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Near and far field contamination modeling in a large scale enclosure: Fire Dynamics Simulator comparisons with measured observations

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Abstract

The occurrence of a fire, no matter how small, often exposes objects to significant levels of contamination from the products of combustion. The production and dispersal of these contaminants has been an issue of relevance in the field of fire science for many years, though little work has been done to examine the contamination levels accumulated within an enclosure some time after an incident. This phenomenon is of great importance when considering the consequences associated with even low level contamination of sensitive materials, such as food, pharmaceuticals, clothing, electrical equipment, etc. Not only does such exposure present a localized hazard, but also the shipment of contaminated goods places distant recipients at risk.

It is the intent of this paper to use a well-founded computational fluid dynamic (CFD) program, the Fire Dynamics Simulator (FDS), a large eddy simulation (LES) code developed by National Institute of Standards and Technology (NIST), to model smoke dispersion in order to assess the subject of air contamination and post fire surface contamination in a warehouse facility. Measured results are then compared with the results from the FDS model. Two components are examined: the production rate of contaminates and the trajectory of contaminates caused by the forced ventilation conditions. Each plays an important role in determining the extent to which the products of combustion are dispersed and the levels to which products are exposed to the contaminants throughout the enclosure. The model results indicate a good first-order approximation to the measured surface contamination levels. The proper application of the FDS model can provide a cost and time efficient means of evaluating contamination levels within a defined volume.

Keywords: Fire Dynamics Simulator; Contamination; Computational fluid dynamics

1. Objectives

This paper examines a case study in which toxic by-products of smoldering combustion are dispersed throughout a large warehouse by numerous forced ventilation systems and air handling equipment. A computational fluid dynamics model was constructed and run to determine the extent of smoke contamination within the enclosure. The model allows for the migration of the contaminants to be examined at all areas within the enclosure as a function of time. The results of the model are compared to actual surface contamination samples from the case study.

2. Overview of the FDS model

The Fire Dynamics Simulator (FDS) was used to perform the computational analysis. FDS is a program, which is the result of research and development at the National Institute of Standards and Technology (NIST), Building and Fire Research Laboratory. FDS utilizes a large eddy simulation (LES) technique to model turbulence within the fluid dynamics model. The methodology provides a computationally efficient method of calculating fluid flow and temperatures in a fire environment.

FDS is a public domain software program and is available free of charge from NIST. A review of the available scientific literature directly related to the development, use, and validation of FDS demonstrates acceptance of the code for both research and practical application. In addition, the theory behind the FDS code has been described in peer-reviewed documents, along with validation studies and examples of practical applications.

An FDS model requires several inputs by the user: (1) the geometry of the area of fire origin and all adjacent spaces, (2) passive and active ventilation locations and magnitudes, (3) material properties for the compartment boundaries, and (4) the fire specification (e.g. location, energy release, and smoke production as a function of time). These inputs and the underlying

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physical calculations of the code allow for a fire and the products of combustion to be mathematically modeled.

In this case, the fluid flows, which transport the contaminants through the space, are the issue of importance. The dominant mode of transfer, which would affect the dispersion of contaminates, is the active and passive ventilation contained within the enclosure and the air handling equipment. The ventilation in the enclosure is composed of two components: the active ventilation located on the roof and passive ventilation located along the wall and the roof. The air handling equipment consists of fans suspended from the ceiling and mounted to the building support columns as well as the process equipment, which has a positive or negative draw. Each of these items plays a crucial role in the distribution of the contaminants throughout the space.

3. Literature review of input parameters

It is first necessary to describe the manner in which the contaminates are introduced into the system. In the current study, literature values are used to describe the smoldering source term. Specifically, typical smolder propagation rates of pinewood and the smoke yield under smoldering conditions were researched. Typical smolder propagation rates within the literature varied between 0.001 and 0.01 cm/s [1]. The smoke yield, which is defined as the mass of smoke produced per unit mass of fuel $\left(\frac{g_{\text{smoke}}}{g_{\text{fuel}}}\right)$, varied between 3% and 17% for pyrolysis and smoldering conditions [2]. An average of the range of literature values for smoke yield, 10%, and a conservative smolder velocity of 0.001 cm/s were chosen to describe the smoke production term that is utilized in the FDS model.

4. Smoldering source in FDS

The production of smoke is computed as a function of time based on the propagation rate of the smolder front and the burning objects geometric configuration. The constant smolder velocity extracted from existing literature is used to define this process. Initially, the smolder propagation is computed based on a radial spread in all directions, i.e. a growing sphere. Once the smoldering front reaches the external bounds of the object, the propagation computation is reduced to represent spread solely along the length of the object. Using the results from the spread model and the material properties of the object, an equivalent mass loss is computed for a given time interval.

The equivalent mass loss is divided by the running time at each interval, converting it into a transient mass loss rate of fuel. The average value for the smoke yield, 10%, is then used in conjunction with the mass loss rate of fuel to give a mass production rate of smoke such that

$$\dot{m}_{\text{f}} = \frac{m_{\text{f}_\text{o}} - m_{\text{f}_i}}{t_i} \quad \text{and} \quad \dot{m}_{\text{s}} = 0.10\dot{m}_{\text{f}}$$

where t_i is the time elapsed, m_{f_o} the original mass of the fuel, m_{f_i} the mass of the fuel at time t_i, and $\dot{m}_{\text{s}}$ is the mass of smoke produced. Fig. 1 illustrates the mass-burning rate of smoke as a function of time.

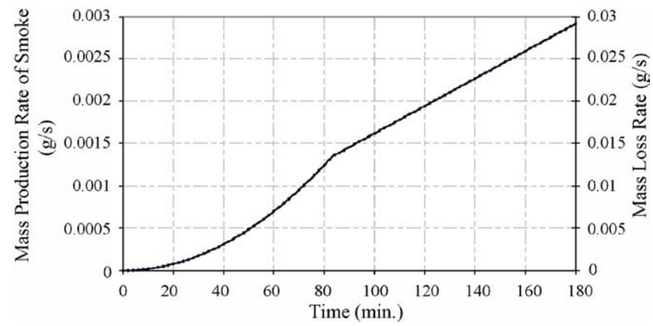

Fig. 1. Source production and mass loss rate as a function of time.

The smoke is introduced into the volume of the enclosure using the velocity ramp feature of FDS. A velocity ramp allows the user to specify the rate at which a fluid, in this case smoke, is being emitted from a source as a function of time. The mass production rate of smoke is converted into a velocity using the size of the smoldering source prescribed in the model and the density of air, Eq. (1),

$$V = \frac{\dot{m}}{\rho A} \tag{1}$$

where V is the velocity, $\dot{m}$ the mass flux, ρ the density of air, and A is the area of the smoldering source. V is the velocity at which the smoke is released from the smoldering source and enters the enclosure. The smoke density is assumed to be that of air. This methodology allows the distribution of contaminates to be examined based solely on the environmental conditions. It is assumed that the air movement induced by the ventilation system plays the dominant role in dispersion and the buoyant forces brought forth by any temperature differences can be neglected. The small amount of smoke produced and the weak buoyant forces associated with smoldering combustion further support the use of this assumption for the case study.

5. Analysis

The FDS model was used to examine the dispersive nature of the smoke as a result of the enclosures forced ventilation system. Particular attention was placed on specific locations within the enclosure consistent with the measured data. Point measurements are extracted from the FDS model based on the average mass fraction within a particular volumetric grid cell. The cell size utilized within the model is 0.478 m × 0.983 m × 0.813 m corresponding to the X, Y, and Z dimensions, respectively. In order to compare the FDS results with the measured results it is necessary to convert the predicted mass fraction of smoke into a density of smoke within the volume using the dimensions of the grid cell and the properties of air. Next, the mass of smoke per unit volume is converted into a mass of smoke per unit area by dividing it by the height of the grid cell (Z dimension).

The experimental samples taken in the case study examined eight specific polycyclic aromatic hydrocarbons (PAHs) and reported a total PAH value for each location in units of pg/cm^2. The mass of smoke per unit area computed from output of the FDS model is further converted into a PAH value by incorporat-

Table 1
Summary of literature values of PAH emission rates for burning pinewood

Polycyclic aromatic hydrocarbons (PAH)	Emission rate per mass fuel (mg/kg)
Phenanthrene	0.47
Anthracene	0.051
Fluoranthene	1.24
Pyrene	1.59
Benzacenaphthylene	0.57
Benzofluorene	0.056
Chrysene/triphenylene	0.98
Benzopyrene	0.62
Total	5.577

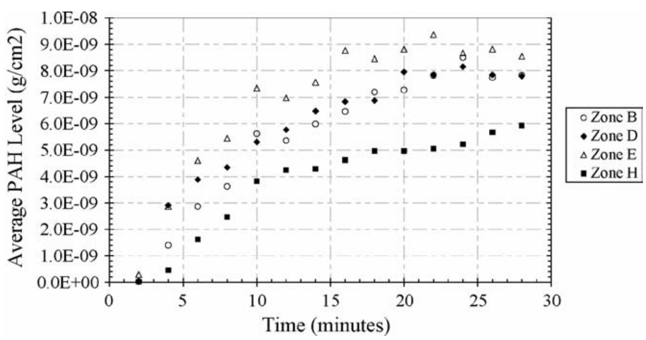

Fig. 2. Convergence of PAH level to steady value for various zones.

ing literature values for emission rates of organic compounds in burning pinewood (Table 1) with the mass loss rate of the fuel and the smoke yield.

Prior to comparing the model results with the sampled values for surface contamination, an overall assessment of the dynamic mixing process is conducted. The PAH values extracted from the model are monitored for the duration of the experiment. The results from the model indicate that within 20–25 min of initiation, the distribution of contaminates remains relatively steady. The relatively steady-state contamination level is directly related to the samples geometric positioning within the enclosure. An example of is provided in Fig. 2, with the presentation limited to four zones for clarity. This initial ramp up period is observed at all locations within the enclosure. Contamination levels increase slightly with time but the change is assumed negligible for the purpose of this study.

To further examine this converging phenomenon an additional calculation is performed which treats the entire enclosure as a simple bulk-mixing problem. The equations used for the bulk-mixing analysis are defined as follows:

$$\frac{dY}{dt} = Q_{\text{in}} - Q_{\text{out}}, \quad \text{where } Q_{\text{out}} = q\frac{Y(t)}{V} \tag{2}$$

and Q is defined as the flow into and out of the enclosure, Y the mass of the air and smoke within the enclosure at a given time, and V is the enclosure volume. By algebraic manipulation and integration Eq. (2) can be rewritten as:

$$Y(t) = \frac{VQ_{\text{in}}}{q}(1 - e^{-tq/V}) \tag{3}$$

Solving the equation using the following values: $V = 96{,}300\ \text{m}^3$; Q_{in}, the production rate of smoke = 0.0078 g/min; q, the vent flow rate in/out of the enclosure = $23{,}800\ \text{m}^3/\text{min}$. This yields Eq. (4), which is plotted over time in Fig. 3.

$$Y(t) = 0.0316(1 - e^{-0.247t}) \tag{4}$$

The results from the bulk-mixing calculation indicate the concentration is approaching steady-state conditions approximately 20 min after initiation (Fig. 3). This bulk-mixing calculation serves as a check on the model predictions to attain steady-state conditions.

6. Results

A quantitative analysis has been conducted between the measured and modeled results. The analysis consisted of breaking the large enclosure into nine zones. Average values from each zone were computed. The measured results consisted of eight PAHs representative of surface contamination levels. FDS was used to model the smoke production and dispersion throughout the enclosure. Literature values were used to present the modeled results in the same form as the measured results.

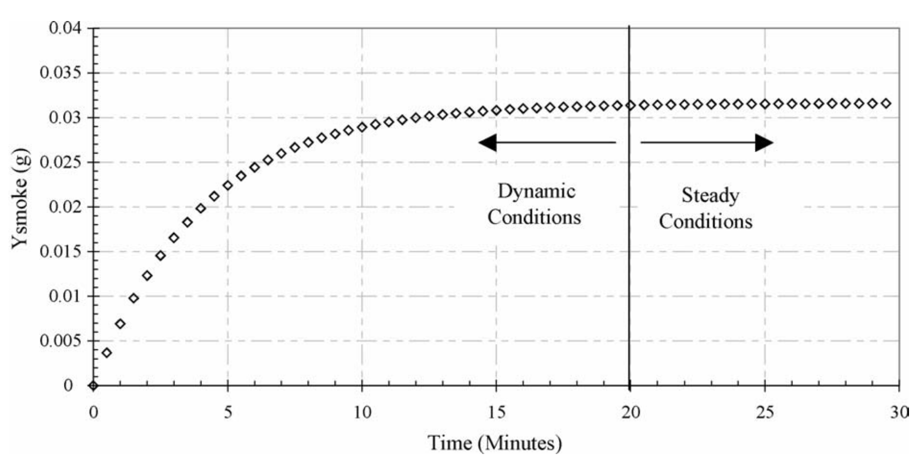

Fig. 3. Environmental contamination level using bulk-mixing calculation.

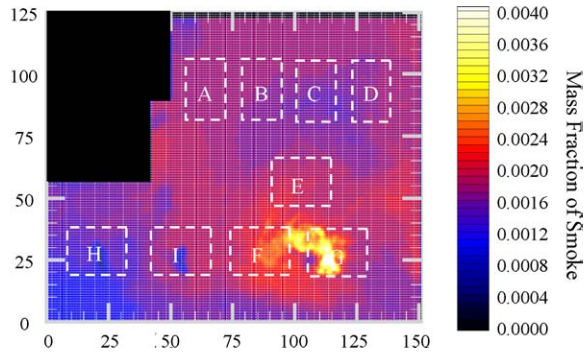

Fig. 4. FDS steady smoke concentration distribution and zone layout (spatial dimensions are in meters).

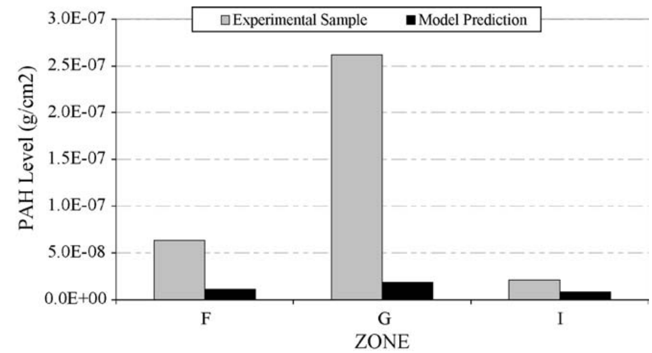

Fig. 6. Contamination level for zones located in the vicinity of the source.

Model results were extracted from FDS at locations similar to those measured. The evolution, concentration, and relative values of contamination were examined as a function of time within the FDS model for each zone. The quantitative image, shown in Fig. 4, is representative of the steady spatial distribution of the smoke/contaminates throughout the enclosure as predicted by the FDS model and depicts the location of the nine zones examined in this study. This figure also shows that there is variation in contamination levels throughout the warehouse due to the turbulent nature of the ventilation system.

A comparison of the nine zones examined in this study provides insight into the models ability to predict surface and fluid contamination levels. A side-by-side presentation of the measured and modeled surface contamination levels for this study is provided in Fig. 5. The accuracy of the model varies based on the geometric location of the zone with respect to the source. However, the overall model results serve as a good qualitative indicator of contamination distribution levels throughout the enclosure. It is evident that the modeled surface contamination levels differ significantly from those sampled in the enclosure near the source location. The results of the model in areas away from the source provide a more accurate depiction of the actual contamination levels. The zones are separated into two groups representative of the near and far field, to better examine the observed differences in contamination levels.

Three zones (F, G, and I) are grouped together to represent the contamination levels near the source. The measured and modeled surface contamination levels for these zones are compared in Fig. 6. Similar trends are observed in the near source zones between the experimental and predicted results. The relative magnitude of contamination levels between zones is consistent internally. Measured contamination levels are much larger then those predicated by the FDS model.

There are several factors that are not accounted for in the model that play a significant role in the surface deposition within the zones close to the source. A detailed deposition model is not included in the model which takes into account the local velocity and the mass of the contaminants. Additionally, though the majority of contaminates were a result of a smoldering source, the combustion did transition to flaming. Once flaming occurred several sprinklers actuated in the vicinity of the source. The introduction of water can play a significant role in the dynamics associated with surface deposition. The dispersion of smoke that was previously dominated by the enclosures ventilation system would be greatly affected by water released from the sprinklers coming in direct contact with airborne particulate. Contaminates that are being forcibly settled out of the air would deposit on surfaces near the source. In addition, the interaction of the fire department near the source may have interfered with the natural deposition of smoke. Such phenomenon would explain the increased deposition levels that are observed in the case study.

The six remaining zones (A, B, C, D, E, and H) are grouped together to examine the far field contamination levels. The measured and modeled surface contamination levels for these zones are compared in Fig. 7. Far from the source, the model predictions are consistently higher then those actually measured

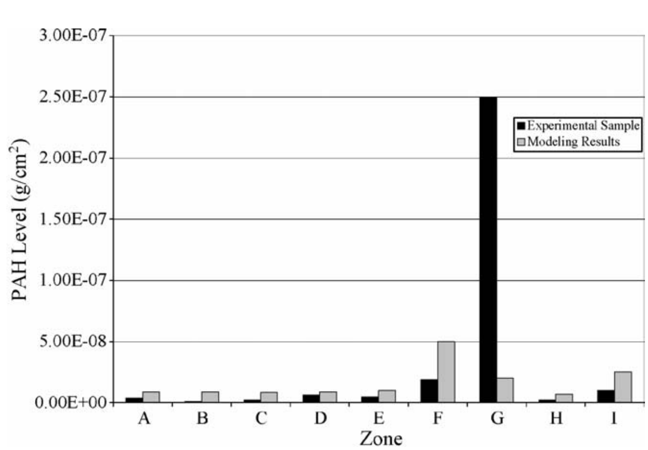

Fig. 5. Modeled and measured surface contamination levels for the nine zones.

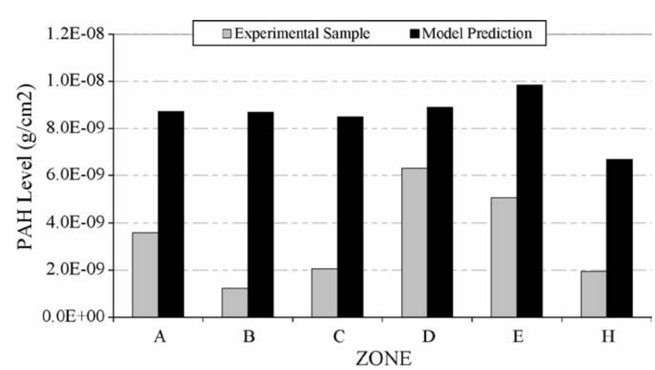

Fig. 7. Contamination level for zones located far from source.

within the enclosure and remain relatively constant from zone to zone. The measured deposition levels vary considerably between zones. There does not appear to be a linear relationship between the measured results and the predicted results when solely examining concentration, though they are on the same order of magnitude.

7. Conclusion

The level of contaminates predicted by the FDS model indicates a good first-order approximation of the measured accumulated surface contamination levels. The near steady exposure conditions within the enclosure further suggest that the dispersion model serves as a useful tool in examining the distribution of surface contaminates. The discrepancy between the results of model and the measured values imply that several factors that are not accounted for in the model make it difficult to determine the exact accumulated values, such as particle agglomeration, settling, and sprinkler interaction. However, the model accurately depicts the presence of contaminates and the relative contamination levels throughout the enclosure. A more detailed examination of dynamic surface deposition may be useful in determining a correction factor that will allow for a more precise modeling tool. The results of this case study allow for a first-order approximation to be made and provide a good foundation for future work regarding the modeling of surface contamination.

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