Jian F, Jayas DS (2016) Engineering considerations for creating uniform distribution of applied gas during controlled atmospheres and fumigation. Pp. 361–370. 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.

Engineering considerations for creating uniform distribution of applied gas during controlled atmospheres and fumigation

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ABSTRACT

Controlled atmospheres containing high carbon dioxide, high nitrogen or low oxygen, and fumigation using chemicals or mixture of fumigants are two important methods to minimize grain deterioration caused by molds and insects. Both methods require a proper storage period with desired concentration (dosage) of toxic gas, certain gastightness of the storage structure, and correct monitoring before, during, and after the atmosphere treatment or fumigation. Therefore, successful controlled atmosphere and fumigation techniques require knowledge of the movement and distribution of the applied gas inside the storage structure. This article analyzes the reasons for uneven distribution of applied gas and the factors influencing the distribution of applied gas. The analyzed factors include gastightness, diffusion, free convection, advection, sorption, grain type and condition, ambient environment, and empty and grain filled space. To create an even distribution of the applied gas, creating an even distribution of pressure gradient is important. The methods of creating an even pressure gradient are also discussed. The use of mathematical modelling and simulation in the estimation of gas movement and distribution is suggested from the engineering perspective. Article also highlights the proper engineering requirement for gas tightness and leakage and the effect of airflow resistance on the distribution of the applied gas.

Key words: Airflow resistance, Controlled atmosphere, Convection, Diffusion, ECO_2 FUME, Fumigation, Gas distribution, Gastightness, Pressure gradient, Recirculation

Fumigation and fogs are the processes using a fumigant or an aerosol in sufficient lethal concentration to control insect pests and/or microorganisms at the required temperature, pressure, and relative humidity. A fumigant is a chemical existing in the gaseous state, while aerosol is in the state of particulate suspensions of liquids or solids dispersed inside intergranular air or storage structure. In this article, we used fumigation in its broadest sense, i.e. to include use of aerosols, fumigants, or mixture of fumigants (such as ECO_2 FUME®). In controlled atmospheres (CA) storage, intergranular gas composition is altered by injecting carbon dioxide (CO_2) or nitrogen (N_2) to create lethal concentration of high CO_2 or low oxygen (O_2) atmosphere. Fumigation or controlled atmosphere of stored products is carried out in enclosures and structures such as chambers, warehouses, silos, food stores, containers, railway box cars, aircrafts, barges, ships, under gas-proof sheets, portable enclosures, mills, or food factories. We refer to all these as enclosures, structures, or bins synonymically. To successfully control insect pests, the processes of fumigation and controlled atmosphere ideally require uniform distribution of the applied gases inside the entire storage structure. The uniform distribution of applied gases at the required lethal concentration for the entire treatment period is the best approach to control insects and prevent insects from developing resistance. The uniform distribution requires the penetration of the applied gas into the pores among the grain kernels in the bulk. Though this penetration ability gives the applied gas a big advantage in controlling insects living in or among grain kernels, this same advantage creates problems such as gas sorption and leakage. The toxic gases that escape from the structure are lethal to humans, livestock and other animals. Leakage also results in uneven distribution of the applied gas.

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Therefore, introduction, movement and distribution of the applied gas should be studied.

Studies show leakage is one of the main reasons for failure of fumigation and controlled atmosphere. There is a general optimism that a properly constructed and sealed structure can reach the required gas concentrations throughout the structure and maintain the concentration for the required period, which will result in a successful control of insect pests. Based on engineering principles, this might not be true under some situations. Either not following or not applying fundamental engineering principles correctly might be reasons for the poor distribution of applied gas which results in the failure of treatment. The reasons causing the uneven distribution of applied gas are analyzed in this article. Failure due to wrong operation by fumigators was not considered in this analysis. We also suggest solutions to this uneven distribution issue.

FACTORS INFLUENCING DISTRIBUTION OF APPLIED GAS

Gastightness

The importance of structure gastightness for a successful fumigation or controlled atmosphere has been studied (Bond, 1984; Annis, 1989; Mills et al., 2001). Australian research group developed the half-life pressure (HLP) value to evaluate the gastightness of the bin. The established HLP value by the Australians is determined as the time taken for a fall of gage pressure from 250 Pa to 125 Pa in a structure. It is categorized as a 'sealed bin' if the HLP value is 5 min for an empty bin or 3 min for a bin filled to capacity. The HLT is the half loss time of the applied gas and is also used in the evaluation of gastightness of the structure. There is already interest in applying vacuum tests to evaluate the seal of vinyl plastic encased stacks (Navarro, 2000). There can be no perfect airtight structure for stored grain fumigation or controlled atmosphere, or even economically feasible airtightness, because high cost of building a 'minimal leakage' structure with a 'high airtightness' (>5 min of HLP). The injected gas from the application of fumigant or controlled atmosphere will gradually increase the pressure inside the structure. As the gas is injected and differential atmospheric pressure builds, the structure will begin leaking. When the gas dosage is completed, the gas leakage from the structure should be at or below the design allowable leakage rate.

Even for the fumigation or controlled atmosphere without injection of gas, pressure gradients induced by ambient wind or external barometric pressure fluctuations will also result in leakage (Annis, 1989). Rapid loss of fumigant at the downwind side of the storage was reported (Mills et al., 2001). Therefore, HLP and HLT values should be used with caution because these might not be good indicators for a successful treatment under certain conditions such as when the pressure inside the structure is much higher or lower than outside and the structure cannot hold the pressure difference. Zation (2014) reported that fumigant distribution was not influenced by the HLP value. Silos that are less leaky (higher HLP value) develop a significantly lower concentration of phosphine (PH_3) gas above the position of the leaking hole than those storages that are leakier (lower HLP value), and take longer to reach an even distribution of PH_3 (Zation, 2014). Therefore, structures with a high gastightness will mainly help to hold the applied gas inside the structure; but it cannot assure that the applied gas will be evenly distributed.

Perfectly sealing bins is neither a practical nor economical option because the structure might be also used for drying, aeration, loading and unloading grain, and inspecting. To complete these tasks, manholes, channels, and small holes are made through the roof, walls, and/or foundation of the structure. Extensive effort is required to seal these holes, channels, and small cracks. Also, some structures such as floor-stored grain bulks present special or unusual sealing challenges (Navarro, 2000). Therefore, the main purpose of increasing gastightness should be to minimize leaking, and maintain a desired level of gas concentration as uniform as possible for the required time for complete kill of all stages of insects, and to monitor and regulate the leakage and replenish and distribute the gas to maintain a minimum level of the required lethal concentration throughout the structure.

Diffusion

If there is no free convection and advection, diffusion will dominate the movement of the applied gas. Diffusion velocity is strongly related to the density (molecular weight) of the fumigant, temperature, relative humidity, sorption, commodity fumigated, air passages (void spaces between kernels) inside porous bulk, and shape and size of fumigated structure. Gas movement due to diffusion is a slow process and is strongly influenced by temperature. For example, diffusivity of applied gas is of the order of 10^{-5} m^2/s (PH_3: 1.6 $\times 10^{-5}$ m^2/s, methyl bromide: 9.9×10^{-6} m^2/s, sulfuryl fluoride: 1.1×10^{-5} m^2/s, CO_2: 3.7 to 5.3 $\times 10^{-6}$ m^2/s, O_2: 5.4 $\times 10^{-6}$ m^2/s at 20 to 25ºC). For a PH_3 fumigation without any free convection or advection inside the bin when tablets of aluminum phosphide were dropped at the top of the grain mass, Zaiton (2014) found that the PH_3 front continuously diffused down for approximately 10 days, and the grain at the bottom was never exposed to the concentration required to kill insects. The HLT of sulfuryl fluoride and methyl bromide under pure diffusion is 3.24 and 3.42 years inside grain mills (Cryer, 2008). These facts are also supported by the mathematical model of pure diffusion which shows that pure diffusion cannot predict the distribution of applied gas concentration accurately (Alagusundaram et al., 1996; Chayaprasert et al., 2010). Diffusion can only help to move applied gas for a short distance. Smith and Jayas (2001) proved that the CO_2 front moved downward through the grain bed with the velocity of the air induced by the gravity and injection of the CO_2, while the width of the front increased due to diffusion of the injected CO_2. From the viewpoint of the fumigant distribution inside a bin, $ECO_2FUME^{®}$ fumigation (using mixture of phosphine and CO_2) might not help to create an even distribution of the applied mixture because diffusivity of fumigant is usually lower than 10^{-5} m^2/s and there might be no synergetic effect on the movement of the mixture.

It is almost impossible to reach a uniform distribution of applied gas inside a bin with holes in its walls if diffusion is the dominant factor influencing the distribution of the applied gas, because air will leak into or out of the bin through these holes. This process will dilute the applied gas at and near the leaking locations. Diffusion coefficient of CO_2 gas is direction dependent due to the gravity of the applied gas and pore structure of the grain bulk (Singh (Jayas) et al., 1984; Alagusundaram et al., 1995). Resistance to diffusion in vertical direction is larger than that in the horizontal direction because most elongated grain kernels lie with their major axes horizontal when a bin is filled (Jayas et al., 1991; Alagusundaram et al., 1995). This will produce an un-even diffusion during early stages. Therefore, the following statement will only be valid after a very long time and hence may not be valid during a relatively short fumigation period: "if a storage enclosure is well sealed and adequately dosed with an insecticidal atmosphere, the applied gas has the potential to come in contact with every grain in the storage, thereby giving a high probability of complete disinfestation" (Annis, 1989). Similarly, the statement "phosphine is rapidly diffused in air because it has a similar density to that of air. Consequently, fumigation with phosphine generally does not require any circulation system for distribution within the fumigated space" (Chaudhry, 1997) is only partially correct, as diffusion of phosphine throughout the structure does not mean uniform concentration throughout the structure.

There will never be uniform gas concentration in a reasonable fumigation period in large or tall storage structures, as there is not adequate diffusion or convection to spread the gas. Dr Ronald T. Noyes, a Grain Storage Engineer and an Emeritus Professor in the Department of Biosystems and Agricultural Engineering, Oklahoma State University, OK, USA, conducted a series of tests in 30 m concrete silos at Douglas Elevator, Douglas, OK, USA, before and after minimal sealing of the under-roof air vents, using three methods which were frequently and internationally used by fumigators. The first method was to place tablets on the grain surface. After 6 to 7 d, PH_3 was not detected at the bottom and very little below the mid-point of the silos. The second method was to divide the dosage into three parts and dosed 1/3 after about 3 m of grain was filled, then 1/3 at midpoint, and 1/3 when the silo was about 90% filled. The third method was "the uniform dosage by turning the grain from silo to silo – one silo has to be empty – using a pellet distributor". The last two methods also did not improve the distribution of the fumigants. Based on his fumigation experience, Dr Noyes suggested that these methods might be the major reason of PH_3 resistance of grain storage insects (*Personal communication*).

Free convection

Distribution of applied gas inside a structure is mainly influenced by the bulk movement of air. Pressure gradients are one of the driving forces of the bulk movement of air and the applied gas. Pressure gradients can be induced by temperature gradients which cause free convection due to thermal buoyancy. Velocity of free convection varies widely inside different stored bulks. The speed of free convection is about 11×10^{-4} m/s inside corn under tropical climatic conditions (Gough et al., 1990), in the range of 10^{-6} to 10^{-8} m/s inside canola (Jian et al., 2015), and about 10^{-4} to 10^{-7}m/s inside wheat (Smith and Sokhansanj, 1990) under temperate climatic conditions. The speed of free convection will vary under different geographical regions and at different locations inside a bin due to the differences of temperature gradients. For the air velocity of 10^{-8} m/s inside a bin with 6 m height of wheat, the applied gas which is released at the bottom of the bin will need about 166, 667 h to reach the top of the grain $((6/10^{-8})/3, 600 = 166, 667)$. When the air velocity is less than 10^{-6} m/s, the time required for the air to reach the top of the grain is exponentially increased (Fig. 1). Therefore, the free convection is an extremely slow process when temperature gradients and kernel sizes of the stored grain (such as sorghum, canola, flax and millet) are small.

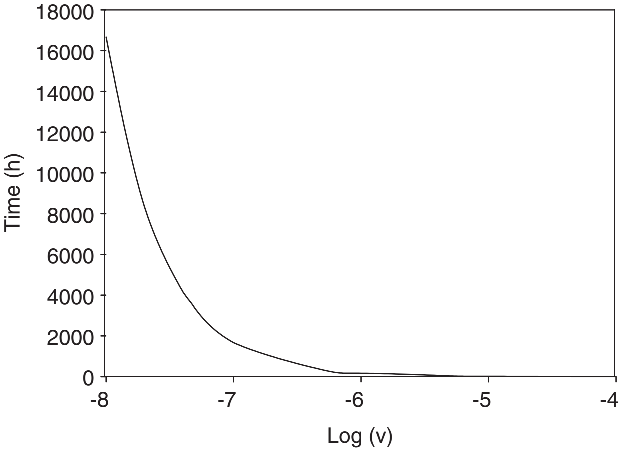

Fig. 1. Time (h) of different velocities of air moving through grain bulk from bottom to top of a 6 m bin. The v is the air velocity (m/s).

The direction of the free convection at the centre of the bin is usually in the opposite direction of that at the periphery of the bin. Based on the two dimensional simulation, Nguyen (1987) found grain structures contained two identical free convection cells, which rotated in opposite directions induced by non-horizontal temperature gradients, and a single cell driven by the horizontal temperature gradients. The direction of free convention inside a larger size bin (such as > 10 m diameter) or warehouse will be much more complex than that in the simulated two dimensional grain structures (Khankari et al., 1995). If the fumigant is not applied at both top and bottom of the bin, the free convection will be in the opposite direction of the applied gas movement at some areas. Free convection can also result from air movement through open windows or cracks (Birdsall and Meroney, 1995). Therefore, free convection might only help the gas movement in certain areas of the treated structure, while inducing excessive leakage near wall or roof openings.

Harvest grain is usually warmer than the ambient air at the beginning of the storage period. In tall upright bins filled with the warm grain and surrounded by cool ambient air in Canada and northern USA, chimney effects will induce the upward movement of applied gases in bin centres (Flinn and Reed, 2008). This upward movement could reach 0.3 m/h after the PH_3 is generated at the bottom of the concrete bins (Flinn and Reed, 2008). Free convection under this condition might help to create approximately uniform distribution of the applied gas.

Advection

Fan forced air movement and gas injection will produce pressure gradients which will result in advection. Under fan pressure, the air will move much faster than 10^{-4} m/s and the air will reach the top of the grain in a short time period (less than a few hours or even minutes depending on the size of fan and pressure gradient, Fig. 1) when the forced airflow is introduced at the bottom of the bin. It is optimally assumed that advection will create a homogeneous distribution of gas. This assumption is only true when large enough pressure gradients with a uniform distribution duct system exists inside the treated structure.

The main principle of the recirculation fumigation system [such as ‘J’ or ‘CLF’ system (Noyes and Kenkel (1994)] and continuous injection system [such as Siroflo® (Winks, 1993)] is to continually create pressure gradients. Introduction of a steady pressure gradient within the entire structure will dominate the natural air movements and diffusion which can ensure effective delivery of applied gas to the entire structure if the pressure gradients are evenly distributed. The recirculated gas can not only decrease the total usage of the fumigant, it will also help to create an even distribution of the applied gas by the steady pressure gradient created by the recirculated air. Compared with recirculation system, the continuous injection system requires less gas tightness of the structure, while using more applied gas. Therefore, for a structure with a low HLP value, the recommended method is to continually monitor the recirculated gas concentration at the recirculation blower, and add applied gas as needed to maintain the minimum required dosage, and recirculate the applied gas periodically.

Current recommendations by Dr Ronald T. Noyes (*Personal communication*) for CLF are to operate the CLF blower during the initial application until the recirculation gas concentration is relatively uniform, then stop the CLF blower, and monitor headspace PH_3 concentration levels by operating the CLF for a few minutes every 6 to 8 h. When headspace gas concentration is below the target concentration required to kill all stages of insects, operate the CLF blower only long enough until the headspace gas reaches a peak value. When headspace gas does not reach target concentrations by pushing gas upward from the grain bulk, then adding more PH_3 is recommended. Following this recommendation will avoid pumping gas out of the structure, and also to create the required pressure gradients. If the pressure gradients are not uniformly distributed, multi injecting points should be considered.

Sorption

During fumigation or controlled atmosphere, the gas concentration within structures gradually depletes, due to sorption of the applied gas by the treated materials and leakage. Phosphine gas penetrates into grain kernels before it converts to the non-volatile, non-toxic forms of phosphorus. Phosphine uptake by the grain has been regarded as partially due to physical sorption and partly to chemical reaction (Banks,1990). The amount of sorbed gas is mainly influenced by the physical and chemical properties of the applied gas, the treated materials and their previous treatment history, filling ratio of the treated materials, temperature, moisture content, exposure period, and dose (Reddy et al., 2007). Reddy et al. (2007) found the percentage of phosphine absorbed by different commodities varied and could be more than 60% of the applied gas. Different crops and crop varieties have different sorption percentage of PH_3 (Banks, 1986; Reddy et al., 2007). Absorption by grain with higher moisture content is higher than that of grain with low moisture content (Hilton and Banks, 1997a; Hwaidi et al., 2015). Initial concentration of applied gas may or may not influence the total sorption of applied gas and varies with the fumigated materials and the applied gas (Banks, 1986; Hilton and Banks, 1997ab; Reed and Pan, 2000; Hwaidi et al., 2015). Sorption can continue for as long as the applied gas is maintained and this depends on the initial concentration and period of fumigation. All of the above mentioned factors will result in an uneven distribution of the applied gas in the interstitial spaces of the treated materials due to the heterogeneous property of the treated materials. For example, increase of sorption with increase of temperature has been observed with PH_3 (Berck, 1968; Banks, 1993), methyl bromide (Hilton and Banks, 1997a), and ethyl formate (Hilton and Banks, 1997b). The locations with high temperature will absorb more fumigant gas and result in a low concentration of the applied gas. Therefore, the best solution for this issue is to increase the air movement inside the treated structure, so the absorbed gas can be replenished.

Grain type and condition

Various grains have different characteristics that can affect the distribution of pressure gradients. The two main factors influencing the distribution of pressure gradients of the applied gas and air are the pore structure (void space) among grain kernels (size, shape, connectivity, tortuosity of the pores, and orientation of the pore to the airflow direction) and properties of fluids (air velocity and viscosity). The following factors influence pore structure: (i) shape, size, surface texture, and moisture content of grain kernels; (ii) dockage, fines, foreign materials, and broken grain kernels (DFM) in the grain mass; and (iii) compaction of the grain (function of overburden grain depth). These factors are influenced by other factors, such as the storage period, filling method, compaction effect of the grain, insect and mould infestation, and vibration of the grain mass by rail and road traffic.

One of the conventional methods of PH_3 fumigation is to mix the tablets or pellets of aluminum phosphide with the grain stream at the grain loading point. The basic assumption of this application is that the tablets of aluminum phosphide will be homogenously distributed inside the grain bulk. This assumption might be wrong because tablets have different shape, size, and density than that of the grain. When the grain mixed with the tablets and DFM will be dropped from the loading port, the tablets and DFM will be heterogeneously distributed inside the bin (Jayas et al., 1987). Another method of the application is to introduce all the tablets to a portion of the grain. This method is mostly used to control the insects at the target area. This method might also fail if the factors influencing the movement of applied gas are not considered.

High percentage of DFM also attracts insects to multiply and produce isolated pockets, which creates moisture accumulationin ‘hot spots’. The infested grain with high percentage of DFM will produce high resistance to air flow when the size of the DFM is smaller than the size of grain. Therefore, when an isolated ‘hot spot’occurs, applied gas may by-pass such moist dense spots. Unfortunately, DFM and infested grain at the hot spots also absorb more applied gas (such as CO_2) than the grain at lower temperature (Jian et al., 2014). Therefore, eventhough the applied gases can penetrate into these hot spots, the concentration of the applied gas inside the hot spots might be lower than at other locations.

Ambient environment

Environmental factors leading to leakage from enclosures have been summarized by Banks and Annis (1984). They found the most significant driving force for leakage of fumigant is governed by the external wind speed. Pressures increase non-linearly as the wind speed increases (Chayaprasert et al., 2010). Positive pressures were exerted on the structure in the upwind direction, while negative pressures were exerted in the downwind direction. Mills et al. (2001) reported: “during calm periods there was very little short-term fluctuation in the pressure but during windy periods, the pressure cycled through as much as 20 Pa (typically 8–12 Pa) with a period of about 4–5 min”. Chayaprasert et al. (2010) reported wind pressure can reach 35 Pa. The air in the bulk is compressed when the wind pressure rises, and a small volume of outside air must move into the bulk diluting the applied gas if the structure is rigid. When the pressure falls again the reverse occurs, and the air in the bulk expands and some of it moves out at leaking locations. Wind at the roof is usually larger than that at the ground. This high speed wind will draw air out of the roof vents or leaks and results in low concentration of applied gas inside the headspace. The HLT of methyl bromide and sulfuryl fluoride inside a fumigated flour mill are correlated with the ambient wind speeds (Chayaprasert et al., 2010).

Major barometric atmospheric pressure changes, usually accompanied by medium to high winds, can cause major losses of gas from a sealed structure in 1 to 2 h, even when the structure is tightly sealed. Dr Noyes experienced these conditions during USEPA ECO$_2$FUME certification tests in small tightly sealed steel bins at OSU in 1995. These 10 bins, which averaged over 200 ppm of PH_3 at the end of the 7 d test, registered between 35 and 60 ppm PH_3 inside the headspaces, sufficient to kill live adult insects in 28 d from the start of EPA tests (*Personal communication*).

Roof and wall panels facing the sun receive more solar radiation during day than shaded panels. This results in the increase of temperature and volume of the air inside the headspace. During a sunny summer day in Canada, roof temperatures can vary by 30°C around the circumference of a metal grain silo (Jian et al., 2009). Flinn and Reed (2008) found PH_3 concentration in headspaces of concrete bins increased and decreased daily, reaching maximum at mid-morning and minimum at late evening.

Empty and grain filled space

Distribution of applied gas in the empty space is different from that in the grain filled space (Alagusundaram et al., 1995). The main reasons causing this difference is that the higher resistance to diffusion and bulk movement inside grain bulk than that in the empty space. The coefficient of diffusion of CO_2 through air is about three times greater than in a grain bulk (Singh (Jayas) et al., 1984). Therefore, process of fumigation or controlled atmosphere inside an empty structure should be different from that inside a grain filled structure. Introducing the applied gas inside the grain bulk by using a fan might help create an even distribution inside a grain filled bin, while the fan might not be needed for an empty structure fumigation if the structure is small and the introduction location of the applied gas is correct. Gastightness for a grain filled bin should be higher than that inside an empty bin. However, this might not be true for an empty structure exposed to high and variable winds.

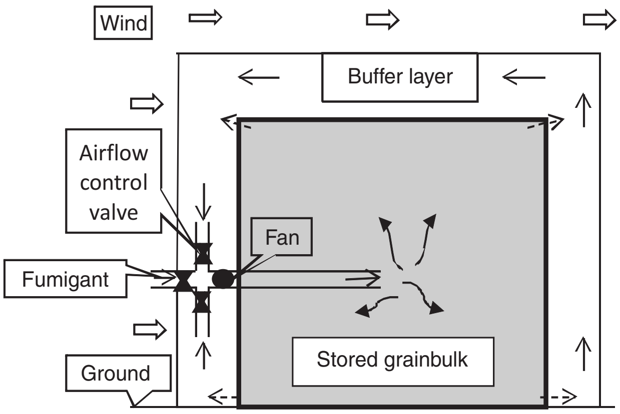

Fig. 2. Schematic (not to scale) of a double layer system for fumigation or controlled atmospheres. (In the graph, the solid arrows show the supplied and recirculated fumigant, the dash arrows indicate the regulated leaking positions of the inner layer, double line arrows show the wind direction, and the curved arrows demonstrate the movement of fumigant).

CREATING UNIFORM DISTRIBUTION OF APPLIED GAS

Leaking regulation

There are many ways to regulate leaking. The traditional method is to seal the structure with similar airtightness at any place of the structure. This is the costliest method and might be infeasible under some conditions (such as to seal a tall building). For a large building, high HLP values are required. If the required HLP value for a structure cannot be achieved, another method is to seal the structure with different gas tightness at different locations. For example, gas tightness at the area close to the gas injection position should be higher than that at the far end of the gas injection location. If required, opening holes at the far end from the gas injection location will help create an even distribution of the pressure gradient. This method can be used for less toxic gas such as CO_2, and N_2 or short life gas such as ozone (O_3).

If there is no pressure gradient, there is no convection and advection movement of air and applied gas. To control the leakage induced by wind, the ideal condition is to make the inner pressure at the wall of the structure be equal to the wind pressure. Compared with the wind pressure, pressure inside a structure is usually stable. Therefore, creating a stable wind velocity might help balance the inner and outer pressures if the structure has a low gastightness. For as small structure, a wall blocking the wind might help. For a large structure, the airtightness of the structure on the area in the upwind direction should be higher than that in the downwind directions. Therefore, analysis of local wind data can be used to regulate the leakage of the structure (Chayaprasert et al., 2006).

Creating appropriate pressure gradient

Injecting and recirculating fumigants are the conventional methods to create the pressure gradient. These methods will not create a uniform distribution of the applied gas if the design or installation is not correct, because air and applied gas will move in the direction of the largest pressure gradient; and direction, location, and rate of the injected gas influence the distribution of the pressure gradient (Alagusundaram et al., 1995). Dr Noyes found that lack of circulation of PH_3 was the primary cause of recirculation fumigation failures (*Personal communication*). Therefore, the design of these methods should consider other factors influencing airflow distribution inside the grain bulk. Other methods such as forcing or pulling air should be considered in the design. Regardless of pulling or pushing air, a pressure gradient must be created inside the entire structure. The velocity of the applied gas should be much higher than that of the maximum free convection (1.1×10^{-3} m/s). Otherwise, there will be no air movement in areas without a pressure gradient. Mills et al. (2001) tested a positive pressure system to fumigate floor-stored grain bulks, and found 1.83 m^3/min for a 250 tonnes of floor-stored wheat bulk could provide an even distribution of PH_3 and the concentration was larger than the required lethal concentration except at one position. This system did not work well under high wind speed due to the difficulty in sealing floor-stored grain bulks. Therefore, methods of the leaking regulation should be considered.

If fumigation is conducted without forcing into or pulling the air from the structure, both the distribution of grain temperature and ambient temperature should be considered. Under this condition, the distribution of the applied gas was mainly influenced by the free convection induced by the temperature gradients in the stored grain. Direction of the free convection inside a structure is usually in different directions in different areas (Nguyen, 1987). Therefore, the best operational method is to use the ‘chimney effect’. To create the ‘chimney effect’, the entire grain bulk should be at the same temperature or have a small temperature gradient. The density of air inside the grain with higher temperature than outside will be lower than that of the ambient air. This density difference will drive the interstitial air to move up and escape from the headspace of the bin. If the bottom of the bin is not sealed, incoming ambient air will replace the escaped air. This moving air will help to distribute the applied gas. The introduction location of the tablets of aluminum phosphide should consider the direction of this chimney effect (Flinn and Reed, 2008). Exhaust roof air should be monitored to detect when gas has reached the top of the structure, so that bottom and roof openings can be sealed. Turning or aerating grain creates a uniform temperature distribution inside the structure. Therefore, “chimney effect” might be applied after the grain is turned or aerated.

For a structure with low gastightness, continually injecting the applied gas and recirculating the applied gas might be the best choice to attempt to achieve an even distribution of the applied gas. This method is usually conducted by moving the applied gas with a low velocity. This low velocity with a single injecting location has the risk of non-uniform distribution of pressure gradient and applied gas. Therefore, multiple injection points should be considered. Australians use the Siroflo multi-point release fumigation method with a flow of 35 ppm ECO_2FUME for 21 d to achieve a positive kill in grain warehouses.

Fumigation or controlled atmosphere with double layer sealing

For fumigation or controlled atmosphere of a small structure such as a bag stack, an air buffer layer created by using double layers of PVC film (Fig 2) may help maintain a uniform concentration of applied gas. The concentration of the applied gas inside the buffer layer can be monitored and regulated. Concentration inside the buffer layer will be the minimum concentration of the applied gas, if the injection port is located at the centre of the grain bulk. The pressure inside the buffer layer should be smaller than that inside the inner layer and higher than the average wind pressure. The airflow of the recirculated air and injected gas can be controlled based on the concentration inside the buffer layer. At the beginning of the fumigation, negative pressure can be applied. After the negative pressure reaches the minimum, the applied gas under positive pressure can be applied. The principle of this double layer design can be used for other structures.

MATHEMATICAL STUDY OF GAS DISTRIBUTION

An understanding of movement of applied gas inside a structure is the first step to create an even distribution of the applied gas. Though some physical principles can be used to estimate the distribution of the pressure gradient and applied gas, the distribution cannot be accurately predicted or generalized without laboratory and field tests and mathematical studies. The distribution principles of the fumigant and controlled atmosphere gases inside structures are lacking studies probably due to the difficulties of this research area (such as the risk of toxication and monitoring of the applied gas). Traditionally, fumigation and controlled atmosphere are conducted based on experience (such as the development of HLP). Therefore, engineering design based on mathematical modeling modeling study might play a role. The suggested mathematical studies listed in this section might help design a more efficient system to create a uniform distribution of applied gases.

Effect of the DFM distribution on airflow resistance

The DFM has a heterogeneous distribution inside grain bins (Parker et al., 2005). Though this non-uniformity of DFM cannot fully explain the air flow resistance distribution (Lawrence and Maier, 2011), the distribution of DFM affects airflow resistance (Jayas et al., 1987). To predict airflow resistance and distribution, therefore, the following two questions should be answered: how single grain kernels are three dimensionally aligned and how the DFM materials are distributed as a function of the grain loading procedure. Jayas et al. (1987) developed regression equations to explain the relationship among the bulk density, porosity, and amount of foreign materials. There are no mathematical models developed to simulate the distribution of the DFM. Studies should be advanced to relate the distribution of DFM to airflow resistance and distribution.

Airflow distribution under different air velocities in different grain depths

There are studies on airflow distribution in grain bulks at velocities of aeration and drying (Jayas et al., 1990; Goudie et al., 1995; Smith, 1996; Smith and Jayas, 2004; Gayathri and Jayas, 2007). Traverse time of the airflow along the main pressure gradient can be estimated (Hunter, 1986; Smith and Jayas, 2004). In the literature, the stored grain in structure was modelled either as a two dimensional rectangular or cylindrical geometry, while Darcy flow (velocity proportional to pressure gradient) or Ergun flow (Darcy flow with a square velocity correction) was assumed. There are few theoretical and field studies of the velocity distribution of fumigant and controlled atmosphere gases forced by a fan with a low airflow velocity (such as the velocity used for the recirculation of PH_3). Under high velocity of airflow (such as drying), the turbulent or transition from laminar to turbulent flows might be dominant inside the grain bulk, while laminar flows might be dominant when velocity of applied gas is low. It is needed to verify whether laminar flows under certain low velocities might be significantly influenced by the non-uniform distribution of resistance to the airflow. Different structures and grain depths will influence the distribution of the resistance. To our knowledge, there is no study of gas distribution under low velocities in different shapes of structures filled with different grain depths and under different storage conditions.

Coupled mathematical model

The mathematical models of the movement of CO_2 and PH_3 by advection, diffusion, and sorption were developed (Smith and Jayas, 2001; Zaiton, 2014). Models considering the effect of leakage (Annis and Banks, 1993; Zaiton, 2014), injection method (Goudie et al., 1995; Smith,1996; Smith and Jayas, 2004), and fumigant as a single component gas (Annis and Banks, 1993; Alagusundaram et al., 1995; 1996) were also developed. These developed models have a limited application for the field practice because these models are not coupled. There is also no coupled model considering the effect of temperature and grain moisture, and the fluctuating weather temperatures and wind pressures. This coupled model should be also coupled with the model of DFM distribution, and the airflow resistance model. These coupled models will help conduct correct fumigation and controlled atmosphere such as to design correct monitoring locations because validated mathematical modelling studies will provide the information about the distribution of the applied gas concentration.

ACKNOWLEDGEMENT

Authors thank Dr Ronald T Noyes, President, Grain Storage Engineering, LLC and Professor Emeritus, Biosystems and Agricultural Engineering Department, Oklahoma State University, Stillwater, OK, USA for reviewing an earlier version of this article and providing valuable feedback to improve the article.

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