MONITORING DISPERSION OF AEROSOLS IN WORK ROOMS USING COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT
In this study, a commercial computational fluid dynamics (CFD) code, CFX4, was used to assess flow field characteristics, and to simulate postulated aerosol release and transport in a large, ventilated work room in the main plutonium facility at Los Alamos. Application of CFD and experiments can have a favorable impact on the design of ventilation systems and worker safety with consideration to facility costs. Steady state CFD results illustrating a complex, ventilation-induced, flow field with vortices, velocity gradients, and quiet zones are presented, as are time-dependent aerosol dispersion results. This paper also explains how results from the aerosol release study were used to evaluate and compare two air monitor placement strategies in terms of predicted worker protection. It was concluded that a quantitative placement strategy was superior to the more traditional strategy of placement in front of outlets in the four room corners.

INTRODUCTION
For over 20 years, the Design Engineering (ESA-DE) and Health Physics Measurements (ESH-4) Groups at Los Alamos National Laboratory (Los Alamos) have been developing new technologies using analytical and experimental tools to aid in the design of nuclear facilities.

These technologies can be used to guide ventilation system design and detector placement decisions for new construction programs, when modifying old facilities, or for evaluation of adequate placement in existing rooms. Also, because research has demonstrated that effective placement of real-time air monitors in large nuclear facilities is critical to radiation safety of workers, we have developed these technologies to aid in decisions regarding placement of aerosol (plutonium) and gas (tritium) detectors. Further, these tools can be used to determine the cause of and help mitigate future nuclear facility accidents involving hazardous aerosol or gas dispersion.

Release of toxic material could occur in Department of Energy research and production facilities such as those located at Lawrence Livermore National Laboratory (LLNL), Sandia National Laboratory (SNL), Savannah River Site (SRS), or Los Alamos. In such facilities, Federal Regulation 10 CFR 835 (DOE 1999a) requires real-time air monitoring using Continuous Air Monitors (CAMs) in normally occupied work areas where an individual is likely to receive an exposure of 40 or more Derived Air Concentration-hours (DAC-hours) in a year. Also, CAMs are needed where there is a need to alert individuals to unexpected increases in airborne radioactivity.

CAMs are used to protect workers by monitoring the level of radioactive materials within a room. Once a preset radioactivity level is exceeded, a CAM alarm is triggered alerting the workers to potential hazard and prompting them to evacuate the room. Knowledge of aerosol dispersion patterns in work areas is important to ensuring the CAMs are located in quantities and in positions that provide adequate worker protection. Traditionally, CAMs at Los Alamos have been located at room exhaust points in the four room corners. But, recent studies have shown that worker protection could be improved using a different placement strategy.

The main purpose of this study was to use CFD to evaluate a ventilation-system-induced flow field, calculate aerosol dispersion, and compare two CAM placement strategies in terms of predicted worker protection. This technology was applied to a Los Alamos nuclear facility process room with complicated geometry.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>DF</td>
<td>Dose fraction</td>
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<tr>
<td>( C_{bz} )</td>
<td>Concentration at the breathing zone</td>
</tr>
<tr>
<td>( t_a )</td>
<td>alarm time</td>
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NUMERICAL METHOD

CFD codes sometimes offer advantages over experimental techniques in investigating fluid flow. These
advantages can include savings in time and cost associated with the alternative, namely, constructing and performing large-scale experiments. In addition, CFD codes allow detailed flow visualization, as well as the ability to conveniently perform parametric sensitivity and optimization studies, and the ability to evaluate room re-configurations. Finally, CFD analysis is the only possible approach to investigate flow fields and aerosol dispersion in a room that is in the design stage.

The flow field and aerosol dispersion in the room studied here was simulated using CFX4, a commercially available CFD package. CFD models provide a simultaneous numerical solution of continuity, Navier-Stokes, and energy equations for a flow-field geometry with specified boundary conditions. CFX4 uses a finite volume (finite difference) scheme based on the SIMPLEC mathematical algorithm discussed by Van Dormaal and Raithby (1984). A predecessor of this algorithm, SIMPLE is given by Patankar (1980)

ROOM CONFIGURATION AND NUMERICAL MODEL

The room geometry is shown as a plan view in Fig. 1. The workroom studied contained five rows of glove boxes and an overhead trolley. Four inlet air diffusers on the ceiling and four outlet registers on the walls near the floor were modeled. The flow rates at the inlets and outlets were measured with a hot wire anemometer and found to corresponded to 10 air exchanges per hour. From measurements of the exit flow, it was determined that not all four outlets exhausted the same amount of air. This finding was incorporated into the outlet boundary conditions.

Outlets were modeled using a constant mass flow rate boundary condition. Inlet air was modeled with a circumferential velocity angle of 28° relative to the ceiling to simulate the effect of the diffusers.

An isometric view of the interior of the room is shown in Fig. 2. The glove box bottoms are 3.17 ft from the floor; glove boxes 2 and 3 are 7.5 ft high and portions of the other glove boxes reach 9 ft. Glove boxes are represented as simple rectangular parallelepipeds. The computational flow domain is the open space in the room with four inlets and four outlets.

Glove box surfaces were treated as solid walls. The three-dimensional model consisted of multi-block assembly with body-fitted grid. This technique was used to partition the three-dimensional computational space into 233,000 volumes with an approximate linear resolution of 0.5 ft per side. The spacing of this grid was optimized to capture the boundary layer flow near the walls of the room and glove box surfaces.

The air in the room was treated as incompressible and isothermal. The three-dimensional, steady state, flow field was computed using the k-ε two-equation turbulence model. People or other heat sources inside the room were not considered in this study. The solutions were obtained on Digital Equipment 600 MHz Alpha machines in about 32 hrs for the steady state solution, and 36 hrs for the transient solution.

VELOCITY FIELD AND AEROSOL DISPERSION

Velocity vectors in horizontal and vertical planes, obtained from the steady-state CFD solution, are shown in Figs. 3 through 5. The flow in the room is surprisingly complex and undesirable from the standpoint of worker safety. The inlets, outlets, glove box configuration in the room, and boundary conditions determine the details. High velocities are noticed at the inlets and along the ceiling and room walls.

Figure 3 shows that re-circulation zones are developed between glove boxes. Velocities as high as 2.7 m/s at the inlets are recorded, but in general the velocities are in the 0.25 m/s range. For future reference, notice in Fig. 3 that the flow between glove boxes 2 and 3 in the region 0 < x < 30 ft, 15 ft < y < 18 ft, is from right to left. There is considerable mixing of air in the room before it exits and not all of the air may exchange 10 times in one hour. A large mixing zone in the room is formed between glove boxes 2 and 4 and in front of glove box 3, which can be seen in Figs. 3 through 5.

For various locations in the room, accidental releases were simulated using a short burst or "puff" of an idealized aerosol (dilute, mono-disperse, neutrally buoyant particles). This scalar contaminant method provided a good approximation for aerosol particles that have an aerodynamic diameter of less than about 1μm. As a first approximation, this method is less CPU intensive than a multiphase simulation, which would have been required to simulate an aerosol with a size distribution or with different densities.

The steady-state CFD solution was used as input in solving dispersion patterns for the aerosol releases. Transient calculations of the aerosol dispersion by advection, turbulent diffusion, and molecular diffusion over a seven-minute period were performed, and aerosol concentration versus time was recorded at twelve potential sampling locations. An example of one aerosol release (from location 2 shown in Fig. 1) calculation at an elapsed time of 60 s is shown in Fig. 6. Notice that the movement of aerosol in the region 0 < x < 30 ft, 15 ft < y < 18 ft is consistent with Fig. 3.

EXPERIMENTAL VALIDATION OF CFD MODEL

Results from computational models are approximations. If practical, it is always desirable to check CFD results with an experiment. Here, CFD-predicted concentration time histories were compared with experimental data obtained at the same room locations and for the same conditions.

In the experiment, short duration (60 s) releases of tracer aerosol were made from release location 11 in the room (see Fig. 1) and particle concentrations were measured with laser particle counters at sampling locations D8, D13, and D15. Figure 7 shows experimental
concentration time histories at these locations. This data can be compared to CFD model predictions in Fig. 8.

The general shapes of the aerosol concentration versus time profiles as well as the lag times and times to peak concentrations compare well between Figs. 7 and 8. The numerical values of concentration in these two figures are not directly comparable because each laser particle counter measured the number of particles in its measurement volume, whereas the CFD code calculated aerosol mass concentration at specific locations. These two quantities are related by a simple conversion factor.

The data in Figs. 7 and 8 suggest that the CFD model calculations yield aerosol dispersion results that are in general agreement with experimental measurements. Similar validation work in the test room at the Los Alamos Group ESH-4 operated UHTREX test facility has also shown general agreement between simulations and empirical measurements (McAtee, et al., 2000). These findings establish that CFD modeling is capable of sufficient accuracy in representing patterns of room airflow and contaminant transport as to be a useful tool for optimizing the number and placement of detectors during design phases. In addition, it is anticipated that the CFD process will provide a better understanding of any spatial flexibility that operations personnel might have in placing the CAMs in an optimal configuration.

TWO DETECTOR PLACEMENT STRATEGIES

The metric chosen to compare placement strategies was dose fraction (DF). The DF, defined by Eq. (1), is the ratio of the integral of the concentration at the "breathing zone" from the time of the release to the time when the CAM alarms to the same integral of concentration for seven minutes. This metric was chosen because it allows an analysis of interplay between predicted worker exposure and CAM alarm response. Other metrics were proposed and may be worthy of investigation (McFarland, et al., 1997).

\[
DF = \frac{\int_{0}^{t_a} C_{hz}(t)dt}{\int_{0}^{7\text{min}} C_{hz}(t)dt} \quad (1)
\]

The CAM alarm time, \(t_a\), was defined as the time elapsed from the start of the release to the time that the CAM would alarm. These CFD-simulated alarm times were obtained by integrating the concentration over time until the CAM alarm threshold concentration was exceeded. The concentration at which the CAM alarmed was assumed to be 8 DAC-hours = \(9 \times 10^{-10} \text{ kg/s/m}^3\) (for Pu-239) which is typical for newer CAMs and low radon concentrations. The alarm times were recorded for each potential sampling location and were used to estimate the inhalation exposure of a worker co-located with the accidental release. The worker’s breathing zone was defined as a space slightly above the release point, and the contaminant in this area was assumed to be inhaled by a nearby worker.

The release rate for the aerosol (scalar) release was calculated and discussed in the report LA-UR-xx (McAtee, et al., 2000). If the release took place over 30 sec, the release rate would be \(8.33E5 \text{ dpm/s or 5.899E-9 kg/s} \) (where dpm is decentigrations per minute ). These numbers were used in determining the scale factor in processing the CFD results where the scalar was released at a rate of 0.1 kg/s for 30 s.

Results from two different placement strategies consisting of six sampling locations (detectors) per strategy are presented here. These two strategies were tested against each other to investigate if one strategy might provide better worker protection. The first strategy is denoted "4+2" and consists of four detectors placed in the traditional four corners of the room in front of the outlets, plus two more detectors in the interior of the room. The location of six detectors for the "4+2" strategy is shown in Fig. 9.

To determine the location of six detectors for the quantitative placement strategy, aerosol from a point source was released over 30 seconds at a rate of 0.1 kg/s from ten representative locations in the room. For each release, aerosol concentrations were monitored and recorded at 99 locations for 7 minutes.

The average DF for all possible combinations of six detectors was calculated, and the combination that produced the lowest average DF was selected as the quantitative strategy. To remove the strong bias from detectors very close to the release points, the DF for these detectors were replaced by the average DF. In theory, this provided for placement that was more suited to the general release condition.

To test the performance of the two placement strategies, "4+2" and quantitative, nine release locations were selected randomly from 52 possibilities, near, above, and below the glove boxes. Results of DF calculations for four releases from the placement strategy evaluation are shown in Table I. It can be seen in Table I that the preferred strategy (yielding the lowest average of DF minimums for each release) is the quantitative strategy.

CONCLUDING REMARKS

In this study, analytical (CFD) and experimental tools have been combined to form a new technology useful in the design of nuclear facilities. Applications include ventilation system design and detector placement.

CFD velocity field results for a particular Los Alamos nuclear facility are presented, which show complex airflow patterns, undesirable from the standpoint of worker safety. Computed and measured aerosol concentration time history data is compared and shows general agreement.
A CFD-derived, quantitative, detector placement strategy is shown to produce a lower worker dose fraction than a traditional four-corner strategy.

It is believed that, with development, the techniques presented here can lead to ventilation system design improvements, and eventually to the optimization of the number and placement of aerosol or gas detectors in nuclear facilities.

REFERENCES


Figure 1. Top view of the room studied.

Figure 2. Isometric view of the room studied

Figure 3. Velocity vectors at z=4.5'.
Figure 4. Velocity vectors at x=23 feet.

Figure 5. Velocity vectors at y=18’ feet.

Figure 6. Concentration of scalar release 2 after 60 s.

Figure 7. Location of quantitative and “4+2” CAMs.
Figure 8 Concentration over time obtained by experiment for detector 15, 13 and 8.

Figure 9 Concentration over time obtained by CFD for detector 15, 13 and 8.

Table I. Values of the DF for the two placement scheme for the four “blind” releases.