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Detailed and reduced form modeling of structural fumigation in food processing facilities

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Abstract

Modeling fumigation in food processing facilities is complicated as achieving a required lethal CT product is dependant on several factors such as the amount of fumigant, location of gas inlets, fans, the building leakage characteristics and the specific environmental conditions. Computationally predicting the procedure before a job is difficult as the governing parameters may vary drastically. This paper describes the extensive computational modeling of a fumigation procedure in a facility and a rather simple reduced order model to predict the concentration in the mill for dynamic planning. In the computational model the structural details are accurately modeled using ICEPAK and the gas flow pattern and other parameters are predicted using FLUENT™. The building leakage is modeled as diffusion to the outside environment governed by constants related to the structure's half life. Results have a very good match with the actual fumigation data. The reduced form model predicts the concentrations at various locations in the structure to plan the gas dosage and the fumigation process from historically available leak characteristics. The advantage of this method is its simplicity and usefulness in the preliminary prediction of a fumigation procedure as compared to the detailed modeling required in any computational model.

Key words: Fumigant, FLUENT, porous medium, leak characteristics, Reduced Order.

Introduction

Most structural fumigations in flour mills, food warehouses, food processing facilities, and feed manufacturing plants used methyl-bromide as the major fumigant. The phase-out of this led the industry to seek alternative fumigation procedures. Few of the alternatives are heat treatment, ECO$_2$Fume® (98 % CO_2 with 2 % phosphine), Profume® (Sulfuryl fluoride) and a combination of heat treatment, CO_2 and ECO$_2$Fume®. These gases require holding lethal concentrations and high temperature for long exposure periods to achieve over 95 % mortality. The fumigation process can be better optimized and controlled only if we have a better understanding of the physics and dynamics of gas movement in the fumigated space during fumigation. Also it is important to understand the effects of parameters such as gas properties and structural and

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environmental factors on fumigation. This will allow better management of the fumigation procedure and also enable design of automatic control systems to monitor and govern the precise gas dosage.

Efficient fumigation procedure involves the delivery of the precise amount of lethal concentration and exposure per unit volume at the target infestation spots with the minimum fumigant dosage rate (Monro 1969). This can be done by designing a site-specific fumigation plan that will take into consideration the site plans, storage structures, stored commodity properties, environmental conditions (ambient temperature, relative humidity, wind speed and direction, solar heat load), structure pest infestation level, pest(s) and their biology, and fumigant characteristics (physical properties, mode of action, permissible exposure limits).(Dow Agrosciences,2003) Computational modeling using FLUENT attempts to closely model this considering all parameters while the Reduced Order Model is designed to generate approximate predictions for dynamic planning of a fumigation job. Results of these models are validated with data from a fumigation job described below.

Experimental measurements

Fumigation experiments were conducted on a facility with fumigant- Sulfuryl fluoride. This facility typically is infected with Indian Meal Moth (IMM) and the Red Flour Beetle (RFB). The facility consists of a main building with equipment such as grinders, sifters and bench airlocks, and several other structures such as the storage, packaging and office facilities. Figure 1 shows a typical cross-section of a mill floor. There are six such floors and other attached storage structures. The exposed walls of the building are sealed to prevent gas loss, high leak areas are separated. Fumigant doses are shot at several locations. Fans are installed for good circulation of fumigant. A data acquisition system comprising of a laptop, two FieldPoint modules, a Fluke data logger, a Vaisala temperature/relative humidity sensor, a NoveLynx pressure sensor, and a R.M. Young 3D anemometer measured the physical flow properties in the mill. A Hobo weather station located on the roof of the building monitored barometric pressure, natural wind speed and direction, temperature, relative humidity, and solar radiation. Concentration at several key locations was measured using Fumiscopes (Key Chemical and Equipement Co.Clearwater,FL), tubing and a purge system. Figure 2 shows is a schematic showing gas flow in the building. The concentration plots at on each floor are presented

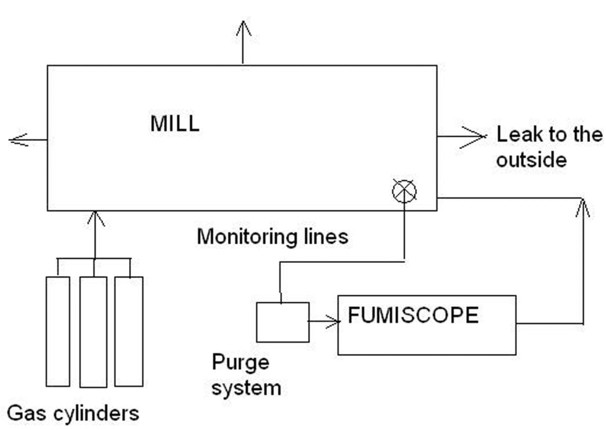


Figure 1. Schematic showing gas flow pattern in the building.

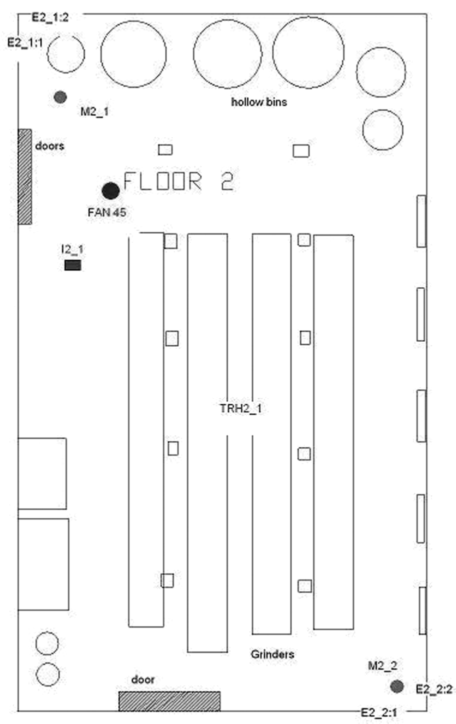


Figure 2. Floor plan for second floor of the mill.

in Figures 5-10 in units Oz/TCF. Our aim in this work is to replicate these plots.

Porous medium model

A critical component of the modeling effort is the representation of the major and minor equipment inside the mill building. The larger structures are relatively straightforward to represent in a computational model. However, much of the mill space is densely occupied by smaller equipment such as grinders and sifters as well as dense forests of pipes and cables. Since the length scales of these structures are much smaller than those of the building and rooms, it becomes computationally intractable to represent these structures faithfully. Modeling approximations are necessary to represent these small scales to engineering precision.

The smaller equipment in the mill are represented using a porous medium model (Bejan 1984), (Kaviany 1995) with known porosity and permeability values. The porous medium models mimic the flow rate/ pressure drop characteristics of aggregates of small-scale geometric features without resolving all the geometric detail. The porous properties are calculated computationally by modeling repeating rows of machines as periodic units (Patankar et al., 1977) with similar flow velocities past them. Figure 3 shows one such unit of a grinder.

Computational model using FLUENT

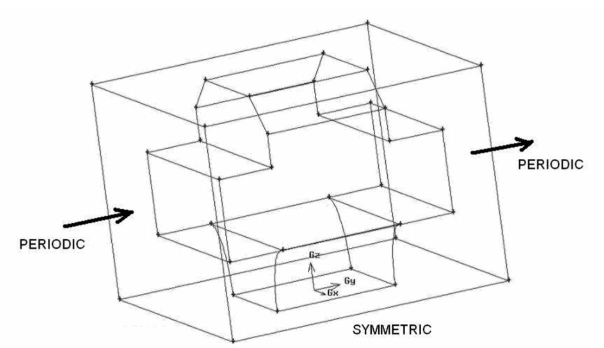
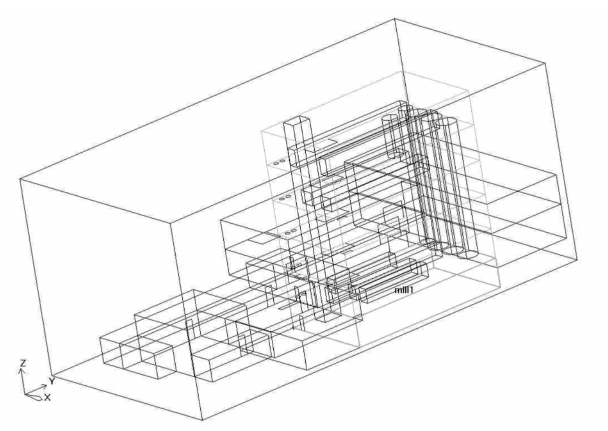


Figure 3. Repeating Unit representing rows of Grinders

The mill structure is modeled in ICEPAK. As shown in Figure 4 each room of the facility is modeled as a cuboidal fluid medium separated by solid walls. The main repeating machinery are modeled as porous media as discussed earlier. The dimensions of each of these has been obtained from industry sources and also manually measured during the fumigation jobs. Small blocks are made representing mass inlets and fans with mass and momentum sources. The locations of these is exactly the same as that in the fumigation job but the size of these are larger as the real mass sources are only tubing coming from the gas cylinders. Fans are the standard 1.5ft radius industrial fans and these have been represented as blocks of the same dimension. The outer walls of the mill are modeled as impermeable walls to which leakage properties will be assigned in FLUENT. A hexahedral mesh is automatically using ICEPAK. The mesh quality and skewness properties were checked.

Figure 4. ICEPAK Representation of the milling



facility and adjoining structures.

Modeling fumigant flow would involve modeling species transport and fluid flow in the domain along with gas leakage to the outside. The mesh generated using ICEPAK is imported into FLUENT. FLUENT solves the Navier Stokes equations along with the species conservation equation listed below on these cells.

$$\frac{\partial\rho}{\partial t}+\nabla.\left(\rho\bar{v}\right)=S_m \qquad (1)$$

$$\frac{\partial}{\partial t}+\nabla.\left(\rho\,\overline{vv}\right)-\nabla p+\nabla.\tau+\rho\bar{g}+\bar{F} \qquad (2)$$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right)+\nabla\left(\rho\bar{v}Y_i\right)=-\nabla\bar{J}_i+R_i+S_i \qquad (3)$$

where S_m is the mass added into the domain and p is the static pressure, v velocity, ô is the stress tensor and ñg and F are the gravitational and external body forces respectively. F also contains the model dependant source terms such as the porous media and user defined sources. In equation (3) R_i is the net rate of production of species i by chemical reaction and S_i is the rate of creation by any user defined sources.

Fumigant doses and fan velocities are accurately specified. The model used is unsteady with incompressible ideal gas properties. The flow in the domain can be considered laminar but there might be areas of low turbulence near the fan and other locations. Therefore a simple turbulence model- turbulent mixing length is used to model the flow. Table 1 lists the material properties of Profume (Sulfuryl Flouride). Variability in gas dosage and fan velocities are considered by specifying user defined functions for mass sources and fans.

Owing to the complexity involved, building leakage is modeled independent of the leak area, seal quality and environmental conditions and defined only by a parameter called the "leak characteristic". This parameter can be estimated separately for different parts of the mill, thereby estimating half life characteristics for different parts of the building. The relation between the above parameters and this quantity can be derived later. Although, this is quite difficult as it would require several fumigations with one parameter varying while holding the others constant.

From the fumigation experiments concentration data is available at key locations. The equation for mass conservation in a structure after the mass addition can be written as

$$V\frac{dC}{dt}\ hAC \qquad (4)$$

$$C\ C_o e^{\frac{hA}{v}t} \qquad (5)$$

ignoring the gas flow to the other structure. Therefore on fitting an exponential curve to the down slope of the concentration data as shown in the Figure 18, the leak coefficient can be estimated from the slope. Here A and V are the exposed area and volume of the structure respectively. For each room of the building such leak characteristics can be estimated from the experimental data. Figure 5 also show the values of leak characteristics used at different locations. This although is only an estimate and the real leak characteristic may be quite different.

A leak equivalent to the total mass loss rate averaged over the whole area is assigned to the entire exposed wall. The walls exposed to the outside are assumed to have a leak proportional to the concentration close to the wall, essentially modeling pure diffusion of gas to the outside. The pressure build in the structure is low compared to the magnitude of the absolute pressure and can

Table 1. Material Properties for air and fumigant

	Units	Air	Fumigant
Density	Kg/m^3	1.225	4.227
C_p	J/kg-K	1005	669
Molecular weight	Kg/kg-mol	28.966	102.06
Thermal Conductivity	W/m-K	0.025	0.01182
Viscosity	$N\text{-}s/m^2$	1.73E-05	1.47E-04

be ignored and hence the assumption of pure diffusion is valid.

Figures 5 shows fumigation concentration data (discrete points) superimposed with FLUENT results (continuous data). The time axis in all these graphs is presented in seconds with zero being the beginning of the first gas shot.

Results

All the graphs show very close match with the experiments-mainly the peaks and decay patterns are replicated closely. Gas concentrations are also accurately replicated in areas with no gas addition. Good match between the experiments and FLUENT data validates our assumption that the

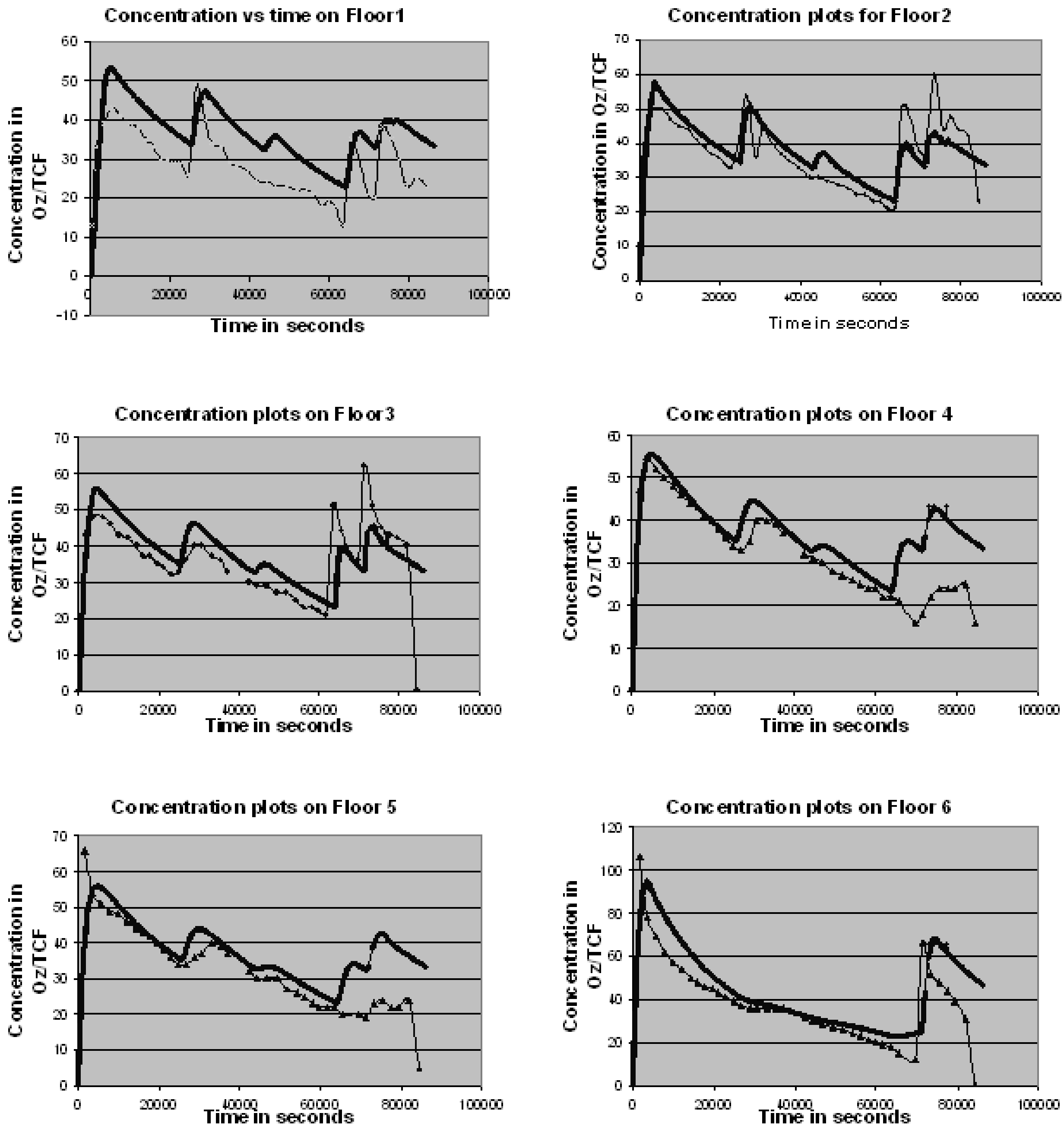


Figure 5. Fluent prediction of concentrations (solids lines) and Experimental data(discrete points) at different locations.

main contribution to the slope of the curves is the leak to the outside of the building. Equal peaks in all graphs show very good mixing in the whole of the mill.

The results also show that the assumption that the leak is proportional to the concentration of the structures is validated. The influence of external parameters such as wind is not seen in the results. This might be due to good sealing of the building or that the uniform wind velocities of about 4m/s have a constant influence on the leak parameter. Gravity effects were not included in the FLUENT model and the results also show no influence of gravity while the fans in the domain are running. The effect of external parameters is embedded in the leak parameters. Constant leak values are used over the 24 hour span and results match. This could be due to the fact that the variation in external parameters in low during this time span. Also the pressure built in the system is low. A relation between the leak constants and pressure difference between the inside and outside can be cast if data is available over several external conditions.

The slight mismatch is due to error in leak coefficients, errors in measuring data using the Fumiscope, difference in open volume specified in the model as compared to the real open volume in the building.

Reduced order modeling of fumigation

As seen in the previous section, modeling the structure and computationally simulating the fumigation procedure is expensive and time consuming. It is not affordable and practical to predict the parameters before the fumigation. A lot of parameters such as the amount of sealing, placement of gas inlets, fans are dependant on the specific mill and fumigation. This shortcoming necessitates a simpler model for approximate prediction of various flow parameters mainly the concentration of gas at difference locations. The main goal is to predict the concentration at various locations in the mill to calculate the CT product. This would help in dynamically planning the gas shots and optimizing the amount of fumigant used and several other factors.

Mathematical representation of fumigation

In a structure, the rate of increase of mass of the structure is equal to the sum of mass addition, the amount of fumigant lost to the outside and the amount of gas leaked into the other parts of the building. The mass can be represented as a product of concentration and volume in the structure. The loss to the outside is assumed to be proportional to the near wall concentration. One major assumption involved in this modeling is assuming the concentration of the whole room is the same. This assumption is reasonable as the concentrations equilibrate in the span of about 1 minute. The amount of mass lost is also dependant on the exposed area of the wall. The loss to other parts of the building can be represented as a pure diffusion term governed by a parameter. Further complexity in modeling gas flow can be incorporated by decoupling these coefficients and increasing the degree of freedom. This may capture both the diffusion of gas and any convective gas flow due to a directional flow field.

$$\frac{dM_i}{dt} = V\frac{dC_i}{dt} = M_{in,i} - h_{leak}.A_{leak}.C_i - h_i.A_{ij}.(C_i - C_j) \tag{6}$$

where C_i is the concentration of the ith room and C_j is the concentration of the adjoining room.

This simple model neglects detailed gas flow patterns and can be used only as an initial prediction. Several other approximations are inherent in the model due to the simplicity assumed in the physics.

To predict the concentration at several locations in the building, such equations are written for locations of interest and locations of mass addition. For locations where there is no mass addition the first term in the equation is absent. This would yield a set of linearly dependant equations. The coefficients would be a combination of leak coefficients of the structures to the outside and to the adjacent structures. The coefficients in equation corresponding to the leak to the outside are related to the half life characteristics of the building. An initial estimate of these coefficients can be got from the historical fumigation data assuming the similar conditions. These coefficients can also be dynamically calculated by observing concentration decay data during the initial hours of the current fumigation. The coefficients corresponding to the flow between structures are dependant on the specific flow characteristics and concentration difference between structures and no prior approximation is possible. Although, a very rough estimate can be made. If the mass added and the volume of two attached structures is similar in magnitude the third component would be negligible since the concentration of the two adjoining structures would be similar. In such situations the coefficients can be assumed as zero. In case of no mass source in the room, all the gas flows in from other adjoint rooms. In such a scenario we can assume the constant to be some large number. It is observed that from the current data it is reasonable for this number to be in the range > = 1.

Results

The Figures 6 to 11 show the comparison between the FLUENT plots and the concentrations predicted using the Reduced Order Model. The leak coefficients were assumed to be only about half of those specified in FLUENT to account for the approximations involved. The flow coefficients connecting floors were specified as 1 enabling good mixing characteristics. Accurate estimate of this number can be found by curve fitting the linearly independent equations to the FLUENT data. Such a process is quite cumbersome and is not considered for the work presented in this paper. Very close match between the two methods is observed. Results in comparison with FLUENT data are presented to avail the advantage of accurate information. It is observed that leak values approximately specified in the range of values traditionally observed also yield very close matches.

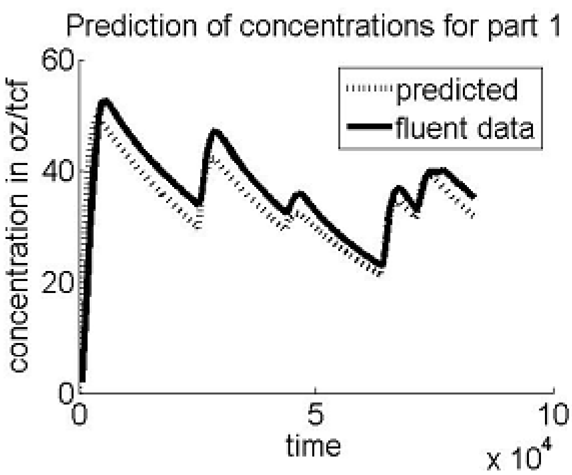


Figure 6. Reduced order model prediction of floor1.

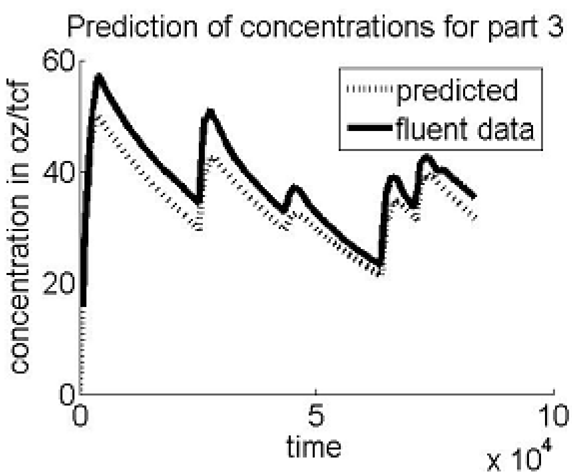


Figure 7. Reduced order model prediction of floor2.

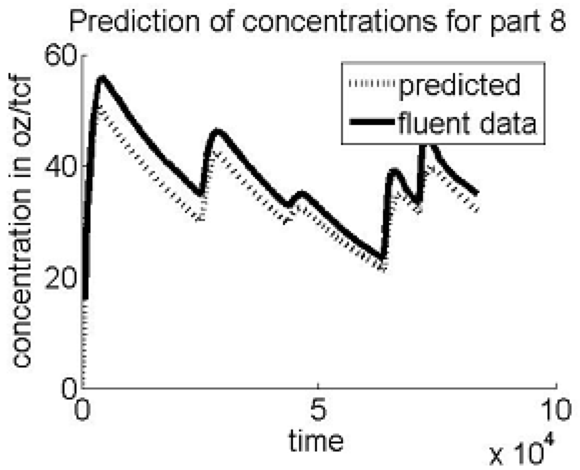


Figure 8. Reduced order model prediction of floor3.

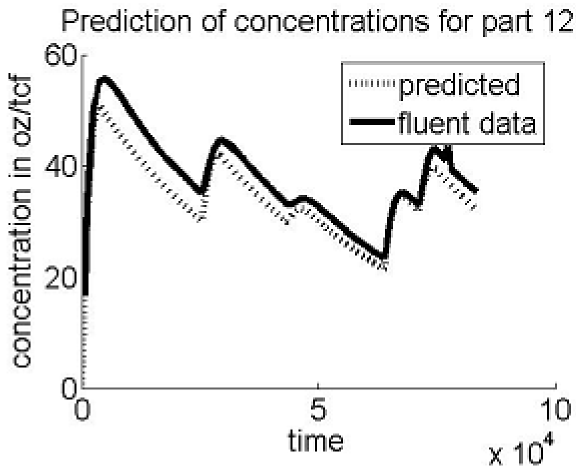


Figure 9. Reduced order model prediction of floor4.

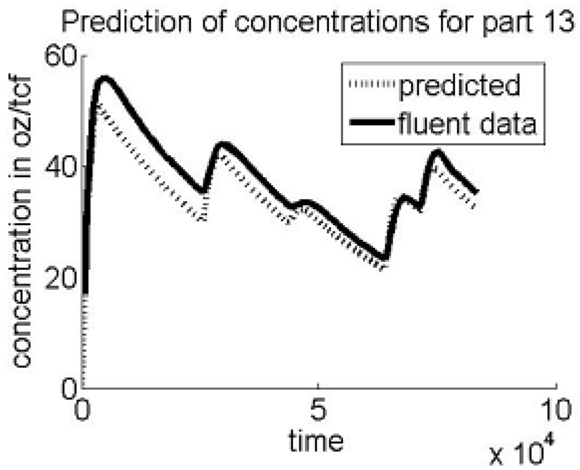


Figure 10. Reduced order model prediction of floor5.

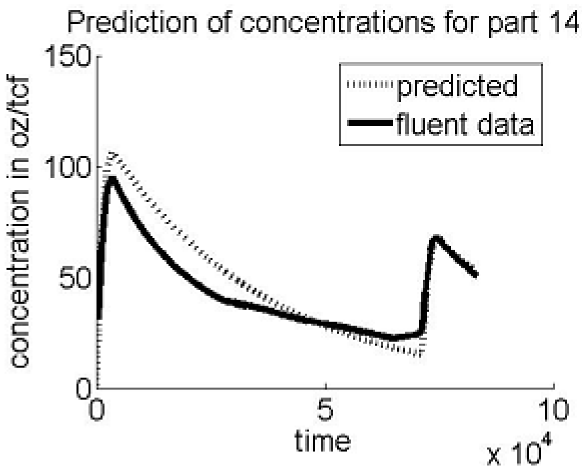


Figure 11. Reduced order model prediction of floor6.

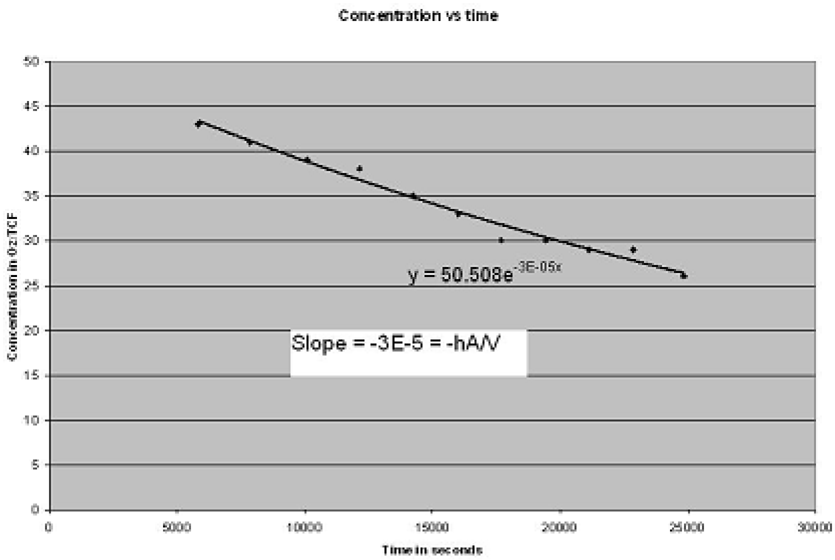


Figure 12. Exponential curve fit for downslope to determine leak coefficients

Conclusion

This work presented the results of two methods developed to computationally model a fumigation process. Extensive computational simulation of the fumigation procedure yields accurate prediction of the fluid flow patterns and gas concentration. Although this procedure is expensive and cannot be done in time for planning a fumigation. Very detailed information regarding gas flow contours, gas velocities etc can be estimated with accurate representation of structure. The reduced order model can be used to obtain information regarding concentrations at various locations in the fumigation space using information regarding current gas dosage and traditionally observed leakage characteristics of the building. Flow between connected rooms is governed by constants. Inaccurate estimate of these constants can result in drastic variation in the resulting concentration plots. Hence it can be concluded that this mathematical representation of the fumigation process is not sufficient and does not accurately replicate the complex gas flow. The physics involved is more complex and only a simple initial prediction can be achieved from this reduced order model. To get accurate gas flow patterns and concentration a detailed Fluent model is required.

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