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Conference Paper · October 2018

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Modeling the distribution of phosphine in cylindrical grain silos with CFD methods for precision fumigation

Efstathios Kaloudis[1], Sotiris Bantas[1], Christos G. Athanassiou[2], Paraskevi Agrafioti[2*], Vasilis Sotiroudas[1,3]

[1]Centaur Analytics, Inc., 1923 Eastman ave, Ste 200, Ventura, 93003 CA, USA
[2]Laboratory of Entomology and Agricultural Zoology, Department of Agriculture, Crop Production and Rural Environment, University of Thessaly, Phytokou str., 38446, Volos, Magnesia, Greece
[3]Agrospecom, N. Kountourioti 3, Thessaloniki, 54625, Greece
*Corresponding author: agrafiot@agr.uth.gr
DOI 10.5073/jka.2018.463.154

Abstract

In the present study, the distribution of phosphine gas in a cylindrical silo was modeled and compared with available sensor data. The cylindrical silo was filled with wheat and a recirculation system was used to enhance the diffusion of phosphine throughout the grain volume. A Computational Fluid Dynamics (CFD) model was developed with OpenFoam software, which accounted for gas transport in porous media and sorption effects of phosphine into the grain. A time-dependent source was used to model the phosphine release from Aluminum Phosphide bags. Furthermore, simulation results were obtained for insect mortality as a function of their exposure to phosphine gas. The phosphine concentration measurements were available from calibrated wireless sensors provided by Centaur Analytics, placed near the silo walls at various heights. As the agreement of phosphine measured data with the simulation results was satisfying, it led to considering that the proposed CFD model (equations, boundary conditions, grain properties, recirculation system approach, etc.) was accurate. Utilizing the capabilities of fumigation modeling, the phosphine concentration could then be determined for every location inside the storage volume and at any given time, thus a prediction method for fumigation duration and success could be enabled. Additionally, as the CFD model correlates phosphine exposure with insect mortality, a methodology for planning precision fumigations can now be established.

Keywords: phosphine, modeling, fumigation, cylindrical silo.

Introduction

Phosphine (PH_3) is the single most relied-upon fumigant to control grain pests, due to its inexpensiveness, ease of application and universal acceptance as a residue-free treatment. Since the use of Methyl Bromide was phased out due to its significant contribution to the destruction of the earth's stratospheric ozone layer, phosphine has emerged as a viable replacement. However, there are several factors that occasionally prevent phosphine fumigations to be successful (e.g. phosphine sorption, leaky storage structures, poor monitoring procedures). Improper use leaves the treated commodity susceptible to insects, increasing the possibility of spoilage, but is also known to lead to tolerant strains among key stored product insects throughout the world (Athanassiou et al., 2016).

In view of the above, it is important to bolster the effectiveness of phosphine fumigation processes and ensure the ecosystem can continue to rely on this important fumigant. To achieve this, an in-depth knowledge and understanding of fumigant behavior are crucial. An efficient method for tackling this is through the combination of field experiments and computer simulation. To the authors' knowledge, there are a limited number of studies in the literature adopting this approach. Except for Lawrence et al. (2013), none of them combine field experiments with detailed numerical simulations. Lawrence et al. (2013) presented a 3D transient heat, mass, momentum, and species transfer model for the stored grain ecosystem which was developed using the finite element method. However, they validate their model against average phosphine concentration measurements which are not indicative of treatment effectiveness. Other relevant publications concerning phosphine simulations are the ones by Boac et al. (2014), Isa et al. (2016), but both are lacking validation with experimental data. Specifically, Boac et al. (2014) studied phosphine distributions in bulk storage structures (bunkers) including the effect of wind phenomena, whereas Isa et al. (2016) made predictions of phosphine flow during grain fumigation in leaky cylindrical silos. Mills et al. (2001) studied a positive pressure system for combating dilution during phosphine fumigations of bulk grain. Nonetheless, their CFD model is not extensively documented. Chayaprasert et al. (2006) used CFD to develop 3D computer models for structural fumigations upon datasets collected at a fumigation treatment in a commercial flour mill. The fumigation models were divided into two parts: internal and external flow models.

In this work, a detailed description of the fumigation treatment inside a cylindrical silo is presented, presenting – for the first time – correlations of numerical (CFD) analysis with wireless gas sensor readings based on a rich sample of phosphine distribution during the entire duration of treatment. Numerical results are employed to provide a map of insect mortality rates, thus binding the analysis with the end objective of pest treatment. Additionally, information about the PH_3 sensing devices as well as the simulation approach is given and a methodology for planning and implementing precision fumigations is outlined.

Materials and Methods

Silo description

The silo under consideration (Fig. **11**) was located in the area of Volos, Greece and the fumigation treatment took place during December. The steel silo diameter was D=15 (m) and its height was H=12 (m). A recirculation system was installed and used during the process. Stored grain (whole wheat) temperature was 12 (°C).

Measurement of phosphine concentration

Data collection of phosphine concentration inside the silo was made with sensor devices provided by Centaur Analytics, Inc. The devices are based on electrochemical sensors thus providing high accuracy, and are equipped with wireless connectivity with the ability to transmit data frequently (e.g. every 2 hours) from inside stored grain. The data were transmitted in real time to Centaur's cloud platform, from which they were downloaded and further processed. Fig. **11** shows the position of the 4 sensors inside the silo, whereas Fig. **12** shows how one of the sensors is installed inside the silo.

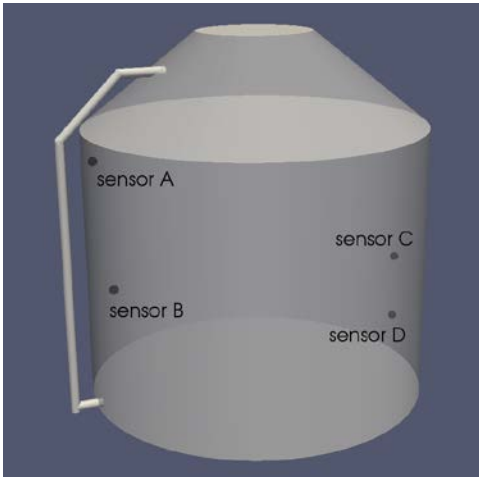


Fig. 11 The three-dimensional model of the cylindrical silo considered in this work

Fig. 12 Installation of sensor B inside the silo

Fumigation parameters

Phosphine gas was generated using Aluminum Phosphide bags. Approximately 10 gr of AlP per tonne of stored product was used, which is equivalent to 2.53 gr of phosphine gas per m^3. The degassing evolution of phosphine is presented in Fig. **13**.

Simulation technique

In phosphine fumigations, it is important to ensure that phosphine concentration exceeds the predefined ppm levels in the entire storage space, to eliminate all insects (for 99.9% mortality). In order to increase the spatial resolution of sensor data, Computational Fluid Dynamics (CFD) models are used. CFD is a branch of fluid mechanics that uses numerical analysis and data structures to solve and analyze problems that involve fluid flows. Computers (typically on the cloud) are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions.

Governing equations

The CFD solver is implemented using OpenFoam v.3.0.1 (OpenFOAM Foundation, Ltd.) in order to solve the following transport equations for incompressible fluid flow, heat, and mass transfer, accounting for porous media effects:

$$\nabla u = 0 \quad (1a)$$

$$\frac{\partial u}{\partial t} + \frac{1}{\phi} u \nabla u = -\phi \nabla p + \nu \nabla^2 u - \phi \frac{\nu}{K} u - \phi \frac{F_e}{\sqrt{K}} |u| u + \phi g \beta (T - T_{ref}) + \phi g \beta_c (C - C_{ref}) \quad (1b)$$

$$\frac{\partial T}{\partial t} + \phi \frac{(\rho C_p)_f}{(\rho C_p)_{eff}} u \nabla T = \frac{k_{eff}}{(\rho C_p)_{eff}} \nabla^2 T \qquad (1c)$$

$$\phi \frac{\partial C}{\partial t} + \phi u \nabla C = \phi \nabla^2 (\frac{D_m}{\tau} C) - \phi B_1 C + B_2 q \qquad (1d)$$

$$\frac{\partial q}{\partial t} = -B_3 q + \phi B_4 C \qquad (1e)$$

In the above equations (1a-1e), u is the velocity vector, and p, T, and C are the pressure, temperature, and phosphine concentration in air, respectively. D_m is the binary diffusion coefficient ($m^2\ s^{-1}$). Buoyancy forces created by both temperature and concentration gradients are considered in the momentum equations using the Boussinesq approximation. Under the Boussinesq approximation, the variation of density ρ with temperature T is linear, according to $\rho = \rho_{eff} - \rho_{eff} \beta (T - T_{ref})$. The volumetric coefficient of thermal expansion β and the species expansion coefficient β_c for ideal gases are given by Eqs. 2a and 2b respectively:

$$\beta = -\frac{1}{\rho}(\frac{\partial \rho}{\partial T})_p = \frac{1}{T} \quad (2a) \qquad and \qquad \beta_c = -\frac{1}{\rho}(\frac{\partial \rho}{\partial C})_p = \frac{1}{\rho_{air}}(\frac{MW_{air}}{MW_{gas}} - 1) \quad (2b)$$

where MW_{air} and MW_{gas} are the molecular weights of air and phosphine gas respectively.

According to Shen et al. (2007) in order to represent the role of porosity on ordinary molecular diffusion, the diffusion coefficient must be scaled with tortuosity. Specifically, an effective diffusivity coefficient could be set as:

$$D_{eff} = \frac{D_m}{\tau} \qquad (3)$$

Neethirajan et al. (2008) calculated τ = 2.4 for wheat.

Porous media approach

In order to account the effect of grains on the gas flow, the grains were assumed to be a porous medium. Flow in porous layers is described by the Darcy-Brinkman formulation. The geometric function Fe and the permeability K of the porous medium are related to the porosity φ based on Ergun's experimental investigations:

$$F_e = \frac{1.75}{\sqrt{150\,\phi^3}} \quad (4a) \qquad and \qquad K = \frac{\phi^3\, d_p^2}{150(1-\phi)^2} \quad (4b)$$

The effective properties $(\rho\, C_p)_{eff}$ and k_{eff} are calculated as a function of the fluid and porous material:

$$(\rho\, C_p)_{eff} = (1-\varphi)(\rho\, C_p)_{solid} + \varphi(\rho\, C_p)_f \qquad (5a)$$

$$k_{eff} = (1-\varphi)\, k_{solid} + \varphi\, k_f \qquad (5b)$$

Sorption effects

Phosphine is adsorbed by grain at differing rates depending on the grain type. Sorption can reduce the concentrations of fumigation doses to sublethal levels before grain has been disinfected. A model to predict fumigant losses due to sorption is considered necessary. Researchers (Darby, 2008) have suggested that the relationship between the fumigant concentration in the interstices between the grain, C, and the average concentration of fumigant within the grain kernel q, is modelled by Eqs 1d and 1e which assert that phosphine is absorbed into the grain and at the same time also degrades in air. The coefficients B_1, B_2, B_3, and B_4, are independent of C and q.

$$B_1 = \frac{S_{sorp}\, k_f}{B_{fill}} \quad (6a), \qquad B_2 = \frac{S_{sorp}\, k_f}{B_{fill} F} \quad (6b)$$

$$B_3 = \frac{S_{sorp}\, k_f}{(1-\phi)F} + k_{bind} \quad (6c), \qquad B_4 = \frac{S_{sorp}\, k_f}{(1-\phi)} \quad (6d)$$

$$B_{fill} = \varphi + \frac{1-R_{fill}}{R_{fill}} \quad (6e)$$

where: S_{sorp} is the specific adsorption surface area, k_f is a linear mass transfer coefficient, F is the partition relation coefficient, k_{bind} is the coefficient for irreversible reaction/binding of the adsorbed fumigant in the grain kernel. For wheat, the above parameters have the following values: S_{sorp} k_f =0.0125, F=0.3, and k_{bind}=0.0569.

Boundary conditions

In order to evaluate accurately the storage (computational domain) interaction with its surroundings, the following convective boundary conditions were used for phosphine concentration and heat transfer (Barreto et al., 2013), respectively:

$$-D_m \frac{\partial C}{\partial x}|_{x=0} = h_m (C - C_{amb}) \quad (7a)$$

$$-k \frac{\partial T}{\partial x}|_{x=0} = h_c (T - T_{amb}) - \alpha_h G + \epsilon\sigma (T^4 - T_{sky}^4) \quad (7b)$$

Coefficients h_m, h are a function of silo geometry (cylinder, orthogonal), fluid medium (air, water) and fluid velocity (e.g. wind velocity). In Eq. 7b, the second term on the right-hand side is the heat gain due to solar radiation and the third term is the net radiation heat loss rate for a hot object which is radiating energy to its cooler surroundings (Adelard et al., 1998):

$$T_{sky} = 0.0552\, T_{amb} \sqrt{T_{amb}} \quad (8a)$$

$$h_c = 10.45 - U_{wind} + 10\sqrt{U_{wind}} \quad (8b)$$

For the purposes of the present study, the time series of ambient temperature, wind velocity, and solar radiation that are used as inputs are presented in **Fig. 14**.

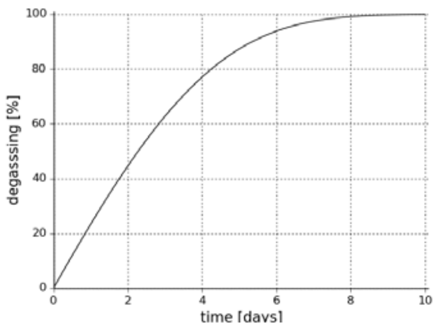


Fig. 13 Degassing evolution of phosphine gas from AlP bags during fumigation (data provided by Detia Degesch)

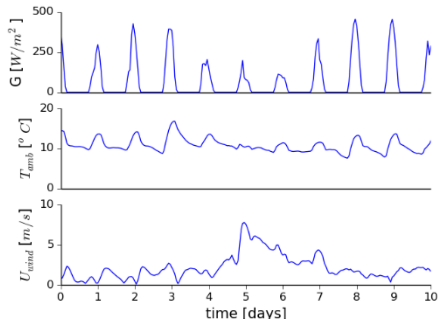


Fig. 14 Time variation of ambient conditions: solar radiation, temperature and wind velocity

Domain discretization

Meshing is the discrete representation of the geometry that is involved in the problem. Essentially, it partitions space into cells over which the equations can be approximate. In the present study, the computational grid used (Fig. **15**) was structured, thus ensuring greater accuracy, and all cells (approximately 85000) were hexahedra. Furthermore, grid-clustering was employed near the side to properly capture large gradients.

Insect mortality

It is known that the effect of phosphine on the mortality of grain insects is due to both the level of the phosphine concentration and the time of exposure (Collins et al., 2005; Isa et al., 2016). An insect mortality indicator function IM(x, t) could be defined as:

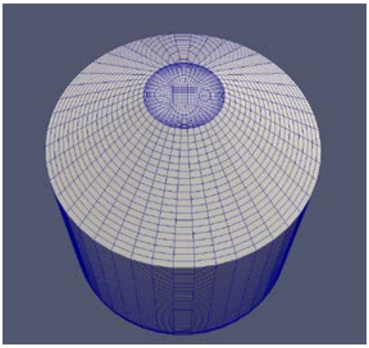
$$IM(x,t) = \frac{1}{K_1}\int_0^t C(x,t)^{K_2}\,dt \qquad (9)$$

The constants K_1 and K_2 are empirical and depend on the species and strain of insect. IM(x,t) account for the period of exposure to phosphine that an insect has encountered. For a given point in the grain, when IM(x,t)<1 there are some insects in the grain still alive. When IM(x,t)>1 at least 99.9% of the insect population have been killed. For the present simulations K_1=4.04 and K_2=0.6105 which accounts for the *Rhyzopertha dominica*.

Results

The simulation model yielded, among other results, the development of phosphine concentration for the entire duration of the fumigation treatment (9 days). In **Fig. 16**, the time evolution of phosphine at the 4 locations is presented. Specifically, sensor data are compared against model predictions. The best correlation occurs for A and B positions which are located on the silo side where the recirculation system was installed. Their maximum concentration is reached at the end of the 4th day, followed by a decrease due to diffusion, losses, and sorption by the stored product. Concerning, locations C and D, sensor data reveal lower concentration values as the model also predicts. A small discrepancy is observed on the time that the maximum value is reached. According to sensor data, phosphine concentration has an upward trend until the end of the 7th day, whereas the CFD model underestimates to the end of the 5th day. Minor fluctuations, with hourly timescales, occur due to natural convection currents which are the result of temperature differences imposed by the unsteadiness of ambient conditions. The currents create upward and downward air movements that transport phosphine along.

The overall performance of the CFD model is considered satisfactory ensuring the validity of the phosphine concentration predictions for the entire silo space as the ones presented in **Fig. 17**. Particularly, **Fig. 17** shows the spatial distribution of phosphine at four time instances. The advantages of using a recirculation system can be clearly seen since at the second day, phosphine has reached every position inside the silo. Until the 6th day, higher concentration values are observed on the top regions of the silo, near the aluminum phosphide bags but as their degassification completes a more uniform phosphine distribution is reached (**Fig. 17**, 8th day). A video showing the model predictions for the entire fumigation process could be found here: https://youtu.be/iISBS7eoWb8



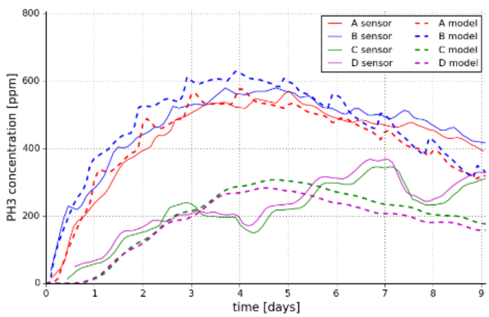


Fig. 15 The computational mesh used for the silo simulation

Fig. 16 Phosphine concentration (ppm) comparison of sensor data (solid lines) vs. simulation predictions (dashed lines) at 4 locations inside the storage.

A useful augmentation of the phosphine concentration profiles is the prediction of the insect extinction. **Fig. 18** shows the areas (red color) in which the Rhyzopertha Dominica species could not survive the fumigation process. As expected, areas near the Aluminum Phosphide bags and at the piping outlet are the first ones that reach lethal levels. According to the simulation, at the end of the 7th day there are still some areas that insects could be still alive. A video showing the insect extinction predictions for the entire fumigation process could be found here: https://youtu.be/54uJ1ZJlkrk

Discussion

A 3D heat, momentum, and species transfer model for stored grain ecosystems was developed in this work, able to predict phosphine concentration changes. As the agreement of phosphine measured data with the simulation results was satisfying, it is safe to assume that the proposed CFD model (equations, boundary conditions, grain properties, recirculation system approach, etc.) is accurate for the purpose. Utilizing the capabilities of fumigation modeling, the phosphine concentration was determined for every location inside the storage at any given time, thus a prediction of fumigation duration and pest elimination success could be provided. The main benefit of the CFD approach is its wide applicability on any type of commodity, storage or phosphine formulation. As the CFD model correlates phosphine exposure with insect mortality, a methodology for planning precision fumigations can be established.

In general, the results presented here illustrate that gas distribution is uneven during the entire treatment period, suggesting that there are large areas within the treated area that are exposed to low concentrations. This may result in increased survival of the exposed insects in these areas, and, to some extent, lead to tolerance development. Circulation of phosphine (through J-system) may be a solution to this implication, but additional experimental work is needed to estimate the relative benefits. In light of the present findings, it is evident that distribution is uneven right after the start of the application, and is likely to exhibit “diurnal circles”, as has been previously reported for other trials (Athanassiou et al., 2016). By the use of sensors, however, monitoring of these variations may provide the inferences necessary for designing a strategy to overcome this phenomenon, under the premise of a ‘precision fumigation’ approach. This was definitely not possible, at least not at an acceptable accuracy level, with the ‘traditional’ phosphine concentration measurement techniques.

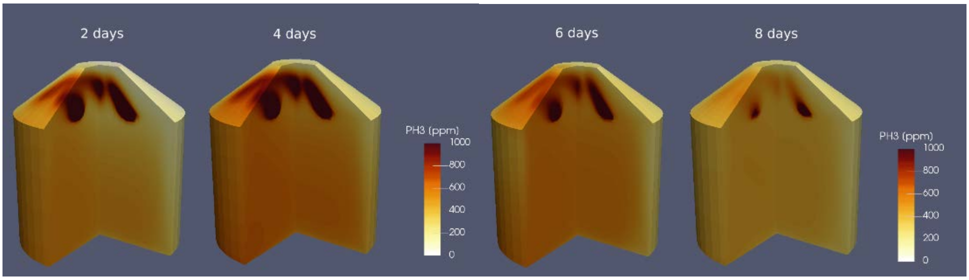


Fig. 17 Phosphine concentration profiles at 4 time instances

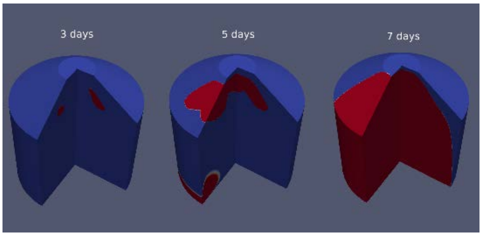


Fig. 18 Extinction of insects at 3 time instances. Red color indicates zones with 99.9% insect mortality.

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