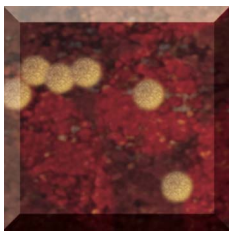

Simulation of Bio-Agent Release in a Room or Office Space

Stephen M. Scorpio, Robert P. Roger, and Alan Brandt

Indoor toxic agent release has become a possibility of great concern. This article presents a numerical flow-field dispersion model used to predict the spatial and temporal distribution of toxins in an enclosed area. The approach is based on assumptions pertaining to the entrainment of small particulates (with properties similar to those of anthrax spores) into the circulation airflow in a typical office. The model simulates the entrainment of spores into the turbulent boundary layer and subsequent transport and dispersion within and out of the room. For the illustrative example given here, it was found that spores would disperse through the room and into the hallway in approximately 5 to 10 min.

INTRODUCTION

Today, there is an increased national awareness of the possibility of toxic agent releases in interior building spaces. Of specific interest, owing to recent events, is the spread of anthrax from contaminated letters into the office circulation airflow. One key aspect for assessing the effects of such releases and for planning mitigation and prevention strategies is the pattern of spread within rooms and buildings. This article describes an APL-developed simulation tool that predicts the propagation and dispersion of particulates through internal building spaces. In addition, the model postulates a mechanism by which particulates, initially deposited on a horizontal surface, are entrained into the ambient air current.

An analysis of the spatial and temporal distribution of a toxic release in a typical room/office has been performed to illustrate the applicability of numerical flow-field dispersion calculations. These calculations provide a basis for studies of agent detection, mitigation, sensor response and placement, ventilation strategies, and evacuation procedures. The analysis was based on assumptions concerning the entrainment of small particulates (with properties similar to those of anthrax spores) into the circulation airflow in a typical office. The study reported in this article provides the methodology for such a simulation, which is illustrated by an example of a hypothetical bio-agent release.

HYPOTHETICAL SCENARIO

The analysis was based on the following scenario. Some anthrax spores have been deposited on a tabletop. The mass and distribution of spores on the table is initially known. The spores are exposed to airflow in the room generated by the ventilation system. Depending on the flow conditions, some of the spores may lift off the tabletop and propagate through the room. The problem is then to determine the rate at which spores

will be lifted from the tabletop and propagate throughout the room.

Anthrax spores are roughly spherical and 2–6 μm in diameter,[1] with a mass of ≈1 pg (personal communication, A. Scorpio, U.S. Army Medical Research Institute of Infectious Diseases, Ft. Detrick, MD, Jan 2002) as shown in Fig. 1.

As an example problem, the following parameters are used:

- One gram of spores is evenly distributed on a 10×10 cm area of the tabletop.
- The average mass of one spore = 1 pg.
- The average diameter of one spore = 5 μm.
- The volume of air occupied by spores on the table $V = 10\text{ cm} \times 10\text{ cm} \times (5 \times 10^{-4}\text{ cm}) = 0.05\text{ cm}^3$.
- The number of spores on the table $N_0 = 1 \times 10^{12}$.
- Ambient airflow outside the boundary layer U_∞ = 1 cm/s.
- The patch of spores is 100 cm from the edge of the table (the start of the boundary layer profile).

MODELING AND SIMULATION

Two aspects of the problem are considered: the entrainment of spores from the tabletop into the ambient room airflow, and transport of the entrained spores within and out of the room. The former requires consideration of entrainment into the air boundary layer along the table, and analysis is based on a turbulent boundary layer model. Flow within the room is modeled using a commercial three-dimensional, computational fluid dynamics (CFD) numerical model with a typical office-like layout and airflow rates.

The exact mechanism or mechanisms by which small particulates would be lifted off and entrained into the ambient airflow is not known with certainty. Three fundamental mechanisms were considered: turbulent diffusion into the boundary layer, liftoff due to mean vertical velocity in the boundary sublayer, and velocity imparted to the particles by near-wall turbulent fluctuations. Only the third mechanism proved to be sufficient to entrain particles of the size considered. Other mechanisms related to wall roughness, horizontal particle motions, particle shape, and electrostatic and other adhesion/repulsion forces require further investigation.

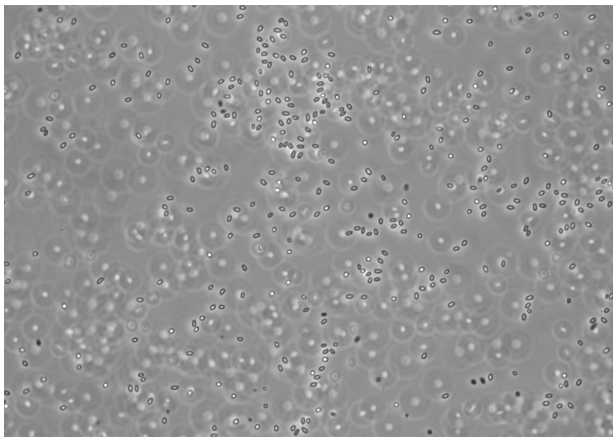

Figure 1. Anthrax spores at 1000X magnification. (Photograph courtesy of A. Scorpio, U.S. Army Medical Research Institute of Infectious Diseases.)

Near-Wall Turbulent Fluctuations

The ambient airflow over the table is defined as U_∞. The spores are exposed to the turbulent boundary layer flow near the table surface. It is hypothesized that anthrax spores are lifted off the table at a rate proportional to the vertical turbulent fluctuation in the boundary layer.

In a statistical sense, the root mean square (rms) vertical velocity will be directed toward or away from the table and thus will hold down half the spores remaining on the table while the other half are lifted off the table. The volume flux through an area A just above the tabletop is then

$$Q = \frac{v_{\text{rms}} A}{2},$$

where v_{rms} is the root mean square vertical velocity fluctuation in the boundary layer.

Mass Concentration of Spores on the Table

It is assumed that the initial mass of spores m_s is known and is evenly distributed over the area A. Let N_0 be the total number of spores initially on the table so that, on average, the mass of a single spore is $\hat{m}_s = m_s/N_0$. Thus for the conditions specified above, 1 g of spores is equivalent to 10^{12} individual spores. The spores are acted on by the vertical turbulent velocity fluctuations. Assuming the spores are lifted off the table at a rate proportional to the number of spores remaining on the table, then

$$\frac{\partial N}{\partial t} = -kN.$$

Here, k is a constant that sets the rate at which the number of spores remaining on the table decreases, N is the number of spores remaining on the table, and t is time. The rate at which spores are entrained into the room airflow is

$$\frac{\partial N_t}{\partial t} = -kN_0 e^{-kt}.$$

Mass Flux of Spores Entering the Flow

The spores are initially distributed uniformly over a 10×10 cm area on the tabletop. The air immediately

above the table will contain spores that have become airborne. The mass flux of spores entering the airflow is

$$\dot{m}_s = \hat{m}_s \frac{\partial N_t}{\partial t} = \hat{m}_s k N_0 e^{-kt} .$$

The constant k is specified using the turbulent boundary layer equations[2] yielding

$$\dot{m}_s = \frac{\hat{m}_s v_{rms} N_0}{2D} e^{-\frac{v_{rms} t}{2D}} ,$$

where D is the diameter of a single spore.

These results, especially the time scale for entrainment, depend critically on the assumption that half the particles remaining on the table are lifted off the surface at each successive time. It is, however, expected that other factors would tend to cause a somewhat larger fraction of the particles to adhere to the surface, increasing the release time considerably. Further research is required to study the details of particulate entrainment into the boundary layer.

Model for Ambient Airflow and Propagation of Spores

A typical office-type room is considered. As shown in Fig. 2, there are three desks and a bookcase. The air enters through the vent on the ceiling and exits through the fully open door. A typical office airflow rate of 5.8 cfs is used, equivalent to a room flushing rate of about 300 times per hour. Three positions of interest are identified. Positions 1 and 2 represent people working at their desks. Position 1 is at the desk opposite the contaminated desk, position 2 is at the desk near the door, and position 3 is in the open doorway. Contaminant concentrations are sampled at these three points.

The flow field analysis was performed on an SGI Origin 2000 workstation using a single 400-MHz R12000 CPU and CFD2000, a commercial CFD software package.[3] A typical run time required 6 days (continuous) for our example problem. The calculation terminates after 12 min of simulated flow. The ambient airflow patterns are presented in Fig. 3. The streak lines shown are colored by flow speed, that is, red = fast and blue = slow.

With the ambient airflow established, material is released from a 10×10 cm square area on one of the desks for 12 min, the simulated time for the case considered.

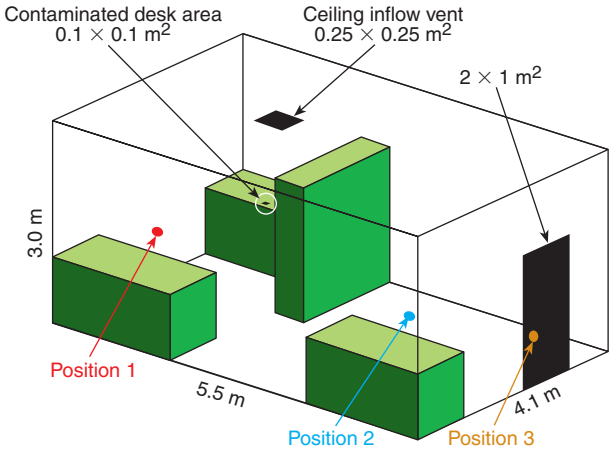

Figure 2. Room geometry used in a model for ambient airflow and the propagation of spores.

RESULTS

Room Dispersion

Figure 4 illustratess the computed contaminant concentration line contours after continuous release for the 12-min period. Concentration contours are shown in a cross plane through the release area and the door, with an enlargement over the table release area.

Spore Distribution

Given the spore concentration ρ_{sx} from the CFD computation, the spore number density is

$$n_s = \frac{\rho_{sx}}{\hat{m}_s} \text{ spores/cm}^3 .$$

Figure 5 shows the number density of spores at the three positions in the room. Positions 1 and 2 correspond to in-room locations at two of the desks in Fig. 2. At these locations there would be ≈4–6 min

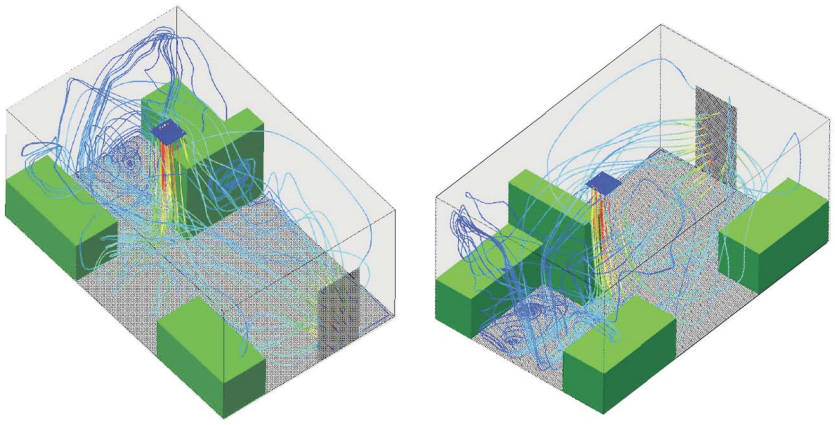

Figure 3. Two views of steady-state room flow pattern prior to contaminant release; streak lines are colored by velocity magnitude: red = fast, blue = slow.

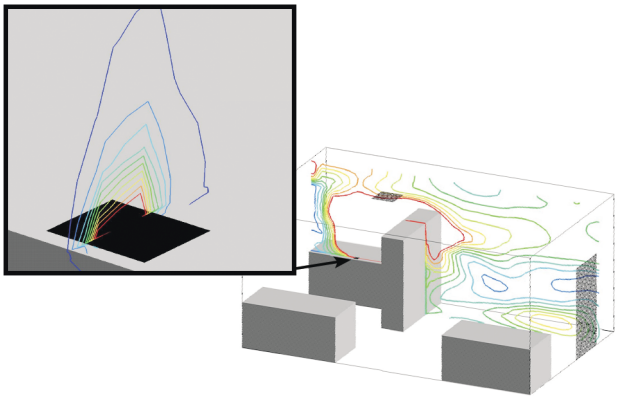

Figure 4. Contaminant concentration contours after continuous release for 12 min in a plane along the room and at the release area (kg/m^3).

before the spores arrived. At the door, Position 3, the spores would arrive after ≈7 min. This analysis indicates the time elapsed prior to exposure and subsequent level of exposure. Such results would be useful in planning sensor placement and evacuation planning.

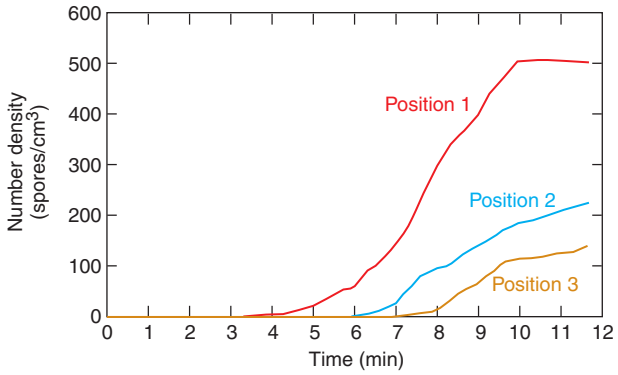

Figure 5. Spore density number at the three positions in Fig. 2.

SUMMARY

It has been shown that the use of boundary layer modeling and CFD can be used to simulate the dispersion of particulates within a room. Coupled with sensor scenarios, dosages experienced by occupants as a function of time can be estimated. This dispersion model procedure can be used as the basis for a toxic agent building simulation and analysis and for design of mitigation and evacuation strategies. Moreover, the approach described here can be extended to other toxic agents (biological and chemical) and to other room and building configurations (e.g., a series of rooms in a HVAC zone or an auditorium).

For the illustrative problem presented here, the exposure level was on the order of 100 spores/cm^3 of air (or 10^5 spores per liter). A dose of anthrax that is lethal to 50% of the exposed population (LD50) is about 50,000 spores. For an adult with a breathing tidal volume of 0.5 L, the exposure would be 1 LD50 per breath. The implication of this analysis is that a single gram of spores deposited on a desktop can result in lethal doses reaching the doorway in as little as 10 min.

REFERENCES

[1]Cieslak, T. J., and Eitzen, E. M., "Clinical and Epidemiologic Principles of Anthrax," *Emerging Infectious Diseases* **5**(4) (Jul–Aug 1999), available at http://www.cdc.gov/ncidod/eid/vol5no4/contents.htm (accessed 19 Aug 2003).

[2]Schlichting, H., *Boundary-Layer Theory*, Sixth Ed., McGraw-Hill Book Company (1968).

[3]*CFD2000 Version 3.0 Users Guide*, Adaptive Research, a Division of Pacific Sierra Research Corporation, Santa Monica, CA (1998).

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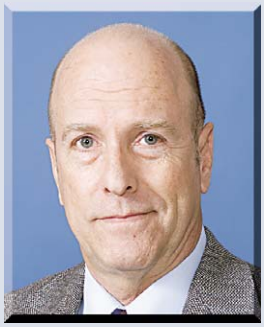

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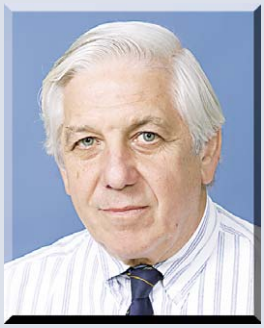

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