A simplified and improved modeling approach for the structural fumigation process using computational fluid dynamics

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Abstract

A 3D Computational fluid dynamics (CFD) model of the fumigation process in the Hal Ross Flour Mill of Kansas State University, Manhattan, Kansas, USA, was formulated for prediction of the gas leakage rate to approximate the gas Half-loss time (HLT) during fumigation with Methyl bromide (MB) and Sulfuryl fluoride (SF). The model consisted of external and internal flow domains. The external domain was used to predict stagnation pressures generated by wind impinging on the mill's walls. The internal domain was used to predict fumigant leakage rates in terms of HLT. Cracks on the mill's walls represented the effective leakage areas on the internal flow domain. This modeling approach had been used by the authors (Chayaprasert and Maier) in a previous study, but it was simplified and improved in the present study. The primary simplification in the modeling approach was exclusion of the flour mill's interior details (e.g., milling equipment), reducing the model formulation and simulation computing times. In the previous study, the gas-tightness of the internal flow domain was identified by varying the flow resistance coefficient of the effective leakage areas until the model yielded a HLT value that was close to the one observed from the experimental fumigant concentration data. In the present study, the domain gas-tightness was verified by building pressurization tests. The model was validated using data from one MB and one SF fumigation experiments. The HLTs provided by simulated fumigations were in good agreement with those determined from the experiments. The result of the present study provides further validation to the modeling approach and emphasizes the importance of building pressurization test for accurate HLT prediction.

Keywords: Structural fumigation, Half-loss time, Pilot flour mill, Computational Fluid Dynamics (CFD), Building pressurization test

1. Introduction

In fumigation of large structures such as flour mills or food-processing facilities, fumigant leakage always occurs because it is not practically possible to perfectly seal the structure. The decay of fumigant concentrations can be described by a first-order kinetic approximation (Cryer and Barnekow, 2006):

$$C_t = \frac{C_i}{2^{\frac{t}{HLT}}} \quad (1)$$

where C_t = current concentration (g/m^3) at elapsed exposure time t (h) and C_i = initial concentration (g/m^3). The half-loss time (*HLT*) is the time (h) at which the concentration reduces by half. The concentration × time (Ct) product (g-h/m^3) achieved at any given time can be calculated by integrating Eq. 1:

$$Ct = \frac{C_i HLT\left(1-2^{-\frac{t}{HLT}}\right)}{\ln(2)} \quad (2)$$

In other words, the needed amount of fumigant (i.e., the initial concentration times the building volume) for any fumigation is a function of the target Ct product, available exposure time, and half-loss time. Given fixed values for the target Ct product and available exposure time, it can be shown through Eq. 2 that the needed amount of fumigant is minimized when the HLT is known (Chayaprasert, 2007). Thus, being able to predict HLT is an essential part of optimizing the structural fumigation process.

Chayaprasert et al. (2008) used computational fluid dynamics (CFD) software, Fluent® (Fluent Inc., Lebanon, New Hampshire, USA), to develop a structural fumigation model for predictions of HLT and Ct product. The CFD model was validated based on a set of data collected during a fumigation experiment conducted by Chayaprasert et al. (2006). Given the same weather conditions, the coefficient (Eq. 4) which specified the gas-tightness of the building in the model was arbitrarily varied until the model was able to predict essentially the same HLT as observed in the experiment. Although the HLT prediction was accurate, this was rather an indirect approach for validating the model because the building gas-tightness was not directly measured. One possible method for measuring building gas-tightness is the equilibrium pressure-flow pressurization test in which measurements of air volume leakage rates through the building envelope are taken at multiple pressure levels. In the present study, the CFD modeling approach used by Chayaprasert et al. (2008) was implemented to construct a structural fumigation model using the Hal Ross Flour Mill, Department of Grain Science and Industry, Kansas State University, Manhattan, Kansas, USA, as the reference structure. The objectives of the study were 1) to simplify the modeling approach so that the model construction and simulation computing times are reduced, and 2) to improve the modeling approach by incorporating the building pressurization test data.

2. Materials and methods

2.1 Model construction

The flows of wind surrounding the mill and fumigant distribution inside the mill were separately simulated. The external flow domain was used to predict stagnation pressure profiles on the flour mill's walls created by prevailing wind. Sixty steady-state flow simulations, each of which was specified with a different fixed wind speed and direction, were performed. Five wind speeds (i.e., 2, 4, 6, 8 and 10 m/s) and 12 wind directions (i.e., 0, 30, 60, 300 and 330 degrees with respect to the north) were selected. Note that Chayaprasert et al. (2008) performed external flow simulations with the six wind speeds (i.e., 1, 2, 4, 6, 8, and 10 m/s) and 24 wind directions (i.e., 0, 15, 30, 330 and 345 degrees with respect to the north). Primary features included in the external flow domain were the flour mill building, surrounding structures, and perimeter boundaries. Figure 1 shows the external flow domain when the wind direction was between 270 and 0 degrees with respect to the north. Note that the north direction used in this paper and as shown in Figure 1 was a fictitious north which was approximately 135 degrees rotated from the true north in the clockwise direction. Given the mill's height H (i.e., 22 m), the distances from the upwind and downwind perimeter boundaries to the mill building were at least 4H and 10H, respectively, to ensure that recirculation flows in the downwind region of the domain did not influence the simulation result. For different wind directions, the upwind and downwind perimeter boundaries were relocated such that this criterion was met. A uniform gauge static pressure of 0 Pa was specified at the downwind boundaries. There was no velocity gradient (i.e., symmetry) through the top boundary.

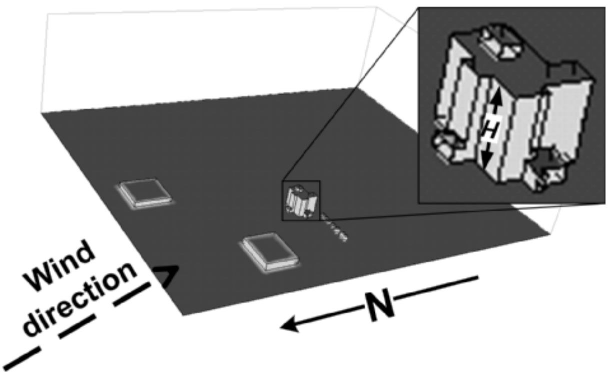

Figure 1 External flow domain when wind direction was 120 degrees with respect to the north. Note that the upwind and top perimeter boundaries are not shown.

To represent the atmospheric boundary layer, the velocity profile at the upwind (i.e., flow inlet) boundaries was calculated as (ASHRAE, 2001):

$$U_h = U_{ref}\left(\frac{h}{h_{ref}}\right)^a \quad (3)$$

where U_h is the local wind speed (m/s) at height h (m) and U_{ref} is the reference wind speed (2, 4, 6, 8 or 10 m/s) specified at a reference height, h_{ref} (m), of 10 m. The exponent, a, was 0.14, representing an atmospheric wind boundary layer in an open terrain. The internal flow domain was a rough representation of the Hal Ross Mill building (Figure 2) which has five floors and a total volume of 9,200 m^3. Unlike the model of Chayaprasert et al. (2008), the flour mill's interior details (e.g., milling equipment) were not included in the internal flow domain, reducing the model construction and simulation computing times. However, major structural features such as elevator shaft, stair wells, and ventilation shafts were incorporated. All the floors were interconnected through various openings which represent opened doors and air vents located on these structural features. A square 0.025 m^3 fluid zone was placed around the middle of each floor. The velocity vector in each fluid zone was fixed parallel to the floor and pointed to the west, simulating a fan flow rate of 0.94 m^3/s. Note that the number and location of this simulated fan were different from those in the experiments in which two 20-inch floor fans with unknown flow rates were placed in each floor. All physical cracks and crevices on the actual building envelope were represented by equivalent leakage zones (ELZs). Two 0.09 m^2 ELZs were placed on each of the north, south, west, east and top sides of the building. The locations of these ELZs were chosen arbitrarily. For the north, south, west and east sides (i.e., vertical walls), the ELZs were located on the first and fifth floors. As an example, the ELZ on the south side of the fifth floor is magnified in Figure 2.

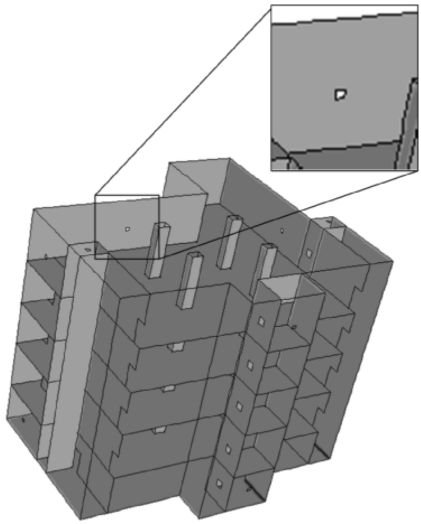

Figure 2 Internal flow domain divided into five floors.

For the top side (i.e., roof), an ELZ was placed at the top of each of the air ventilation shafts. All ELZs were assigned pressure boundary conditions with a flow resistance. The pressure difference, Δp, across each ELZ was calculated as:

$$\Delta p = k_L \frac{1}{2}\rho v^2 \quad (4)$$

where ρ and v are the density and velocity of the gas flowing through the ELZ, respectively. The gas-tightness of the mill building could be changed by adjusting the dimensionless loss coefficient, k_L, which was the same for all ELZs.

2.2 Model validation

The Hal Ross Mill model was validated using data from one 24-h methyl bromide (MB) and one 24-h sulfuryl fluoride (SF) fumigation experiments which are discussed in detail in another paper presented in this conference entitled, "Comparison of Leakage Rates of Methyl Bromide and Sulfuryl Fluoride during Structural Fumigations" by the same authors as this paper. Before each fumigation experiment, a building pressurization test was conducted. During each test, the building was pressurized by a specially calibrated fan to different pressure levels. At each pressure level, the flow rate through the fan and the static pressure difference across the building envelope were measured. The gas-tightness of the mill was characterized by the relationship between the pressure difference (ΔP, Pa) and airflow rate (Q, m^3/s) according to the following equation (ASHRAE, 2001): where b and n are the flow coefficient and pressure exponent, respectively. Instead of performing fumigation simulations with various values of the coefficient, k_L, until the model yields the correct HLT, the loss coefficient of the internal flow domain of the Hal Ross Flour Mill model was determined, before performing fumigation simulations, by simulating the pressurization test. The loss coefficient was satisfactorily determined when the simulated pressurization test provided the flow coefficient and pressure exponent (Eq. 5) that were almost identical to the ones obtained from the actual test.

$$Q = b\Delta P^n \quad (5)$$

One MB and one SF fumigation were simulated. The simulations were unsteady state flows with a time step of one minute. At each simulation time step, the pressure value assigned to each ELZ was a summation of the average stagnation pressure, which was predicted by the external flow model and was different for different walls, and the stack effect pressure (p_s), which was calculated by:

$$p_s = (\rho_o - \rho_i)g(H_{NPL} - H) \quad (6)$$

where ρ_o is the outside air density (kg/m^3), ρ_i is the fumigant–air mixture density in the building (kg/m^3), g is the gravitational constant (9.81 m/s^2), and H is the height of the ELZ (m). H_{NPL} is the height of the neutral pressure level (NPL) which was assumed at the middle height of the mill. Provided that the inner surface temperature of the walls of the internal flow domain was specified equal to the average ambient temperature measured inside the mill, the fumigant-air mixture was obtained from the Fluent® solution. The outside air density was explicitly calculated using the ideal gas law:

$$P = \frac{\rho_o R T_o}{M} \quad (7)$$

where M is the air molecular weight of 28.966 g/mol, and R is the universal gas constant of 8.3145 (m^3-Pa/K-mol). The ambient atmospheric pressure, P (Pa), and outside air temperature, T_o (K), were obtained from the fumigation experiments. Chayaprasert et al. (2008) conducted a simulation of an entire fumigation including the fumigant introduction phase, but in the present study only sections of the exposure period, where the fumigant concentrations were decreasing, were simulated. During the MB and SF experiments which lasted 24 h, three and one HLTs were observed in different elapsed exposure times, respectively. The HLT values and corresponding elapsed exposure times are listed in Table 1. Each elapsed time was simulated separately. For each simulation, the initial concentration was set to the value observed at the beginning of the respective period. At each time step, the average concentration in the internal flow domain was recorded. To determine the HLT, the resulting average concentration data were fitted to Eq. 1.

Table 1 Comparison between the average HLTs calculated from the actual concentration curves and those from the simulated curves. The last column lists the average wind speed measured at the flour mill during each elapsed exposure time.

Fumigation	Elapsed exposure time (h)	HLT (h)		Avg. wind speed (m/s)
		Experiment	Simulation	
MB	5th-10th	111.0	29.6	1.65
MB	10th-15th	16.4	17.0	3.52
MB	17th-24th	10.2	10.5	7.12
SF	5th-24th	19.7	20.0	3.67

3. Results and discussion

The pressurization test results for the MB and SF fumigations are plotted in Figures 3a and 3b, respectively. For both tests, the flour mill was pressurized between 20 and 80 Pa. The mill could not be tested for pressure levels lower than 20 Pa because prevailing wind was interfering with the test results, yielding unstable flow rate and pressure readings. On the other hand, simulations permitted pressurization tests for this lower pressure range. It can be seen that the results of the simulated pressurization tests were in good correlation with those of the actual test. This provided prior confirmation that the internal flow domain had essentially the same gas-tightness as the actual mill building. Comparing the two fumigations, the flow coefficients (0.10 versus 0.11) and pressure exponents (0.65 versus 0.63) were similar, indicating comparable sealing effectiveness.

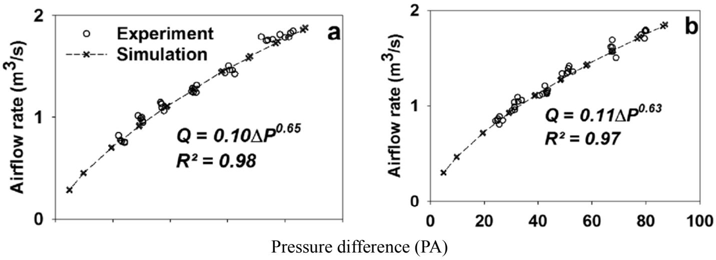

Figure 3 Experimental and simulation results of the pressurization tests for (a) MB fumigation and (b) SF fumigation.

The actual measurements of fumigant concentrations at all monitoring locations during the MB and SF fumigations are compared with the average concentrations obtained from the simulations in Figures 4a and 4b, respectively. By observation, it can be seen that the SF fumigation showed a relatively constant HLT, while the HLT for the MB fumigation changed as the fumigation progressed. Therefore, the entire exposure time of each fumigation was divided into sections according to the observed HLT values and each elapsed exposure time was simulated separately. For both fumigations, the differences in the observed concentrations within the mill were within 5 – 6 g/m^3 for most of the time, implying even fumigant distribution. At any point in time of each elapsed time, the simulated concentration curve stayed within this 5 – 6 g/m^3 band and followed the decreasing trend of the corresponding actual concentration curves relatively well. Table 1 compares the average HLTs calculated from the actual concentration curves with those from the simulated curves. While the simulation predicted a relatively long HLT (i.e., 29.6 h) for the first elapsed time of the MB fumigation, it was substantially different from the HLT calculated from the experimental concentration curves (i.e., 111 h). This substantial difference can be explained by the fact that at low fumigant leakage rates changes in the HLT are highly sensitive to changes in the gas. Given the initial concentration = 16 g/m^3 and elapsed time = 5 h, it can be shown using Eq. 1, that the final concentration will be 15.51 and 14.23 g/m^3 when the HLT is 111 and 29.6 h, respectively. While the difference in the final concentrations is approximately 8%, the difference in the HLTs is 73%. Except for the first elapsed time of the MB fumigation, the HLTs were accurately predicted with error of less than 1 h.

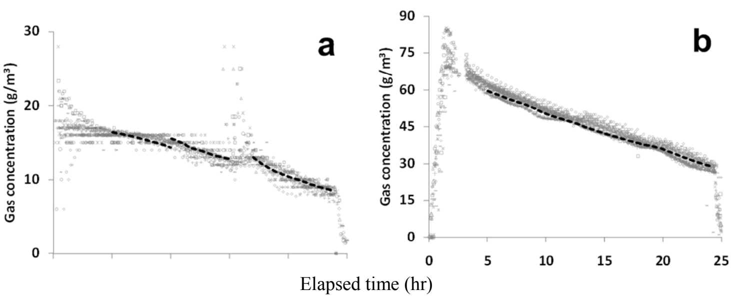

Figure 4 Comparison between the actual and average simulated gas concentrations for the (a) MB and (b) SF fumigations.

Variations in the environmental conditions, especially the wind speed, had a noticeable effect on the HLTs. The average measured wind speed for each elapsed exposure time is also given in Table 1. It is clear that the HLTs were well correlated with the wind speed measured at the flour mill during the fumigations. An argument could be made against the validity of the modeling approach of Chayaprasert et al. (2008) because these authors selectively varied the loss coefficient, k_L, until their model provided a satisfactory HLT prediction and the gas-tightness of the reference building was not directly quantified. A slightly different modeling approach was implemented in the present study. The environmental effect on fumigant leakage rates was effectively captured by the CFD model as indicated by the accurate HLT predictions after the leakage characteristic of the simulated building had been quantitatively specified to match that of the actual building. This shows that the CFD modeling techniques, mainly the implementation of ELZs and separation of the internal and external flows, used by both the previous and present studies are acceptable. In addition, exclusion of the milling equipment in the internal flow domain appeared to have negligible effect on the HLT prediction accuracy.

4. Conclusions

A CFD model of the structural fumigation process in the Hal Ross Flour Mill was formulated using the modeling methodology established by Chayaprasert et al. (2008). The model was validated using data sets from two fumigation experiments conducted in the flour mill. The actual building gas-tightness before the fumigation experiments was quantified by building pressurization tests. This quantified gas-tightness was incorporated into the model. While the model was simplified by reducing the number of external flow simulations and excluding the milling equipment in the internal flow domain, it was able to accurately predict the HLT values observed in the experiments. The result of the present study provides further validation to the modeling approach and emphasizes the importance of building pressurization test for accurate HLT prediction.

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