adoption of a recirculation system in these cases can improve fumigation results. Summarizing, our tests clearly indicated that phosphine sensors were quite effective in measuring phosphine concentrations and can play an important role in the future in IPM-based programs during the post-harvest stages of agricultural commodities. Hence, sensors can be used as a "precision fumigation" tool and provide real-time estimates for insect control.

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Use of a 3D Finite Element Model for Post Fumigation Phosphine Movement Analysis

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Abstract

Phosphine is a dangerous gas commonly used in fumigations throughout the world. Grain that has not fully released the phosphine it absorbed during fumigation may continue to desorb phosphine into the headspace of a storage structure. U.S. OSHA standards for handling phosphine state the acceptable limit at 0.3 ppm. If this limit is exceeded grain handling may become dangerous. It is important to understand the process of phosphine venting and desorption in order to ensure safe handling of fumigated grain in silos and during shipments. In order to achieve this, the venting and release of phosphine was studied on location in a well-sealed grain silo in Lake Grace, Western Australia, to serve as a set of data for verification of a computational model. This situation was then modeled using a 3D finite element model and compared to the real world results. Results were calculated using two fumigant desorption models based on previous literature, a reversed sorption model and an air-grain equilibrium model. Simulations reproduced accurate trends of desorption but did not accurately reproduce the quantity of fumigant, with a 55.5% error for the model based on reversed sorption equations and 86.3% error for the air-grain equilibrium based model. For both models, simulations were conducted to compare the effectiveness of existing grain venting regulations at producing grain that is within safe handling limits. These results highlight the necessity for continued desorption research and the importance of following venting guidelines.

Keywords. Finite Element Modeling, Fumigation, Phosphine, Stored Product Protection

1. Introduction

A successful fumigation relies on exposing each insect within a grain mass to the specific concentration of fumigant for a specified amount of time needed to kill all insects present at all life stages. There is a significant amount of literature available on the bio-efficacy of fumigants such as phosphine against a range of stored product pests at multiple life stages (Chaudhry, 2000; Price and Mills, 1988), however, information on the fumigant activity within the commodity during a fumigation is very limited. Therefore, modeling the behavior of gas fumigants in the interstitial air volume of the stored grain mass is helpful in determining what factors may cause fumigation failures, and how those factors can be affected by environmental conditions. A previous attempt at developing such a fumigation model was made by Isa et al. (2016) using the program Fluent instead of an independent computer code. They also simulated vertical gas flow in a silo using Fluent and Comsol (Isa et al., 2011). While using any of the available fluid dynamics software packages has several advantages, such as ease of use and ease of visualizing results, it has disadvantages as well. Their fumigation model simulates both sorption and leakage losses, but the leakage losses are not influenced by weather condition or operational variables which is not realistic. Since the boundary conditions are set inside Fluent, loss prediction was implemented with point losses only. The amount of loss was then controlled only by pressure half loss time. This strategy may be insufficient not only for fumigant loss that is affected by weather, but also in its inability to consider the combined effect of many small leaks over the entire external surface of the silo.

The M-L 3D finite element ecosystem model was previously developed to investigate stored grain environments and has the capacity to monitor chemical concentrations throughout the grain mass (Lawrence, 2010; Lawrence and Maier, 2011). In order for this model to accurately predict fumigant concentrations the model had to be improved with the added capacity to account for fumigant loss. The primary sources of fumigant loss are fumigant leakage from the silo and fumigant sorption into the grain.

Sorption of gas by grain was listed as one of the factors most likely to cause inadequate fumigation conditions in Australia (Darby, 2011). Wheat at higher temperature sorbed a greater amount of phosphine than lower temperature wheat. After 96 hours in a container with initially 1 mg/L phosphine, the fumigant concentration in the interstitial airspace of stored wheat at 35°C was below 0.1 mg/L, whereas in wheat at 15°C it was around 0.5 mg/L (Darby, 2011). That result was supported by Reed and Pan (2000), Sato and Suwanai (1974) and Dumas (1980) who reported phosphine sorption increased with higher grain temperature and moisture content. An increase of temperature also caused faster rates of sorption of phosphine in wheat independently from moisture content. An increase from 24°C to 35°C caused the sorption rate constant to increase from 0.0064 to 0.186 (Banks, 1986; Berck, 1968). Increased adsorption of phosphine to the surface of cereal grains with increasing temperature was also shown in Sato and Suwanai (1974).

There are a number of factors that may deter the efficacy of a fumigation where enough fumigant was applied to theoretically control the insects. According to Banks and Annis (1984) these factors are excessive overall loss of fumigant, inadequate fumigant dosage in localized regions, excessive delay between application and fumigant reaching particular regions, or a combination of these factors occurring simultaneously. To observe whether any of these effects were occurring in a fumigation would be difficult and would require excessive monitoring of fumigant concentrations at a number of locations in the silo. Even with such controls, there could be regions that are not monitored and experience problems, or environmental conditions that are abnormal or unforeseen. How environmental factors and operational procedures influence a fumigation can be more easily and thoroughly investigated using a fumigant model that incorporates sorption and fumigant loss. A better understanding of such influences would allow applicators to take more effective corrective actions to prevent fumigation failures.

2. Materials and Methods

2.1 Effect of Sorption

To estimate sorption loss of phosphine gas in a grain silo, an equation for concentration as a function of time was obtained from Daglish and Pavic (2008). The equation is valid at a 1 mg/L application, and 0.75 fill ratio, resulting in an R^2 value of 0.96 at 25°C and 55% relative humidity. The equation presented in the literature was adjusted to fit the time step and units in the code, i.e., an hourly time step and units of kg/m^3. Additionally, to calculate the amount of phosphine lost due to sorption, the equation was modified by taking the derivative with respect to time. The resulting baseline sorption equation was:

$$C = 0.0000026e^{-0.0017t} \qquad \text{Eq 1}$$

where,

C = fumigant concentration lost [kg/m^3], t = time [h]

Fumigant sorption also varies due to other factors that are important variables in our experiment, such as temperature and moisture content of grain. To account for these variables, Eq [1] was multiplied by factors dependent on temperature and moisture content. The effect of temperature on phosphine sorption was studied by Darby (2011) who determined sorption losses at 35°C were about five times as large as losses at 15°C, at a constant equilibrium relative humidity of 65%. Therefore, this result can be modeled with an exponential equation dependent on temperature, where the value at 35°C is five times the value at 15°C. The value for this expression is set to equal one when the temperature is at 25°C, because that is the temperature of the baseline equation from Daglish and Pavic (2008). This means that when the temperature equals that of the baseline equation, the overall equation should be unchanged. The effect of moisture content on the sorption of phosphine was studied by Reed and Pan (2000). They determined fumigant loss for several temperatures at two values of wheat moisture content, i.e., 11% and 13.5%. The sorption at the higher moisture content was 1.8 times greater than the sorption at the lower moisture content at 25°C. This was modeled with an exponential equation which was set to 11.5%, the equilibrium moisture content of the wheat from the baseline Daglish and Pavic (2008) equation. The resulting equation for fumigant loss due to sorption into the grain mass when modified to account for changing temperatures and moisture contents is therefore:

$$C = 0.0000026e^{-0.0017t} * 0.13365e^{0.0805T} * 0.067e^{0.235M} \qquad \text{Eq 2}$$

where,

C = fumigant concentration lost [kg/m^3]

t = time [h]

T = temperature [°C]

M = moisture content [%], wet basis

Implementing this equation into the fortran computer code required that the fumigant concentration lost due to sorption is subtracted from the current fumigant concentration at each node for each time step but only if the current fumigant concentration at that node is higher than the sorption amount to be subtracted. If the phosphine concentration at a node is less than the concentration that would be lost to sorption, the phosphine value at that node is set to zero instead.

2.2 Effect of Silo Leakage

To estimate the amount of fumigant lost due to leakage from the silo, estimates for individual sources of leakage were taken from Banks and Annis (1984) along with additional information from the other sources to extrapolate estimates of fumigant loss as a summation of losses from various sources. The most significant sources of fumigant loss result from: (1) concentration differences between the inside of the grain silo and the ambient conditions, (2) chimney effects due to temperature differences, (3) chimney effects due to concentration gradients, and (4) wind effects.

To implement these equations into the computer code, the calculated fumigant concentration lost is subtracted from the current fumigant concentration at each node along the vertical silo wall at each time step but only if the fumigant concentration at that node is higher than the leakage amount to be subtracted. If the phosphine concentration is less than the amount to be subtracted, the concentration is set to zero.

The final equation to predict fumigant leakage from the silo due to effects of fumigant sorption and loss, and modified for changed environmental conditions is therefore:

$$C = \frac{5}{x} * \frac{Nn}{Nb} * (0.0002233e^{0.4621Sw} * Ci + 0.0000248\, e^{0.1386Tc} * \, Ci + 0.0000326e^{0.1386Td} * \, Ci + 0.0029962Ci^2) \quad \text{Eq 3}$$

Where,

C = fumigant concentration lost [kg/m^3]

X = pressure half loss time (minutes)

N_n = number of nodes

N_b = number of boundary nodes

Once equations were developed to predict phosphine loss from sorption and leakage from the fumigation in question from factors such as the effects of weather, they could be used to determine the sensitivity of fumigations to changing environmental conditions. The original 10-day fumigation was conducted from Aug 31 to Sept 9, 2015 in Manhattan, Kansas. Weather data for that time period was acquired from the Kansas State University Mesonet database (http://mesonet.k-state.edu/). This weather data was modified by changing hourly values of each key parameter (wind speed, ambient temperature, relative humidity) by +/- 25% and +/-50%. The modified simulations were compared to a base case that used the original weather data to simulate the fumigation described in Cook (2016).

2.3 Simulated Fumigation

A mesh with 2,587 nodes was created in the Abaqus finite element software for the simulation based on the dimensions of the silo supplied. While the dimensions were modeled precisely, the major discrepancy is that this silo contains a cone shaped bottom, and our model is limited to a flat bottom silo. For this reason, the cone was left off, but the extra distance may have provided space for more mixing of the fumigant before it arrived in the region of the simulation. For this reason, fumigant was applied across the entire lower boundary of the simulation, excluding boundary nodes. Weather data for the period in question was taken from the Kansas State University Mesonet database (http://mesonet.k-state.edu/). As phosphine cannot be directly input into the model, a phosphine application method was implemented in which the base nodes of the silo, excluding edge nodes, were set at a starting amount that was held for 24 hours to approximate the phosphine release time in the experiment (Cook, 2016).

3. Results and Discussion

3.1 Simulation Accuracy

With model parameters such as loss and leakage quantified, the model was verified by comparison of the simulated fumigant concentrations to the experimental values measured by Cook (2016) with a gas release period of 24 h. Both the experimental and simulated results indicate a rapid increase of phosphine at the beginning of the fumigation, followed by a loss of phosphine that continually slows until the end of the fumigation, as seen in Fig. 1. While the trends are similar, the maximum average concentration is greater when only considering the points available in the experimental data. This effect demonstrates the potential for over predicting phosphine concentration when not measuring points along the sidewall of the silo.

The quantitative comparisons between the measured and predicted values are based on results reflecting the same locations and time readings. The root mean square error of this verification was 47.5 ppm, the average difference was 0.1 ppm, and the average of the absolute values of the differences was 38.6 ppm. The overall average experimental fumigant concentration was 283.3 ppm, therefore, the average percentage error compared to predicted values was 13.6%. The major discrepancy between the results seems to begin the evening of the first day of fumigation, around 1830 to 1930, when the increase in phosphine in the experimental data begins slowing and the predicted data do not. This coincides with the beginning of a decrease in night time temperature. This may be similar to the night time phosphine drop noted in Australian experimental data that was made available to the authors by the PBCRC (data not shown). This culminates in the largest difference between experimental and predicted data, at 1100 the next morning, after which the experimental phosphine readings begin to climb back to levels predicted by the simulation. The low temperature that night was 21.8°C, the afternoon highs for August 31st and September 1st were around 33°C. A similar effect appears to happen at a smaller scale the next night, with the values dropping slightly and then rebounding in the morning of September 2nd. The temperature that morning was around 25°C. After the second night, night time concentration drops are not seen in the experimental data, either because they did not happen, their effect was smaller due to lower phosphine values, or they were missed due to lack of night time phosphine sampling. The net effect, however, is that the predicted values appear to be a few hours ahead of the actual values. The night time decrease may also explain why the simulation slightly over predicted the amount of phosphine reported. This, along with an over prediction of the low phosphine levels seen late in the experiment, comprise the major differences between the simulation and experiment.

3.2 Temperature of Ambient Air

Shown in Fig. 2 are the predicted average concentrations of phosphine for five simulations with a varying ambient temperature, expressed as percentages of the ambient temperature for the model verification (i.e., 100%) in degree Celsius scale. As expected, when ambient temperatures were increased, total average phosphine concentrations in the silo decreased. The effect of increasing temperatures is not directly proportional, as the effects of temperature changes decrease as the temperature increases. When temperatures were decreased, total average phosphine concentrations increased by a higher amount. Halving the ambient temperature resulted in a phosphine concentration that when averaged over all locations and times was 26% greater than the concentration from the verification. At 1.5x the ambient temperature, overall average phosphine concentration was 27% less than the overall average concentration from the verification. Fumigations with lower ambient temperatures achieved higher maximum phosphine concentrations (416, 410, 400, 380, and 364 for 50-150%, respectively). The scale of the effects builds with time, becoming larger as the simulation progressed (Fig. 1). By the end of the simulation the percentage differences from original were 102%, 57.3%, -47.1%, and -67.9%, for the 50%, 75%, 125%, and 150% ambient temperature situations, respectively. The temperature decreases caused 57% and 102% increases in phosphine concentration for the 75% and 50% temperature cases, respectively.

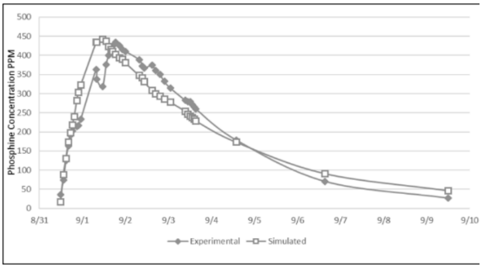

Fig. 1 – Comparison between average experimental and predicted phosphine concentration (ppm) results considering only data at the same locations and times from which data were recorded by Cook (2016) between August 31 and September 9, 2015, with a 24h fumigant release.

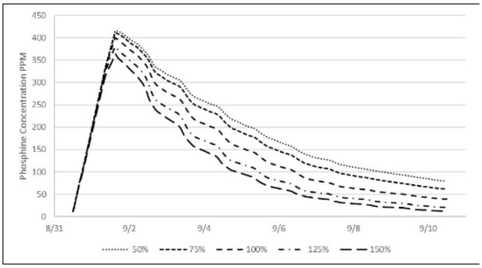

Fig. 2 – Overall average phosphine concentration (ppm) for five temperature conditions, expressed as a percentage of the temperatures (100%) used in the verification conducted between August 31 and September 9, 2015.

Increasing the ambient temperature by a factor of three (i.e., from 150% to 50%) decreased the overall average Ct-product by 71.5%, i.e., from to 47500 ppm-h to 27700 ppm-h (Table 1). Doubling the ambient temperature of the silo (i.e., from 75% to 150%) decreased overall average Ct-products by 39.1%, from 43800 ppm-h to 27700 ppm-h.

Table 1 – Cumulative average Ct-products (ppm-h) and the difference from original (%) for five ambient temperatures, expressed as a percentage of the ambient temperatures (100%) used in the verification conducted between August 31 and September 9, 2015.

	50%	**75%**	**100%**	**125%**	**150%**
ppm-h	47500	43800	37700	31400	2,700
Percent Difference	26.0	16.1	0.0	-16.6	-26.6

The primary reason for this relationship is found in the fumigant loss equation and its reliance on temperature. Based on baseline equations developed in Banks and Annis (1984), fumigant concentration loss increases as a function of grain temperature along the silo wall, and with increases in the difference between the silo temperature and ambient temperature. Additionally, temperature increases also increase the fumigant loss due to sorption as detailed in Daglish and Pavic (2008). Increasing and decreasing ambient temperature does not have an equal influence on overall fumigant concentrations. This is due to the previously discussed effect on increasing leakage from the silo. As the leakage rates increase at high temperatures, the effect diminishes because the leakage effect due to temperature difference comprises only two terms in the overall leakage equation, which is additive. This can be seen clearly in Table 1, as increasing from the 100% case to 125% had a larger effect than increasing from 125% to 150%, and decreasing from 100% to 75% had a larger effect than decreasing from 75% to 50%.

The effect of temperature is of particular interest in subtropical grain growing regions such as Australia, where temperatures are high and grain is commonly fumigated in the summer. Higher temperatures cause increased gas leakage, making sealing even more important. While high temperatures cause a decrease in phosphine concentrations in the grain mass, phosphine is more effective against insects at higher temperatures (Bond, 1989; Sun, 1946) in large part due to their increased activity and higher respiration rates. If, however, the silos were well sealed, increased leakage caused by higher temperatures would be mitigated and insect susceptibility to the fumigant would be maximized.

3.2.3. Wind Speed

Shown in Fig. 4 are the predicted average concentrations for phosphine for five simulations with varying wind speeds, expressed as percentages of the wind speeds from the model verification (i.e., 100%). As expected, phosphine concentrations were higher for silos with lower wind speeds. Halving wind speed resulted in a phosphine concentration that when averaged over all locations and times was 10.4% greater than the concentration from the verification. At 1.5x, the same overall average phosphine concentration was 13.3% less than the overall average concentration from the verification. Fumigations with lower wind speeds achieved higher maximum phosphine concentrations (407, 404, 400, 393, and 386 for 50-150%, respectively), as leakage begins taking effect before the maximum values are reached. Percentage changes resulting from the five simulations are shown in Fig. 5. By the end of the simulation the percentage differences from original were 25%, 14%, -15%, and -29% for the 50%, 75%, 125%, and 150% wind speed cases, respectively.

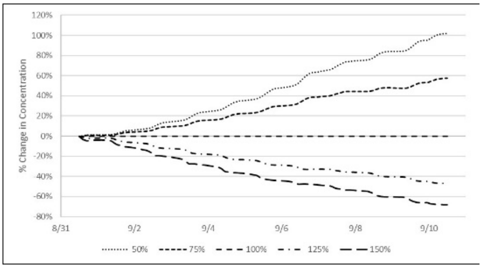

Fig. 3 – Change in overall average phosphine concentration (%) for five temperature conditions, expressed as a percentage of the temperatures (100%) used in the verification conducted between August 31 and September 9, 2015.

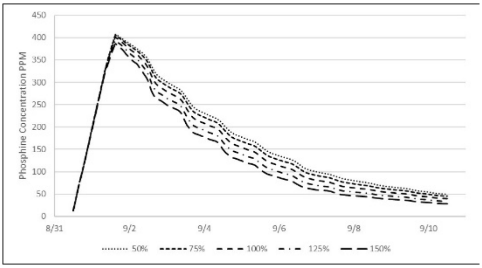

Fig. 4 – Overall average phosphine concentration (ppm) for five wind speeds, expressed as a percentage of the wind speeds (100%) used in the verification conducted between August 31 and September 9, 2015.

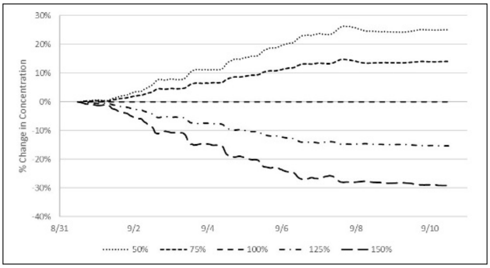

Fig. 5 – Change in overall average phosphine concentration (%) for five wind speeds, expressed as a percentage of the wind speeds (100%) used in the verification conducted between August 31 and September 9, 2015.

Increasing the wind speed by a factor of three (i.e., from 50% to 150%) decreased the overall average Ct-product by 27%, i.e., from 41600 ppm-h to 31700 ppm-h (Table 2). Doubling the wind speed of the silo (i.e., from 75 to 150%) decreased overall average Ct-products by 21%, from 39900 ppm-h to 31700 ppm-h.

Table 2 – Cumulative average Ct-products (ppm-h) and the difference from original (%) for wind speeds, expressed as a percentage of the wind speeds (100%) used in the verification conducted between August 31 and September 9, 2015.

	50%	75%	100%	125%	150%
Ct-product	41600	39900	37700	35200	31700
Percent Difference	10.4	6.0	0.0	-6.7	-13.3

For temperature and leakage effects, any change in conditions that resulted in an increased loss of fumigant had a smaller proportional change as higher amounts of loss were reached. In this case, the effect of increased wind speeds did not decrease at higher wind speeds, and in fact had a slightly larger impact on phosphine concentrations. The value in the exponent of the wind speed equation adapted for the model in Plumier et al. (2018) is more than three times the exponent in the temperature equations. Thus, the exponential effect of increasing wind speed will be much more pronounced than changes in temperature or leakage as seen previously. The exponential increase in fumigant concentration loss due to higher wind speeds was slightly more than enough to overcome the diminishing returns of increasing leakage, and will be more relevant given the likelihood that weather events can cause wind speed changes greater than those tested, which is unlikely for temperature. These results also agree with the results of Chayaprasert et al. (2015), which demonstrated increasing wind effects at higher velocities. The influence of wind speed on a fumigation is often more variable than the influence of ambient temperature, due to the overall percentage changes that occur. While the temperature effect continued to increase consistently over the course of the simulation, the wind effect was more dependent on varying weather conditions. The low wind speed conditions that were observed beginning on September 8 caused the effects of changing wind speed to level off, as seen in Fig. 5. These results indicate that weather events that cause high wind speeds are capable of having a large disruptive impact on phosphine concentrations in a silo. This points to the importance of best fumigation management practices such as seal testing a silo before a fumigation and monitoring gas concentrations during a fumigation. Monitoring phosphine concentrations helps detect increased fumigant loss due to sudden increases in wind speed.

4. Conclusions

- The verification demonstrates that the model effectively predicted the trend of phosphine concentrations, and predicted the overall Ct-product of the fumigation reasonably accurate.
- The accuracy of this fumigation model was found to be sufficient to use the model as a tool for conducting future simulations on predicting fumigant concentrations as a function of environmental conditions and operational variables.
- Increasing temperature and wind speed decreased phosphine concentrations, with temperature changes having a more significant impact overall than wind speed changes at tested levels. However, given the larger variability of wind effects possible beyond tested levels and the greater impact of increasing wind speeds relative to temperature, high wind weather events such as thunderstorms have the potential for substantial disruptive impact on phosphine concentrations.

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A Novel Engineering Design of Small Scale Metallic Silo for Food Safety in Rural India

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Abstract

Wheat is an essential component of the human diet for most of the world. In India wheat is an important staple food crop and it is used for the preparation of a diversity of products like *roti*, *parantha* (semi fried), *puri* (fried), bread, pasta, noodles, buiscuits etc. It has been reported that ~60-70% of wheat produced is stored at home or farm levels for domestic consumption. In order to understand the rural grain storage system, an extensive field study was carried out in villages of Haryana state (India). The field study revealed that ~95% of families store their grains in metallic silos of different sizes (300 to 2000 kg) and only Aluminium phosphide tablets (locally called sulfas) are used to protect grains from storage pests. Aluminium phosphide (AlP) tablets are used in an unscientific manner to control insect pest infestation, resulting in residues in stored grain. An experimental study of 12 months was carried out to identify the problems associated with pest management in conventional metallic silos. The storage period was divided into two parts, i.e., summer and winter, of 180 days each. Ambient temperature and relative humidity (RH) were recorded continuously for the entire period and temperature inside the silos was also recorded at different locations. The emergence of 'hot spots' was found during May-June when the temperature ranged from 37.6 to 42.7°C inside the silo during the summer season. During this period ambient temperature and RH ranged from 22.6-44.2°C and 37-82%. At this stage, convection current caused moisture migration at the top and bottom of the silo, whereas in the winter season moisture migration inside the silo was observed only at the top layer. Wheat samples from the topmost layer, in the vicinity of the "hot-spot" and from the bottom layers were collected and analyzed for various quality parameters.

The wheat samples near the "hot-spot" emergence were found most deteriorated in every aspect, for instance, in terms of protein content (decreased by 21.77%), fat content (decreased by 64.05%), germination capacity (decreased by 84.06%), thousand kernel weight (decreased by 22.09%), ash content (decreased by 41.96%), acidity (increased from 3.07-6.23 mm/gm) and insect-damaged kernels (increased by 80%). The results confirmed that even in a very small silo of 100 kg capacity if grains are stored without any fumigation treatment,