

TECHNICAL BRIEF

Monitoring dispersion of aerosols or gases in enclosures using CFD

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. Federal regulations require real-time air monitoring using Continuous Air Monitors (CAMs) in normally occupied work areas where an individual is likely to receive a specified exposure. 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 (Whicker, 1996). But, recent studies have shown that worker protection could be improved using a different placement strategy.

CFD has been used in studies to evaluate a ventilation-system-induced flow field, calculate aerosol dispersion, and compare CAM placement strategies in terms of predicted worker protection. This technology was applied to a Los Alamos nuclear facility process room with complicated geometry.

CFD codes offer some 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) discretization scheme.

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 using hot wire anemometry 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.

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.

Velocity vectors in a horizontal plane, obtained from the steady-state CFD solution, are shown in Fig. 2. 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 were observed at the inlets and along the ceiling and room walls. Such data is useful to guide and evaluate nuclear facility ventilation system design.

Figure 2 shows that re-circulation zones are developed between glove boxes. Such zones can trap aerosols or gases. 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. 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.

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 1 μ m. As a first approximation, this method is less data processor 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.

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.

Results from computational models are approximations. In 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 3 shows CFD model predictions. These results can be compared to experimental concentration time histories at the same locations in Fig. 4.

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. 3 and 4. 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. 3 and 4 suggest that the CFD model calculations yield aerosol dispersion results that are in general agreement with experimental measurements. Such results 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.

REFERENCES

Whicker, J.J., Konecni, S., Parietti, L., Buhl, T., Hoover, M., Hoover, P., Martin, R., Morgan, R., Rodgers, J., Voss, T., Wannigman D., 2000, "Placement of continuous air monitors in PF-4 plutonium laboratories: consensus findings and recommendations," Los Alamos National Laboratory Report in preparation.

Whicker, J.J., Yang, Y., Rodgers, J.C., Spore, J., "Experimental characterization and computational modeling of indoor aerosol dispersion and their applications in optimizing of continuous air monitor placement," *Proceedings of the 1996 ASME Fluids Engineering Division Summer Meeting*, July 7-11, San Diego, CA, 1996.

FIGURES

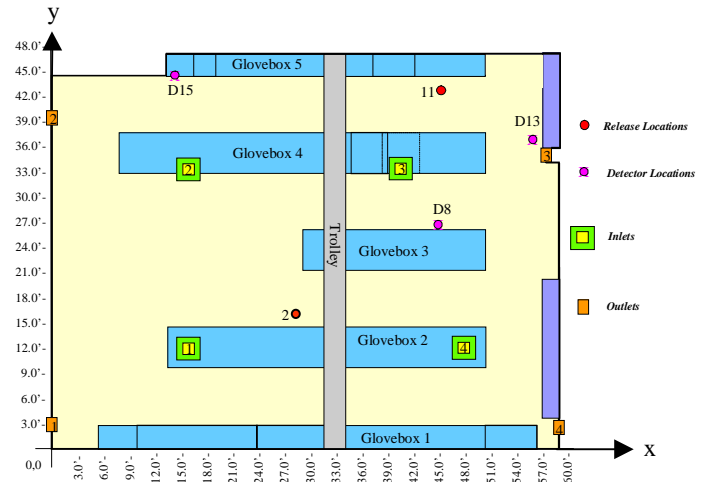


Figure 1. Plan view of the room studied and locations of releases 2 and 11, and detectors 8, 13, and 15 in Cartesian coordinates.

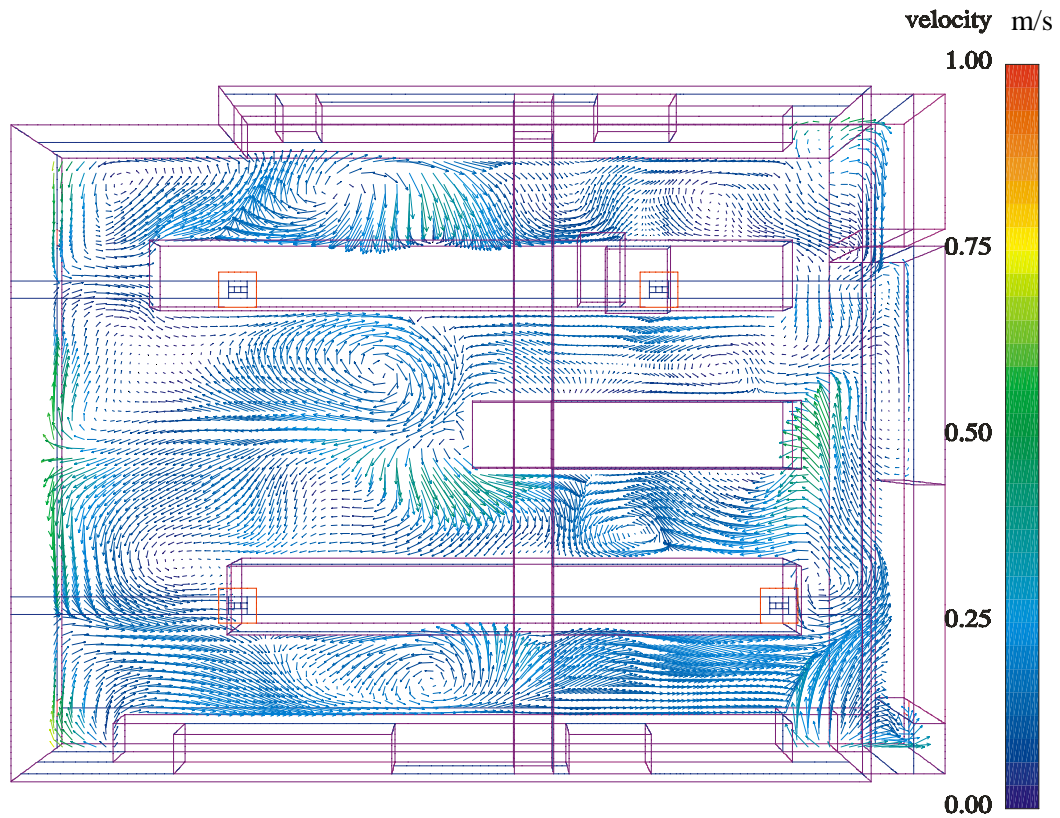


Figure 2. Horizontal components of velocity vectors at height = 4.5 ft

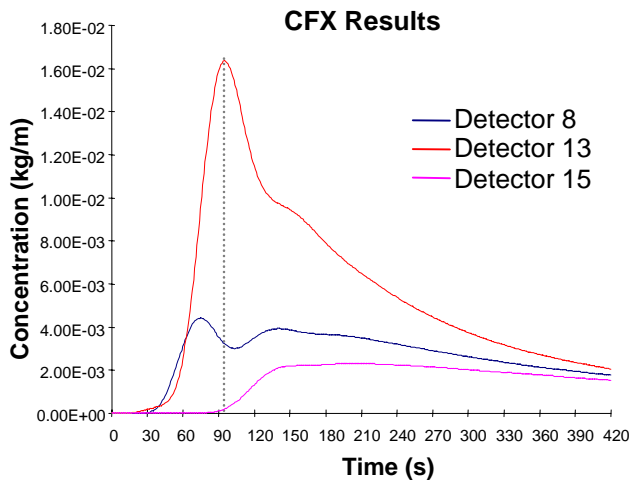


Figure 3. Concentration versus time obtained by CFD for detectors 8, 13, and 15.

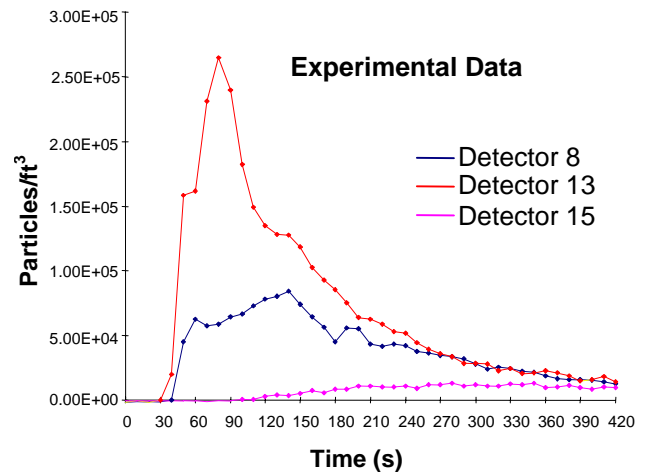


Figure 4. Concentration versus time obtained by experiment for detectors 8, 13, and 15.