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# MODELLING THE OZONE PENETRATION IN A GRAIN LAYER

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**Abstract.** Studies of grain drying with ozone-air mixture were carried out to detect the ozone penetration patterns through the grain mound of various moisture content ( $14.6 \le w_0 \le 23.0\%$ ) at different ozone concentrations ( $500 \le C_0 \le 1250$  ppb) in the supplied air. The ozone penetration through the grain layer depends on the initial ozone concentration in the supplied air, ozonation time, velocity of the supplied air, height of the grain mound, initial grain moisture content and mycobiotic contamination of grain surface. It was determined that in a 60 cm height of the grain layer ozone is first recorded after 12 h, and at 105 cm – only after 34 h at  $w_0 = 19.0\%$ ,  $C_0 = 500$  ppb. If the initial concentration of ozone is higher, it is first recorded sooner. Ozone penetration through the grain layer with higher moisture level is slower, and ozone reaction with grain surface and microflora present on it is longer.

Hypothesis about the adequacy of the model (how it reflects the real process) has been verified by calculating reproduction and adequacy variance. The mathematical model could be applied for prediction of the course of grain ozonation process.

Keywords: environmental processes modelling, grain mound, ozone penetration.

## 1. Introduction

One of the most important modern challenges is to ensure the production and supply of food industry with high quality, undamaged raw materials free from chemical contaminants and undesirable propagules of microorganisms.

Harmful activity of microorganisms results in the annual loss of about 14% of wheat grain worldwide, and in some countries even up to 50% of the total yield of grain crops (Jayas 1999; Singrün 2002). A widespread group of microorganisms - microscopic fungi or micromycetes, often adversely affect not only the quality of food of plant origin, but also the human environment. In order to achieve beneficial balance in nature, their activities must be limited and adjusted towards human-friendly direction (Lugauskas 2007). Micromycete activity and the induced damage significantly increase when the grain is injured in the process of harvesting. Grains damaged in the crop combine bunker are by one third more infected with micromycetes than the intact grains (Lugauskas et al. 2007). Therefore, the working parts of the combines should be adjusted so as to minimize the damage of grain (Špokas, Steponavičius 2010).

Development of micromycetes can be restricted or suspended by drying grain in dryers or applying active ventilation, thus reducing the moisture content to 13–14% (Muir, White 1997). However, the mentioned measures do not ensure complete destruction of micro-organisms in grain (Glushchenko, L. F., Glushchenko, N. A. 2003).

Technologically created environment affects biological processes in a stored grain layer. Formation of a suitable environment is the main issue in the post-harvest period.

The researchers acknowledge that a broad variety of chemicals used to maintain the grain quality (sodium hypochlorite, a variety of antioxidants, etc. (Andrews *et al.* 1997; Nesci *et al.* 2003)) has caused a lot of sanitary, social, public health and energy problems (Kim *et al.* 2003; Murphy *et al.* 2006; Ryden *et al.* 2003). In addition, the listed substances are expensive and environmentally hazardous. The costs associated with many chemical treatments can be significantly higher than the cost of drying. Besides, chemical treatments can be corrosive, as is the case with propionic acid, sulfur dioxide, and phosphine. They also can affect grain quality, result in dry matter loss, and have negative health and environmental impacts (White *et al.* 2010).

Biological materials have also been used to eliminate micromycetes: propion ferment, modified mananooligosaccharide, yeast, etc. (Cuglenok *et al.* 2005). Technology of biological agents' application is complicated, preparations are lengthy, and the desired effects are not always achieved. In some countries the attempts to inactivate micromycetes developing on grain surface applying essential oils were made, but it reduced the grain germi-



nation (Hsu *et al.* 2007; Paster *et al.* 1995). The scientific literature provides evidence that physical means of disinfection: grain cleaning, thermal treatment, application of a high-frequency electromagnetic oscillation, electron flow, etc. are among the most promising and least harmful to the environment (Aziz, Youssef 2002; Cutrubinis *et al.* 2005; Kalinin *et al.* 2001; Požėlienė *et al.* 2005). However, implementation of the majority of listed technologies is very expensive, and efficiency of some technologies is insufficiently studied.

In many countries of the world one of the most important questions is a rational usage of natural resources and environmental protection from different-origin pollutants, damaging not only to the environment, but to humans as well (Baltrenas, Zagorskis 2008). Regarding the fact that lately the problems of human health and related issues of nutrition as well as reduction of environmental pollution have become of utmost relevance, new ecological tools for grain purification from micromycetes are needed. One of such tools could be the application of ozone (trioxygen  $O_3$ ) at selected concentrations.

Ozone has long been used for water disinfection (Lunin et al. 1998) and reduction of microbiological contamination of the indoor air (Storchevoi 2003). Ozone is the relatively stable molecule, only at high ozone concentrations or elevated temperatures it decomposes to oxygen at a significant rate (Valuntaite et al. 2009). The study of ozone-disinfected grain showed no changes in its biochemical composition (amino or fatty acids) (Mendez et al. 2003; Kreimeris et al. 1986). Only at very large concentrations of  $O_3$  (over 2 g·m<sup>-3</sup>) the contents of total nitrogen and fat in grain reduce (Krivopishin 1988). However, short ozonation with high concentration is more damaging to biologically active substances (enzymes, etc.) of the treated product (Krivopishin, Pygin 2000); therefore longer ozonation with lower concentrations is more viable and environmentally friendly.

White *et al.* (2010) investigated the effects of ozone treatment on dry matter loss of high-moisture maize stored under extreme (32 °C) environmental conditions. They found that ozone treatment was effective at decreasing dry matter loss in 22% moisture content maize stored at 32 °C for 9 days. It has been established that the grain drying process with cold air can be improved when gaseous ozone is added to the air (Aboltins *et al.* 2010). Besides, the ozonized grains were characterized by higher germination energy (Tkachev, Gorskij 2004).

Ozone concentration and ozonation time are among the most important factors determining the cessation of the development of ozone-treated micromycetes (Nicoué *et al.* 2004; Butko *et al.* 2005). Even small ( $300 \pm 50$  ppb) concentrations may be effective for suspension of some micromycete growth (Palou *et al.* 2001). The high ozone concentrations ( $350 \text{ mg} \cdot \text{m}^{-3}$ ) eliminated most of the micromycetes in less than 2 minutes (Aleksandrova *et al.* 1983).

Ozone is classified as ecological chemical disinfectant. One of its advantages is that excess ozone rapidly autodecomposes to produce oxygen, and leaves no residues in food (Tiwari *et al.* 2010). After the reaction of ozone with the grain surface microflora, the grain remains free of any toxic residues (Kim *et al.* 2003); therefore ozonation is considered a viable tool reducing the mycobiotic contamination of grain surface. The research data show that low concentrations of ozone (about 30  $\mu$ g·m<sup>-3</sup>) produce a positive effect on both plants and animals, but ozone concentrations higher than 180  $\mu$ g·m<sup>-3</sup> are already dangerous to human health (Ryden *et al.* 2003; Krivopishin, Pugin 2000). However, due to the oxidation processes taking place during ozonation the color of the treated product may slightly alter (Kim *et al.* 1999).

In addition, energy input required for ozonation process is significantly lower compared with the expenditures for thermal, radial and microwave electromagnetic field treatment. For ozone processing of one ton of grain the energy input was 4–5 kW·h. For comparison, the energy requirement for drying make about 128 kW·h, and for the processing applying microwave electromagnetic fields – from 91 to 130 kW·h (Tkachev, Gorskij 2004).

Although the issue of ozone use is presented in many scientific papers, but its application to disinfect the grain surface as well as the interactions of ozone and grain under the influence of the drying environment factors have not yet been sufficiently studied.

While investigating the use of ozone for grain disinfection, it is very important to assess its initial concentration, ozonation time and efficiency, the height and moisture content of grain mound, and concentration of emerging ozone (Kells *et al.* 2001). The diffusion process describing the self-dispersion and distribution of ozone particles in the grain layer also depends on the air filtration velocity through the grain mound (Raila *et al.* 2006).

Intensity of ozone uptake in the grain layer is also predetermined by the grain characteristics, grain variety and mycobiotic contamination.

The aim of the work – to explore the patterns of ozone penetration through wheat grain mound of different height and moisture content and to create mathematical model of factors influencing ozone penetration, which could serve for prediction of the course of grain ozonation process.

#### 2. Materials and methods

# **2.1.** Investigations on grain drying by active ventilation with ozone-air mixture

Investigations of the ozone dispersion through the dried grain layer were performed at the Laboratory of agricultural products storing and processing technologies of the Department of Heat and Biotechnological Engineering at Lithuanian University of Agriculture. The setup used for tests consisted of: centrifugal ventilator "KVKE 250 L TW", chamber of constant static pressure and ventilated cylinders (Raila *et al.* 2006).

In order to determine the impact of ozonation on the intensity of grain drying, we used two ventilated cylinders. Each 0.18 m in diameter 1.2 m high cylinder contained  $22.0 \pm 0.5$  kg of wheat grain. Under the first cylinder two ozonators and under the second cylinder five ozonators were placed. The ventilation intensity was adjusted by a valve at the bottom of each ventilated cylinder. Changing

the position of valve, in both cylinders equal velocity ( $v_f = 0.24 \pm 0.05 \text{ m} \cdot \text{s}^{-1}$ ) of air filtration through the grain layer was set. In the air supplied for drying the concentration of ozone produced by ozonators located under the first cylinder was  $500 \pm 5$  ppb, while in that located under the second cylinder  $-1250 \pm 5$  ppb. Grains of winter wheat variety 'Tauras' with 14.6% of moisture content were poured into the cylinders; the grain was ventilated for 72 hours. Similar experiments were performed with grain having 17.5, 20.3, 22.0 and 23.4% of moisture content.

During the investigation, the mass of dried grain was recorded by weighing the cylinders with grain with mechanical scales "RP-200Š13" every eight hours. Air temperature and relative humidity were measured by ALMEMO sensors FH A646-21 (temperature reading error  $\pm 0.1$  °C, relative humidity error  $-\pm 2\%$ ). Measuring results were stored in the secondary device ALMEMO 3290 every 10 minutes.

Velocity of the air emerging from the cylinders was measured using a widening conical tube (Fig. 1), which was positioned on top of the cylinder.



**Fig. 1.** Air velocity detection device: 1 - measurement aperture; 2, 4 - straight part of the tube; 3 - conical part of the tube

In order to avoid significant air leaks, during measuring the cylinder sides were covered with an impermeable material. Thermoanemometer (OMEGAFLO HH - 600 model 615 M) was inserted through a hole 1 in the cone. The measurement results were observed in the scale of the meter on the screen.

Ozone concentration in the grain mound was recorded by ozone meter 10 (AHLBORN Ozon-Sonde FY A600-O3;  $C_{\text{max}} = 300$  ppb, measuring error  $\pm 2$  ppb) and "GasAlertmicro" alarm sensor ( $C_{\text{max}} = 1300$  ppb, measuring error  $\pm 10$  ppb) every half-hour in each measuring height of the ventilated cylinders. Ozone concentration was measured at 15, 30, 45, 60, 75, 90 and 105 cm height of the grain layer.

After summarizing experimental results the empirical equations of ozone concentration changes in grain mound were designed; their values were used in creating generalized mathematical model of factors influencing the changes of ozone concentration. Coefficients of regression equation of the model were determined employing the "Matlab" program; graphs prepared using "MS Excel" spreadsheet.

#### 2.2. Determination of grain moisture content

Grain moisture content was determined by the dry residue after full evaporation of water from grain. From a well mixed sample the grain was placed in beforehand weighted special weighing dishes. The weight of prepared samples was determined using scales "Scalter SPO 51", and the samples were placed in a drying chamber. The samples were being dried at 105 °C until stabilization of the weight of the weighing dishes with grain.

The weight of the dishes with dry grain was determined, and the amount of evaporated water and the grain moisture content w (%) were calculated.

## 2.3. Grain premoistening

Grain moistening purpose was to prepare the grain of the desired moisture content to be used in the study of ozone penetration. In order to moisten the known quantity of grain to the desired moisture content, it is necessary to calculate the amount of required water:

$$m_{\rm H_2O} = m_d - m_0,$$
 (1)

where  $m_{H_2O}$  – water amount required for grain moistening till the desired moisture content, kg;  $m_d$  – moist grain weight kg;  $m_0$  – initial (dry) grain weight, kg.

$$m_{\rm H_2O} = \left[\frac{m_0 \left(100 - w_0\right)}{\left(100 - w_d\right)}\right] - m_0, \qquad (2)$$

where  $w_0$  – initial (dry) grain moisture content, %;  $w_d$  – desired grain moisture content, %.

For moistening the grain was spread on a polyethylene film laid within a wooden container, and the calculated water amount  $m_{\rm H_2O}$  was added over. The grain was stored in containers for 2–4 days, depending on the quantity of added water, stirring periodically 2 times a day so that water is evenly distributed throughout the grain mass.

Before placing the grain into the cylinders, a sample was taken to determine grain moisture content.

#### 3. Results and discussion

#### 3.1. Ozone penetration in a grain layer

In order to create a mathematical model of factors influencing ozone penetration, the research data of the grain drying with ozone-air mixture are essential. Grain of 14.6%, 17.5%, 20.3%, 22.0% and 23.4% moisture content were used for ozonation. The grain was continuously ozonized for 72 hours.

Patterns of ozone penetration through grain mound of different moisture content, at different ozone concentrations  $C_0$  in the supplied air: 500 ppb (Fig. 2) and 1250 ppb were determined (Fig. 3).

The research data have shown similar character of concentration changes during a 72-hour period in separate heights of the mound. Ozone, supplied with the ventilation air, begins to penetrate starting with the lower layers of grain mound. It has been observed that ozone penetrates very slowly through separate grain layers; considerable



**Fig. 2.** Ozone dispersion in grain mound, at initial ozone concentration  $C_0 = 500 \text{ ppb} = 1070 \text{ }\mu\text{g}\text{\cdot}\text{m}^3$ , air filtration velocity  $v_f = 0.24 \pm 0.05 \text{ m}\text{\cdot}\text{s}^{-1}$ 

 $O_3$  sorption is observed. The first record of ozone in separate layers of grain mound occurs only after a certain period of time, which strongly depends on the grain moisture content and ozone concentration in the supplied ozone-air mixture. These studies confirmed preliminary conclusions of the earlier studies (Raila *et al.* 2006) that the higher is the grain moisture content, the slower is ozone penetration through it, i.e.  $O_3$  absorption is higher.

In previous works researchers have revealed that the ozone penetration in the grain layer depends on the ozone concentrations  $C_0$  in the air supplied to the grain and ozonation time *t* (Ksenz 2003), velocity of the supplied air  $v_f$  (Kells *et al.* 2001; Mendez *et al.* 2003) and temperature  $\tau$  (Allen *et al.* 2003). These experimental studies have shown that the ozone penetration in grain layer (and hence the rate of grain disinfection) is affected not only by those parameters, but also the moisture content of the



**Fig. 3.** Ozone dispersion in grain mound, at initial ozone concentration  $C_0 = 1250 \text{ ppb} = 2675 \text{ }\mu\text{g} \cdot \text{m}^3$ ; air filtration velocity  $v_f = 0.24 \pm 0.05 \text{ }\text{m} \cdot \text{s}^{-1}$ 

ozonized grain w. Ozone penetration through the grain layer of higher moisture content is slower, and ozone reaction with grain surface and microflora present on it is longer. Since the duration of the interaction of ozone with grain surface is longer, the conditions for the development of microflora are less favorable. When ozone is recorded in the air emerging from the grain mound it means that all layers of the mound are already ozonized. However, at 1250 ppb ozone concentration in the supplied air, ozone in the upper layer (1.05 m) is recorded only after 28.5 hours, while in the air emerging from the grain mound (1.20 m) – only after 32.8 hours (Fig. 3, d).

As the ozone penetration over the entire grain mound takes so long, and within this time mycobiotic contamination of the upper layers could have significantly increased, for effective ozonation the computercontrolled process is essential. Applying active ventilation with ambient air the grain is dried, and, if the air is enriched with ozone, the grain is also disinfected. If the process is automatically managed, during the first hours of grain ozonation the ozone concentration in the supplied air could be increased so as to ozonize the top layers of the mound as soon as possible, and limit the development of micromycetes on the grain surface. Subsequently, the ozone concentration could be reduced to prevent ozone pollution.

# **3.2.** Mathematical model of factors influencing the ozone concentration changes

After summarizing the experimental data, a mathematical model of factors influencing the variations of ozone concentration in grain mound was created (Fig. 4).

The impact of the factors on the ozone penetration in a ventilated grain mound is described in equations C = f(t), C = f(h),  $C = f(C_0)$  and  $C = f(w_0)$ . The influence of each factor upon the ozone dispersion was determined (Fig. 2 and Fig. 3). The factor variation range corresponds with those set in the methodology of the study:  $2 \le t \le 60$  h;  $30 \le h \le 105$  cm;  $14.6 \le w_0 \le 23.0\%$ ;  $500 \le C_0 \le 1250$  ppb.



**Fig. 4.** Principal scheme of the mathematical model: t – ozonation time, h – grain mound height,  $w_0$  – grain moisture content before drying,  $C_0$  – ozone concentration in the supplied air, C – ozone concentration in grain mound

After evaluation of all possible products among the four chosen factors (t, h,  $C_0$  and  $w_0$ ), a regression equation with 4 variable factors and 20 regression coefficients was composed:

$$C_{\text{mod.}} = b_0 + b_1 t + b_2 h + b_3 C_0 + b_4 w_0 + + b_5 (t \cdot h) + b_6 (t \cdot C_0) + b_7 (t \cdot w_0) + + b_8 (h \cdot C_0) + b_9 (h \cdot w_0) + b_{10} (C_0 \cdot w_0) + + b_{11} (t \cdot h \cdot C_0) + b_{12} (t \cdot h \cdot w_0) + + b_{13} (t \cdot C_0 \cdot w_0) + b_{14} (h \cdot C_0 \cdot w_0) + + b_{15} (t \cdot h \cdot C_0 \cdot w_0) + b_{16} t^2 + b_{17} h^2 + + b_{18} C_0^2 + b_{19} w_0^2.$$
(3)

Verification of the significance of the model coefficients showed 12 coefficients to be insignificant. Since the coefficients of regression equation are not determined independently of one another, and the irrelevant are eliminated, the values of the remaining coefficients are repeatedly determined. So the resulting regression equation with 8 coefficients was obtained:

$$C = 543.8 + 0.92 C_0 + 18.65 t - 36.61 w_0 -$$
  

$$11.27h - 0.185 t^2 + 0.074 t \cdot w_0 +$$
 (4)  

$$0.036 h^2,$$

where  $C_0$  – ozone concentration in the supplied air, ppb; t – ozonation time, h;  $w_0$  – grain moisture content before drying, %; h – grain mound height, cm.

Hypothesis about the adequacy of the model (how it reflects the real process) has been verified by calculating reproduction and adequacy variance. Calculations showed that the created model is adequate, because the Fisher criterion  $F_{apsk.}$  is lower than the selected from the Fisher table  $F_{lent.}$  (Pollard 1982) when significance level is  $\alpha = 0.95$ .

Analysis of the resulting regression equation. Analysis of the regression equation of the model showed that in the framework of the mathematical model, the character of the ozone concentration changes (Fig. 5) in the ozonized grain mound follows the experimentally determined pattern (Figs. 2 and 3).

The ozone concentration at any place in the mound heightens as the ozonation time t is prolonged and the ozone concentration in the supplied air  $C_0$  is increased. The created model validated the experimentally obtained data that the first record of ozone in separate grain mound layers occurs only after a certain period of time (Fig. 2, c). In a 60 cm height ozone it is first recorded after 12 h, and at 105 cm – only after 34 h at  $w_0 = 19.0\%$ ,  $C_0 = 500$  ppb (Fig. 5, a). If the initial concentration of ozone is higher, it is first recorded sooner. At  $C_0 = 800$  ppb and the same moisture content ozone at 60 cm height of grain mound is recorded already after 2 h and at 105 cm - after 11 h (Fig. 5, b). Employing the created mathematical model it is convenient to predict the process of ozone penetration into grain mound interpolating within the range of determined values ( $2 \le t \le 60$  h;  $30 \le h \le 105$  cm;  $500 \le C_0 \le$ 1250 ppb;  $14.6 \le w_0 \le 23.0\%$ ). This means that all intermediate values of ozone concentration C can be ascertained by the regression equation of the model.



Fig. 5. Ozone dispersion at various heights of grain mound h, calculated by the mathematical model, depending on the ozonation time t



Fig. 6. Ozone dispersion in grain mound, calculated by the mathematical model, depending on the ozonation time *t*, initial grain moisture content  $w_0$  and ozone concentration in the supplied air  $C_0$ 

Employing the created mathematical model it is convenient to predict the process of ozone penetration in grain mound interpolating within the range of determined values ( $2 \le t \le 60$  h;  $30 \le h \le 105$  cm;  $500 \le C_0 \le$ 1250 ppb; 14.6  $\le w_0 \le 23.0\%$ ). This means that all intermediate values of ozone concentration *C* can be ascertained by the regression equation of the model.

The model provides possibility to determine not just temporal ozone concentration but also changes in the concentration depending on grain moisture content (Fig. 6). Regression equation analysis shows that the concentration function  $C = f(w_0)$  is linear.

The examination of the ozone concentration changes at a certain grain mound height (Fig. 7) confirmed the theoretical research data (Petruševičius, Raila 2009), which states that the concentration changes by exponentially descending function. Besides, results obtained by the model regression equation very well coincide (determination coefficient variation threshold  $R^2 = 0.95-0.99$ ) with exponential equations of the mentioned theoretical studies. This confirms the adequacy of the theoretical studies for actual ozonation process, because the consequence of theoretical studies is also an exponential equation.



**Fig. 7.** Ozone dispersion in grain mound, calculated by the mathematical model, depending on the height of grain mound h and ozone concentration in the supplied air  $C_0$ :

$C_0 = 1250 \text{ ppb}$	$C = 1197.3e^{-0.0106h}$	$R^2 = 0.99$
$C_0 = 900 \text{ ppb}$	$C = 1163.8e^{-0.0241h}$	$R^2 = 0.97$
$C_0 = 500 \text{ ppb}$	$C = 878.5e^{-0.0587h}$	$R^2 = 0.97$
$C_0 = 1250 \text{ ppb}$	$C = 1409.9e^{-0.0075h}$	$R^2 = 0.99$
$C_0 = 900 \text{ ppb}$	$C = 1148.5e^{-0.0119h}$	$R^2 = 0.99$
$C_0 = 500 \text{ ppb}$	$C = 1481.5e^{-0.0399h}$	$R^2 = 0.95$

Experimental studies were aimed to determine the ozonation impact and its parameters ensuring safe application of ozone, as of preventative measure, for reduction of grain surface mycobiotic contamination. One of the most important factors is the intensity of ozone dispersion within a grain layer. Therefore, the ozone concentration in the supplied ozone-air mixture as well as ozonation time must be chosen so that the greater ozone portion, after interacting with the grain surface and microflora present there, would decompose in the top layers of the grain mound not reaching the environment.

In summary, it can be stated that the created mathematical model of the factors influencing the ozone penetration through the grain layer (initial ozone concentration, initial grain moisture content, ozonation time and grain mound height) can be applied for the prediction of grain ozonation process.

In the further studies on grain ozonation, the mathematical model should include the evaluation of the initial mycobiotic contamination of grain mound, air filtration velocity and grain mound porosity.

#### 4. Conclusions

1. The ozone penetration in a grain layer depends on the initial ozone concentration in the supplied ozone-air mixture, the initial grain moisture content, ozonation time and grain mound height.

2. Temporal decrease of ozone concentrations in grain mound can be described in the exponential equation. Besides, the concentration linearly decreases with increasing initial moisture content of ozonized grain.

3. The created mathematical model of the factors influencing the ozone penetration in the grain layer (initial ozone concentration, initial grain moisture content, ozonation time and grain mound height) is described by regression equation; it can be applied for the prediction of the grain ozonation process.

4. The ozonation process of grain with different moisture content can be operated by a computer program evaluating the changes in ozone concentrations employing the created mathematical model.

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# OZONO SKVERBTIES GRŪDŲ SLUOKSNYJE MODELIAVIMAS

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#### Santrauka

Grūdų džiovinimo ozono ir oro mišiniu tyrimai atlikti siekiant išaiškinti ozono skverbties per skirtingo drėgnio grūdų sampilą dėsningumus (14,6  $\le w_0 \le 23,0$  %), esant skirtingoms ozono koncentracijoms ( $500 \le C_0 \le 1250$  ppb) tiekiamame ore. Ozono skverbtis grūdų sluoksnyje priklauso nuo pradinės ozono koncentracijos tiekiamame ore, ozonavimo trukmės, tiekiamo oro greičio, grūdų sampilo aukščio, pradinio grūdų drėgnio ir jų paviršiaus mikobiotinio užterštumo. 60 cm grūdų sluoksnio aukštyje ozonas pradėtas fiksuoti po 12 h, o 105 cm – tik po 34 h, kai  $w_0 = 19,0$  %,  $C_0 = 500$  ppb. Padidinus pradinę ozono koncentraciją, ozonas pradedamas fiksuoti greičiau. Ozonuojant drėgnesnius grūdus, ozonas per jų sluoksnį kverbiasi lėčiau, vyksta ilgesnė jo reakcija su grūdų paviršiumi ir ant jų esančia mikroflora.

Hipotezė apie modelio adekvatumą (kaip jis atspindi realų procesą) buvo patikrinta apskaičiavus reprodukcijos ir adekvatumo dispersijas. Sudarytas matematinis modelis gali būti taikomas grūdų ozonavimo procesui prognozuoti.

Reikšminiai žodžiai: aplinkos procesų modeliavimas, grūdų sampilas, ozono skvarba.

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