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Development and validation of Computational Fluid Dynamics models for precision structural fumigation

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Abstract

Three-dimensional Computational Fluid Dynamics models for structural fumigation were developed and validated using Fluent® based upon comprehensive data sets collected during the fumigation of a commercial flour mill. The external flow model, which included the flour mill and surrounding structures, was used to predict stagnation pressures on the mill's walls as a function of the wind speed and direction data. The pressure differences due to density differences between the gas inside and the air outside the mill (stack effect) were estimated using the environmental temperature and relative humidity data. The combined effect of the stagnation pressure and the stack effect was used as the boundary conditions of the internal flow model. The internal flow model incorporated interior details of the mill such as building plans, locations of major equipment, partitions and ducting. Because it was not possible to obtain the actual number and sizes of the cracks in the structure envelope, the idea of representing the cracks as effective leakage zones (ELZ) was adopted. The flow resistance coefficient, k_L, of the ELZs determines the gas tightness of the mill. Nine simulations were conducted with different k_L values. Both experimental and simulation concentration data indicated that the fumigant was uniformly distributed within the entire mill building. Using a manual optimization approach, one specific k_L value was determined for which the models were able to yield a half-loss time (HLT) value identical to the experimental HLT (17 h) and minimize the prediction of the concentration × time (*Ct*) product to within 10.5% of the observed value. Therefore, it was concluded that the models were validated and the assumption of ELZ was reasonable. The modeling methodology established in this paper could be utilized for the prediction of fumigation performance in any type of structure.

Keywords: Structural fumigation modeling; Methyl bromide alternative; Sulfuryl fluoride; Half-Loss Time; Computational fluid dynamics

1. Introduction

Currently, the only fumigation planning tool available to the industry was developed for use with sulfuryl fluoride (SF) fumigant gas. The proprietary Fumiguide™ calculator (Dow AgroSciences, Indianapolis, IN) takes into account various fumigation conditions such as estimated fumigant leakage rate (i.e., half-loss time (HLT)), exposure duration, volume of the structure being treated, target pest, fan capacity, and fumigant introduction rate. Two major limitations of the Fumiguide™ calculator are: (1) its utilization of conditions at the beginning of the fumigation process only and its assumption that conditions do not change at various times during the fumigation treatment, and (2) determination of the HLT value is solely based on the experience of the fumigator. Taking into account the dynamic changes of environmental conditions, fumigant concentrations in the fumigated structure, and their interaction is important for optimizing fumigant gas distribution and maintaining the lethal dosage level.

The analysis of fumigant gas leakage is similar to that of infiltration through an air-tight building. Two main forces that create pressure differences across the building envelope driving natural ventilation and infiltration are the wind and buoyancy (or stack) effects (ASHRAE, 2001). The combination of these two effects characterizes each building and complicates the analysis. Thus, the

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computational fluid dynamics (CFD) method is a proper approach for solving this complex problem. In the heating, ventilation and air conditioning (HVAC) industry, CFD has been used to study the effects of wind-induced pressure on building surfaces (Burnett et al., 2005; Senthooran et al., 2004) and contamination in building spaces (Cheong et al., 2003; Gilham et al., 2000; Sekhar and Willem, 2004). Additional studies by other researchers have also been published on these topics. However, no published study has been found in the literature on the use of the CFD method for modeling the fumigation process in large structures.

In this study, the CFD method was adopted to develop and validate comprehensive models that can be used for prediction of HLT and gas distribution during the fumigation process in a reference flour mill. The flour mill for this study has six floors with an approximate total volume of 28 317 m^3. Chayaprasert et al. (2006) described the methods and findings for a data collection effort undertaken as part of a commercial structural fumigation of a grain-processing facility that yielded the data needed for validating the CFD models. The specific objectives of this paper were to use a commercial CFD solver, Fluent® (Fluent Inc., Lebanon, NH):

- to construct a model of the flow outside the reference structure for predicting stagnation pressure profiles on the structure's walls created by prevailing wind;
- to construct a model of the fumigation process inside the reference flour mill in which the predicted stagnation pressures were used to generate concentration data similar to those observed during the fumigation experiment;
- to verify that the concentration data generated by the models predict a HLT value and a concentration × time (Ct) product similar to those observed during the fumigation experiment, given the same environmental conditions and fumigation practices.

2. Materials and methods

2.1. Simulation tool

The simulation software used in this study was Fluent® 6.2.16 on single-processor 1.8 GHz AMD Opteron machines with 4 GB RAM. Fluent® is a CFD solver based on the finite volume method. It has capabilities of modeling a broad range of fluid flow problems, including incompressible or compressible flows, laminar or turbulent flows, flows with other transport phenomena such as heat transfer and species transport, and flows with chemical reactions (Fluent, 2005). For all simulations in this study, the standard k–ε was used as the turbulence model, the pressure–velocity coupling was solved by the SIMPLE algorithm, and the governing equations were discretized using the first order upwind scheme.

During the structural fumigation process, the exchange between the external fresh air and the gas inside the structure occurs simultaneously through the structure's envelope. Because the length of the flows inside (0.01–0.1 m) and outside (1–5 m) the structure are substantially different; performing CFD simulations of both cases in the same flow domain would require an excessive number of computational cells (several million cells) and an unacceptable computing time (of the order of months). Therefore, in this study the flows of wind surrounding the structure and fumigant distribution inside the structure are modeled separately.

2.2. External flow model

The purpose of the external flow model is to predict stagnation pressure profiles on the structure's walls created by prevailing wind. It was used to perform several steady-state flow simulations based on different fixed wind speeds and directions. Since stagnation pressure is mainly a result of wind, variations in the other weather conditions (i.e., temperature, relative humidity [r.h.], and solar radiation) have not yet been incorporated in the model. Satellite images of the neighboring area (Google Earth 〈http://earth.google.com〉) were examined and no large structures were found within a 530 m radius of the grain processing and storage facility. Therefore, the entire flow domain was set-up as a rectangular volume such that it included the grain-processing building and the surrounding facility structures. The dimensions of these structures were obtained from construction drawings of the facility.

To ensure that the flow around the structures was not affected by the outer boundaries of the domain, these boundaries were placed at sufficient distances away from the structures. Fig. 1 illustrates the external flow domain setup in Fluent® used to simulate the wind effect when the direction of the wind was in the first quarter, i.e., the wind directions were between 0° (wind from the North) and 90° (wind from the West). Assuming that the velocity gradient far above the facility did not change, a symmetry boundary was assigned to the top of the flow domain at a distance of 4H from the flour mill's roof, where "H" is the height of

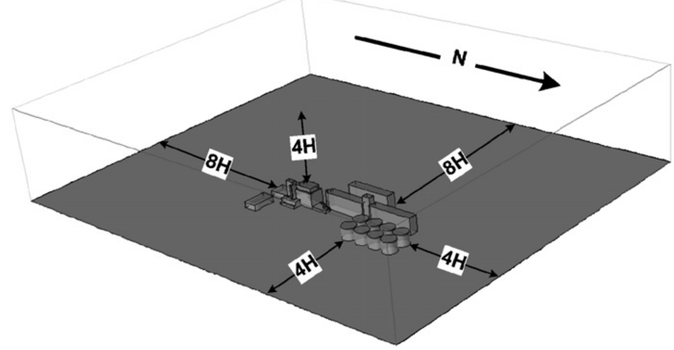

Fig. 1. Geometry of the external flow simulation when the wind direction is between 0° and 90°.