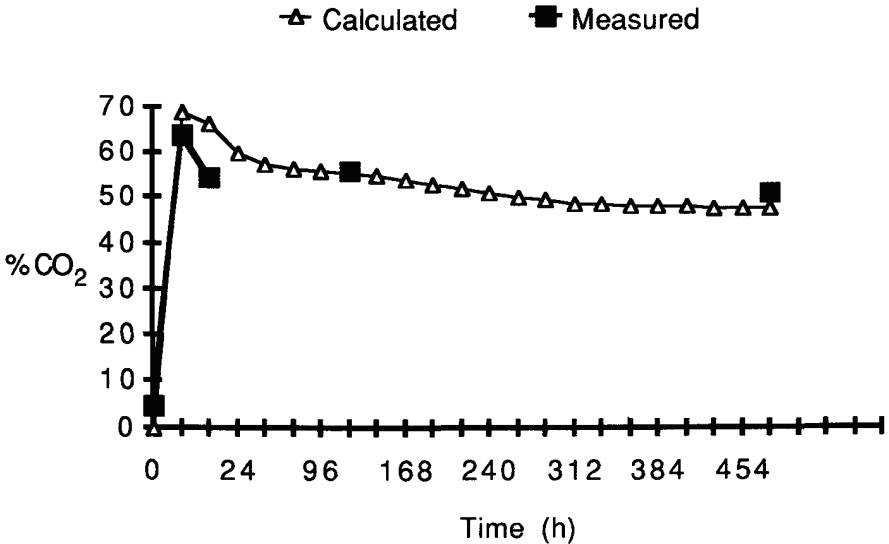
Fig. 3- Calculated and measured average carbon dioxide concentrations in a silo containing 28 tons of wheat at $29^{\circ}C$ with a head space/total volume ratio of 0.5. Calculated gas concentrations were obtained from the numerical experiment.

Table 2 - Parameters used to run the numerical experiments reported in Figures 4, 5 and 6.

| Reference to Fig. No. | Run | Amount of wheat (tons) in the silo of 68 m$^3$ | Pressure relief valve set (Pa) | Pressure decay time (min) from 1500 to 750 Pa | Estimated gas loss in %/day due to leaks | head space /total volume ratio |
|---|---|---|---|---|---|---|
| 4 | 1 | 52 | 1500 | 25 | 0 | 0.1 |
|   | 2 | 40 | 1500 | 25 | 0 | 0.3 |
|   | 3 | 28 | 1500 | 25 | 0 | 0.5 |
|   | 4 | 16 | 1500 | 25 | 0 | 0.7 |
| 5 | 5 | 52 | 10 | 25 | 0 | 0.1 |
|   | 6 | 52 | 500 | 25 | 0 | 0.1 |
|   | 7 | 52 | 1000 | 25 | 0 | 0.1 |
|   | 8 | 52 | 1500 | 25 | 0 | 0.1 |
|   | 9 | 52 | 2000 | 25 | 0 | 0.1 |
| 6 | 10 | 52 | 1500 | 10 | 6,5 | 0.1 |
|   | 11 | 52 | 1500 | 15 | 3 | 0.1 |
|   | 12 | 52 | 1500 | 20 | 1 | 0.1 |
|   | 13 | 52 | 1500 | 25 | 0 | 0.1 |

## CONCLUSIONS

A numerical simulation model of the different factors which influence gas behavior within a treated enclosure has been outlined. The model may be used in grain storage management to assess the need for improvement in the gas tightness of the treated structure or to predict the effectiveness of the planned treatment in controlling insects. Prior to a gaseous treatment, a pressure decay test may be of importance to estimate the level of gas retention. The described numerical model can serve as a tool to estimate the importance of factors contributing to gas loss.

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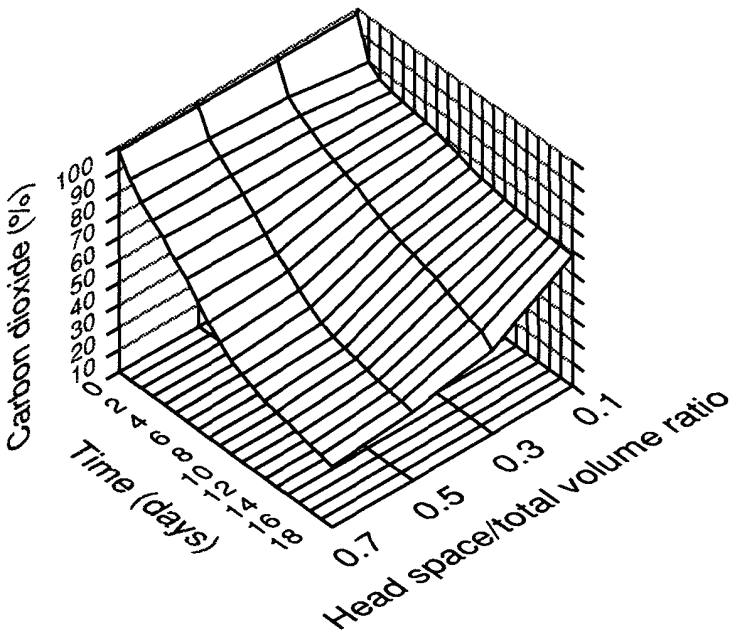
Fig. 4- Results of numerical experiments obtained using the model to simulate retention of carbon dioxide within treated enclosures of different head space/total volume ratios. The main features of runs 1 to 4 are shown in Table 2.
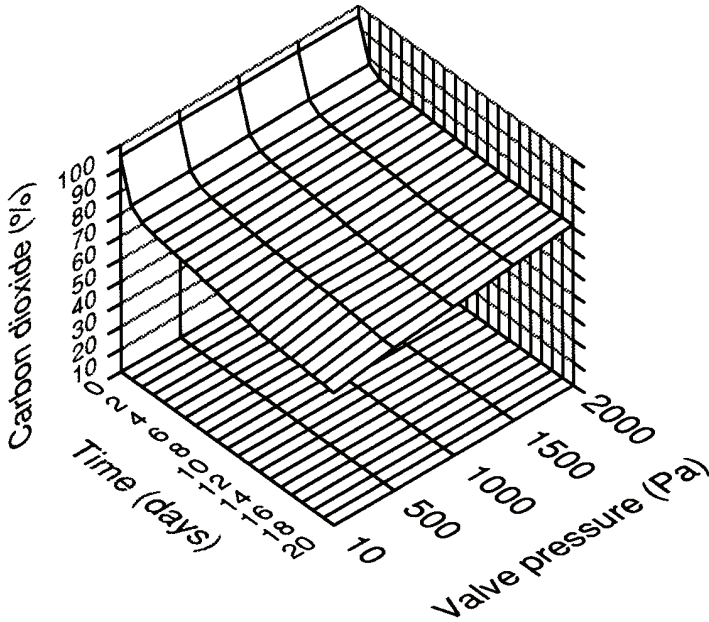
Fig. 5- Results of numerical experiments obtained using the model to simulate retention of carbon dioxide within treated enclosures of different pressure relief valve settings. The main features of runs 5 to 9 are shown in Table 2.
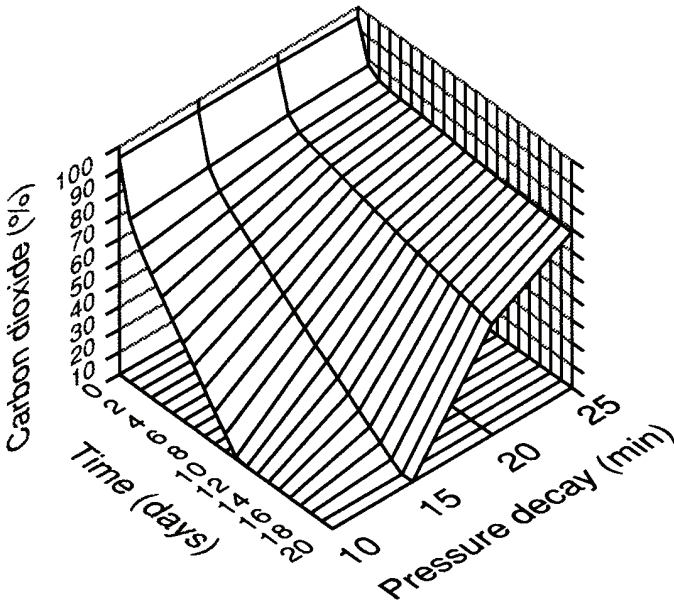
Fig. 6- Results of numerical experiments obtained using the model to simulate retention of carbon dioxide within treated enclosures at different degree of gas tightness as expressed in min for pressure decay from 1500 to 750 Pa. The main features of runs 10 to 13 are shown in Table 2.

# LES APPLICATIONS DES ATMOSPHERES MODIFIEES AU STOCKAGE DU GRAIN

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## RESUME

Les traitements insecticides en atmosphère modifiée (AM) sont entrepris dans le but de créer un environnement létal pour les insectes des magasins de stockage. Cette méthode est la seule alternative à la fumigation et s'offre à de nombreuses applications et traitements sans laisser de résidus toxiques. Cette publication passe en revue les méthodes les plus couramment utilisées.

Les AM peuvent être créées grâce à du gaz liquéfié, soit transporté en vrac dans des camions citernes, soit comprimé dans des réservoirs cylindriques dans le cas de traitements à petite échelle. Une alternative consiste à générer ces AM directement sur le site. Ceci exige l'emploi de générateurs exothermiques de gaz inerte dont le fonctionnement est basé sur la combustion d'hydrocarbures ainsi que sur l'utilisation de compresseurs et de tamis moléculaires produisant de l'azote à partir de l'air. Nous discuterons des possibilités de créer des AM sur site grâce à des sources biologiques, comme le stockage hermétique assisté par bio-génération de AM externe ainsi que du stockage hermétique conventionnel. Les effets des AM sur les insectes les plus communs des stocks ont été étudiés par rapport à la concentration et au temps d'exposition de façon à établir des gammes de doses efficaces. Ces études montrent que les atmosphères air/dioxyde de carbone sont habituellement plus toxiques que les atmosphères pauvres en oxygène. Les méthodes d'application et les gaz nécessaires sont passées en revue en tenant compte de la qualité de construction des enceintes existantes à traiter.