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Mathematical modelling and numerical simulation of phosphine flow during grain fumigation in leaky cylindrical silos

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ABSTRACT

The phosphine distribution in a cylindrical silo containing grain is predicted. A three-dimensional mathematical model, which accounts for multicomponent gas phase transport and the sorption of phosphine into the grain kernel is developed. In addition, a simple model is presented to describe the death of insects within the grain as a function of their exposure to phosphine gas. The proposed model is solved using the commercially available computational fluid dynamics (CFD) software, FLUENT, together with our own C code to customize the solver in order to incorporate the models for sorption and insect extinction. Two types of fumigation delivery are studied, namely, fan-forced from the base of the silo and tablet from the top of the silo. An analysis of the predicted phosphine distribution shows that during fan forced fumigation, the position of the leaky area is very important to the development of the gas flow field and the phosphine distribution in the silo. If the leak is in the lower section of the silo, insects that exist near the top of the silo may not be eradicated. However, the position of a leak does not affect phosphine distribution during tablet fumigation. For such fumigation in a typical silo configuration, phosphine concentrations remain low near the base of the silo. Furthermore, we find that half-life pressure test readings are not an indicator of phosphine distribution during tablet fumigation.

1. Introduction

Phosphine gas has been the most preferred fumigant to kill stored grain insects since the mid-1990s (Collins, 2010). It remains the most relied upon fumigant (Cavasin et al., 2006; Horn et al., 2003; Warrick, 2011) and comprises approximately 80% of the fumigant usage in Australia (Darby and Annis, 2003). The advantages of phosphine over other fumigants are the low price, ease of application, and minimal residue (Boland, 1984; Bullen, 2007; Chaudhry, 2000; Collins et al., 2001; Rajendran, 2007).

However, phosphine sorption into grain kernels has been proven to occur (Annis and Dowsett, 2001; Chakrabarti et al., 1994; Darby, 2008; Darby et al., 2009; Ferrell, 1996; Reed and Pan, 2000; Daglish and Pavic, 2008, 2009). Furthermore, the importance of silo sealing has been mentioned to affect phosphine distribution (Andrews et al., 1994; Mills et al., 2000; Proctor, 1994; Warrick, 2011; White, 2012). Both sorption and leakage contribute to an insufficient application rate, which encourages the development of resistance in grain pests. Such resistance can lead to significance grain loss and has threatened the use of phosphine as a sustainable agrochemical (Collins et al., 2005; Daglish et al., 2002; Lorini et al., 2007; Nayak et al., 2010; Rajendran and Gunasekaran, 2002). To date, however, alternatives to phosphine are limited.

In view of the above, it is very important to carefully conduct fumigation to make sure that there are no chances of insufficient dosage. Hence, preventing the need for multiple fumigation, which encourages the development of resistance. To achieve this, a good understanding of fumigant behaviour is crucial. Performing field experiments is expensive to organize, and hence, mathematical modelling and computer simulation are alternative, possibly beneficial tools.

Unfortunately, little is known about the behaviour of fumigants in grain storage at this point (Collins, 2010). In addition, comprehensive studies on the modelling of phosphine distribution in grain silos are lacking, regardless of the application method of fumigation.

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Commonly, phosphine is applied through a fan-forced system or tablet formulation. Fan-forced fumigation involves injecting gas through an inlet near the base of the silo. In contrast, tablet fumigation involves placing solid tablets on a basket near the grain surface at the top of the silo, which then dissolve via their interaction with air and moisture.

A previous study by Annis and Banks (1993) proposed a mathematical model to predict the average phosphine concentration over time during tablet fumigation. Spatial variation of the gas concentration within the grain is ignored. Given the considerable size of most silos, this is unrealistic. Although leakage and sorption were considered, for simplification, they were both modelled as a constant.

A relatively small number of studies using computational fluid dynamics (CFD) exist in the literature. For example, Bibby and Conyers (1998) predicted the gas flow and heat transfer of a mixture of carbon dioxide and oxygen in a silo with leaky holes at the top boundary. Although a multicomponent gas is considered, sorption of gas into the grain kernel is not accounted for, which has proven to be important (Darby, 2008; Darby et al., 2009).

The work by Mills et al. (2000) investigated the movement of phosphine in a horizontal storage. The fan-forced fumigation involve a gas that is delivered through eight injection inlets and exits through eight recirculation suction outlets. Unfortunately, the model equations are not given. The focus of this work is on the use of CFD to simulate the proposed system. Other examples are the works concerning the distribution of the fumigant, sulphuryl fluoride, in a flour mill (Chayaprasert et al., 2006, 2008, 2010). In these works, the whole building was the attention rather than a single storage bin. In addition, the development of the transport modelling equations is not clear.

For tablet fumigation most of the modelling studies of the fumigant distribution have focused on CO_2 gas rather than phosphine. Those by Alagusundaram et al. (1996a, 1996b), Smith and Jayas (2001), and Smith et al. (2001) look at CO_2 released from dry ice into a cylindrical storage bin. In these models the dry ice is placed at the bottom of the storage rather than on the surface of the grain or inside the silo. Although the transport model is similar to this present study, sorption and leakage are not considered.

Importantly, none of the theoretical modelling studies mentioned here have tried to account for insect extinction.

Experimentally, phosphine gas distribution has been studied by Boland (1984), Bridgeman et al. (2000), Chakrabarti et al. (1994), Jianhua et al. (2000), and Williams et al. (1996). With the exception of Jianhua et al. (2000), the experiment incorporate well sealed, large scale silos that range between 2000 and 7000 tonnes (approximately 2600 m^3–9210 m^3), whereas here, we consider a small scale "on farm silo" (approximately 100 m^3 or ≈ 76 tonne). The experiments by Jianhua et al. (2000) do involve tablet fumigation within a small size silo (240 tonne). However, the silo is equipped with a gas recirculation system, which is beyond the scope of our current investigation as it is not common on farm.

The lack of a comprehensive model for typical small scale (on-farm) grain fumigation practices serves as a primary motivation for this work. In contrast to the reported studies, the present model is developed by considering a binary gas flow (phosphine and air) in a three-dimensional cylindrical silo filled with grain. Absorption of phosphine into the grain, degradation of the phosphine over time in the silo and extinction of grain pests are included in the current model. In addition, both fan forced and tablet fumigation regimes are considered for silos that range in their "integrity" from being air tight to moderately leaky.

This present study focuses on fumigation with phosphine in accordance with on-farm practices. Although grain storage comes in a range of shapes and sizes, a vertical silo is considered here since this is the most popular method of storing grain, constituting 79% of all on farm storage types (White, 2012). Generally, fan-forced fumigation on farms is unusual since for small silos tablet fumigation is considered to be adequate, however, the results obtained here provides a comparison between the two types of delivery method.

2. Model development

Fig. 1 shows the view of the typical cylindrical silo considered here. The coordinate r (m) denotes the radial distance from the origin $r = 0$, θ (radians) is the angle from a fixed axis, and z (m) is the vertical height of the silo. Inside the silo, grain occupies the silo up to the height $z = h$ (m) and is porous, while the region from $z = h$ to $z = L$ (m) is called the headspace and is non-porous.

The model assumes that no water or excess water vapour is present, and that the gas present in the pores is a binary mixture of air and phosphine. Therefore, in the porous zone, the total volume will consist of grain and gas such that,

$$\varepsilon_{gr}(\mathbf{x}) + \varepsilon_g(\mathbf{x}) = 1 \quad (1)$$

where ε_{gr} and ε_g are the volume fractions of grain and gas, respectively. Furthermore,

$$\varepsilon_g(\mathbf{x}) = \varepsilon_{air}(\mathbf{x}, t) + \varepsilon_{ph}(\mathbf{x}, t) \quad (2)$$

where ε_{air} and ε_g are the volume fractions of air and phosphine gas, respectively. The volume fraction of grain, $\varepsilon_{gr}(\mathbf{x})$, is considered to be static over time, which means that any deformation of the grain, for example via the consumption of grain by pests, or compaction due to gravity is ignored.

The gas is considered to be an ideal mixture of ideal gases, such that the total gas pressure, $P_g(\mathbf{x},t)$ (Pa), is the sum of the air pressure, P_{air} (Pa) and phosphine pressure, P_{ph} (Pa), namely,

$$P_g = P_{air} + P_{ph} \quad (3)$$

Furthermore,

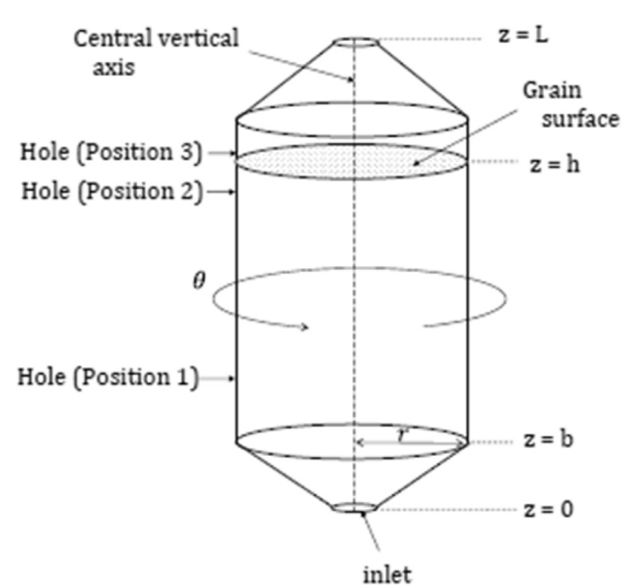

Fig. 1. Schematic of the cylindrical silo (not to scale) considered in this work.