



# Introduction to Applied Computational Fluid Dynamics for the Biological Safety Environment

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## Abstract

*The basics of Computational Fluid Dynamics (CFD) are presented to allow the practicing biological safety professional to have a preliminary understanding of the use of CFD for airflow analysis and contaminant tracking. A discussion of result interpretation is provided to assist in communicating with the applied CFD engineer. Results from two actual buildings, a Biosafety Level 3 (BSL-3) facility and a hospital, provide examples of post-processed CFD data. An overview of the general costs associated with a CFD business unit is provided to facilitate budgeting. Next, a discussion of the ways CFD can add value to a design is provided. Finally, a short list of information required to model a generic space is provided to facilitate project initialization.*

## Definition of Terms

ACH	air changes per hour
BSL-3	Biosafety Level 3
CAD	Computer Aided Drafting/Design
CFD	Computational Fluid Dynamics
RANS	Reynolds Averaged Navier-Stokes
LES	Large Eddy Simulation
$\dot{m}_i$	Mass flow rate of species i
$\rho_i$	Density of species i
$D_{i,j}$	Diffusion coefficient of species i with respect to species j
$C_i$	Concentration of species i
$n_\xi$	Coordinate direction

## Introduction

The objective is to provide a high level technical overview of Computational Fluid Dynamics (CFD) followed by the background necessary to work with an applied

CFD engineer. The background includes some basic information about interpreting results, costs of a CFD study, and the value this adds to a project.

CFD provides a numerical simulation of fluid flow based on the Navier-Stokes equations. Information at the boundaries is required to determine the flow conditions inside a space. Some boundaries require flow to be specified, examples would be ventilation system inlets and returns, biosafety cabinets, and biosafety hoods. Another common specification is heat leaving a boundary, such as a hot machine or computer. Boundaries may be inside the solution areas as well as at the edges. Internal boundaries could be tables and room partitions, while external boundaries are generally walls, doors, or windows. Boundary conditions can be very complicated depending on the model requirements. CFD provides information on the motion of air within a space. In addition to velocities, temperature and pressure are commonly available. Particles and individual gases can also be tracked.

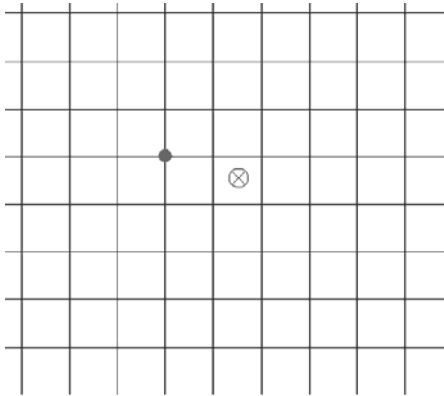
Rather than focusing on equations, the technical discussion will be from a conceptual perspective. Next, a section on interpreting results is provided, followed by an examination of the results from the two cases. Sample results are provided for a simulation of a Biosafety Level 3 (BSL-3) environment and a hospital environment. An overview of the costs and computational equipment required to perform CFD simulations is provided. The cost-value of a CFD study is discussed. The final section focuses on the information required by an applied CFD engineer in order to create a model. While not exhaustive, this information should help both biosafety professionals and CFD professionals communicate.

## Technical Discussion

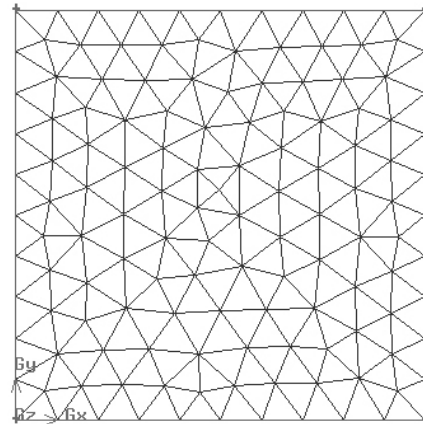
The region to be modeled using CFD must first be divided up, or “discretized,” into cells. The combination of all cells is referred to as the grid or “computational domain.” Individual cells are usually hexahedral (six sides like a brick, [Figure 1]) or tetrahedral (4-sided like a pyramid, [Figure 2]). Depending on the methodology, solutions are obtained either at cell centers or at cell intersections, as shown in Figure 1. (*Technical aside: For an equi-*

**Figure 1**

Hexahedral grid (2-D view) showing finite difference (dot) and finite volume (other) calculation locations.

**Figure 2**

Tetrahedral grid (2-D) view.



spaced orthogonal grid [Figure 1], it has been shown there is no practical difference. For a more typical non-equi-spaced non-orthogonal grid [Figure 2], it has been proven that the finite volume methodology with the solution point in the middle of the cell is more robust, i.e., less likely to cause the solver to crash.) Numerous commercial CFD codes are available to solve the governing equations and obtain the airflow pattern. Also, software independent of the actual solver is often purchased; for example, the application used to create the grid. Additional software is sometimes used to set up complicated boundary conditions (pre-processors) and to provide enhanced visualization of the results (post-processors). In addition to the software, computational resources are required. A simple desktop computer is capable of running small solutions (under 500,000 cells) to steady solution in about a day, but cannot process large-scale problems. A distributed load (parallel) system is required.

The number of grid cells in any domain is a significant factor in determining what can be assessed. As a rule, one cannot “know” anything smaller than the cell size where information is sought. For example, if the cells near a chemical source are six inches away; stating the concentration at three inches from the source would be a violation of the rule. At a minimum, there should be a cell three inches from the source and, preferably, several cells between the source and the three-inch measurement point. For swirling flows, one generally needs at least three tetrahedral cells to capture the motion. Basically, more cells equal better results. However, as the cell count increases, so does the solution processing time. If the cell count is sufficiently high, the simulation can overwhelm computing resources. The number of cells that can be solved and the resolution obtainable are directly related to the computing resources available.

In CFD, a major decision is the type of model to use to simulate the airflow. Some models are best for getting

an average snap-shot of the flowfield while extremely high value/risk situations may warrant the use of more expensive, fully time-varying or “transient” models. Steady-state RANS (Reynolds-Averaged Navier-Stokes) is often sufficient to resolve key information about the flowfield. A steady-state simulation provides a “snap-shot” of the average flowfield. Sometimes an unsteady RANS solution is used for particularly difficult problems in order to keep the solver stable as it progresses to the solution. An unsteady or time-varying solution would be required if the boundary conditions change with time. LES (Large Eddy Simulation) is an advanced unsteady solution method that can provide more data about transient operation, but is more computationally expensive. LES should be carefully considered in light of the information desired, the grid resolution, and the ability to model boundary conditions accurately. The limiting boundary conditions for internal airflow are usually the air inlets. The solution’s representation of the real-world situation is limited by the crudest component of the model. For many situations, a RANS model is adequate, but if accuracy is critical, the additional costs of LES would be justified.

Two key questions in the design of a BSL-3 containment laboratory space are air changes per hour (ACH) and what happens in the case of a contaminate release. RANS can provide an overview of ACH that is more detailed than an analytical calculation by identifying areas of short-circuiting, re-circulation, and dead-air. Species transport is driven by two phenomena, the flow pattern (or streamlines) and Fickian Diffusion, driven by concentrations which is represented by the following formula:

$$\dot{m}_i = -\rho_i D_{i,j} \frac{\partial C_i}{\partial n_\xi}$$

In Fickian diffusion, species move from regions of high concentration to regions of low concentration and they try to do this independent of the airflow. A third consideration is how the airflow behaves in various modes of operation (fume hood on/off, etc).

Room features include standard furnishings, as well as ventilation system components and heat sources (Figure 3). An empty room will not necessarily have the same airflow characteristics as a fully furnished room. Heat sources in a room can create convective currents that alter airflow patterns locally. Laboratory equipment can be re-circulating, partially venting, or fully venting and is an obvious contributor to the motion of air through a room. CFD can include all these effects, provided the vendors can supply information on the devices.

## Interpreting Results

CFD is known for producing color pictures; it has sometimes been called colorized fluid dynamics. Unfortunately, the color pictures often mask the grid used. One cannot tell the grid density from a contour plot. This makes it very difficult for the novice (and sometimes the expert) to assess a CFD simulation on the basis of the images. Furthermore, the graphics can distract from the key points. CFD is being used to validate or to analyze a design. Therefore, there exist key deliverables. In a few cases, the pictures can show “uniform flow” or “a lack of significant recirculation or stagnation regions.”

Figure 4a provides an example of air moving over a block. The picture of velocity contours gives few hints about the grid used to obtain the solution. In Figure 4b, the 670-cell grid is now superimposed on the solution showing a very coarse representation of the domain. The flow as shown is not inaccurate; it is just insufficiently resolved to make any conclusions. If the number of cells is increased to 57,518, there is far greater resolution (Figure 4c). Specifically, the wake region behind the block is improved. Figure 4d shows the streamlines, or airflow pattern, around the block.

The graphics illustrating the anticipated airflow patterns can be useful for a developer or a review board, but the best value of CFD is in the expertise of the person performing the simulations and their skill in interpreting the results. An expert CFD consultant can help improve the design of a space before it is constructed. Valuable information on the actual performance of a facility can be obtained. For example, assume Design 1 has an average of 5 ACH with no region of less than 2 ACH, and Design 2 has an average of 4.5 ACH with no region of less than 3.5 ACH. These are useful quantitative numbers. Without an extensive database of testing, it is best to take the numerical values on a qualitative basis. Design 2 is better than Design 1, but 5 ACH versus 4.5 ACH is not significantly different while the 2 to 3.5 is large enough to be

important. Obtaining quantitative data from qualitative pictures requires post-processing capabilities and adherence to good CFD practices. A skilled CFD provider will help interpret the accuracy of the results for a client. An example of this expertise would be knowledge that, based on the simulation parameters, 0.5 ACH is not significantly different. Because many people who know they need CFD are uncomfortable evaluating the results due to the lack of explicit published guidelines for modeling the indoor air environment, peer review can be a way of ensuring the results are reasonable. To ensure recommendations are valid, peer review can be required as an item in the request for proposal.

While finding a CFD practitioner is easy using the internet, finding a qualified individual is not. Some common criteria to consider, when contracting CFD services, are the academic credentials and personal biographical sketches of the people who will be doing the analysis. Additionally, the core business of the company is relevant. Hiring a company focused on gaseous dispersion in indoor and outdoor environments might be preferable to hiring an automobile, turbine, or rocket focused company to model a laboratory. Finally, requesting references from previous clients is generally a good practice. The authors work for CPP Wind Engineering, a firm experienced in providing CFD services.

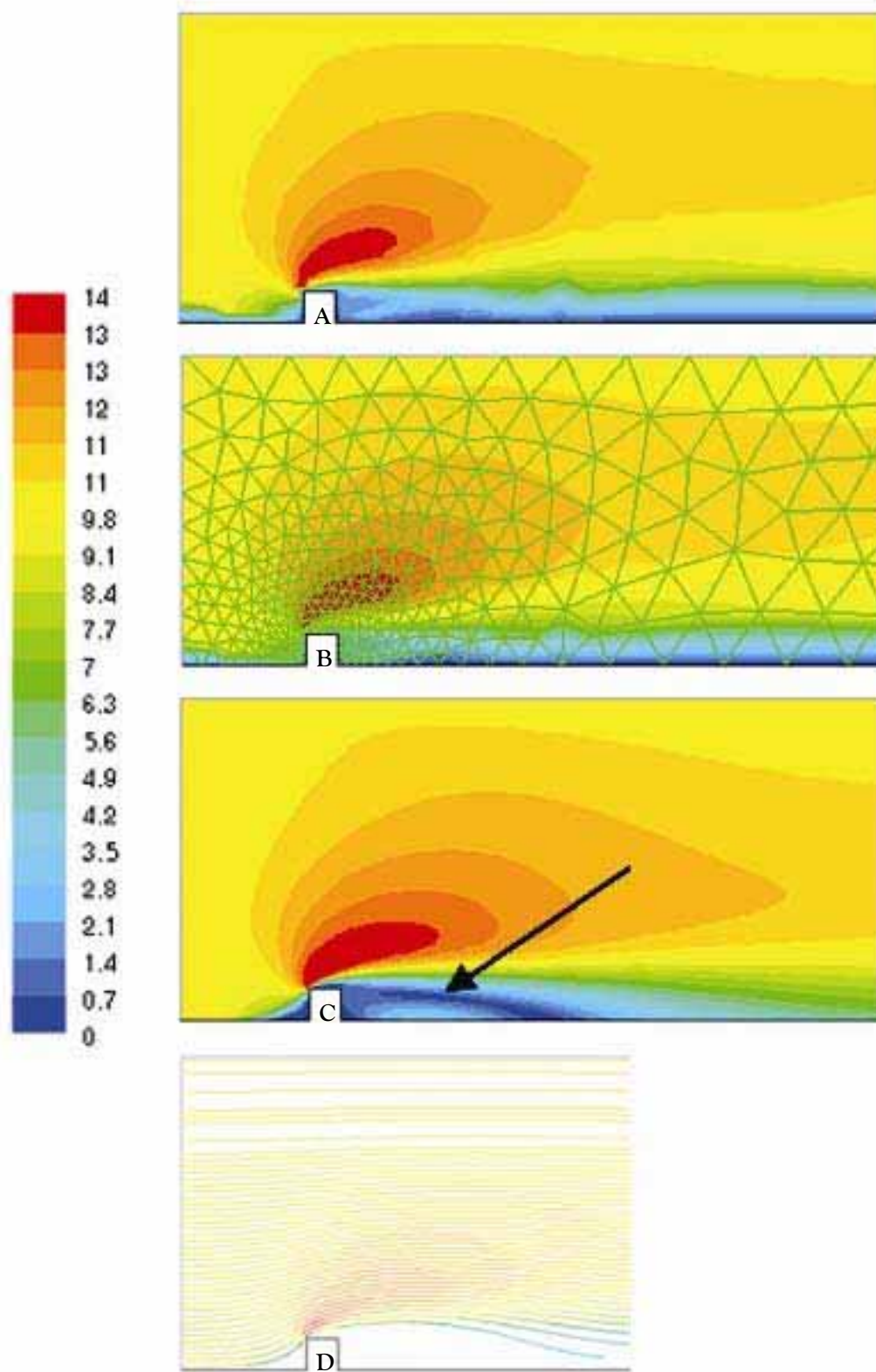
## Results

Sample results are provided for two facilities to familiarize the reader with typical output from simulations. Since the reader will have only limited information on the spaces being modeled, only one case is presented for each facility for demonstration purposes although more cases would typically be analyzed to compare different designs for a client.

An overview of the hospital space modeled is provided in Figure 3. The rooms contain a bed, light, equipment panels on two walls, a computer on a small desk, and some cabinets. The air inlet is colored green and the return is red. The grid cross-section is provided in Figure 5. A total of 76,503 cells were used for the domain. The largest cell size was 10 inches by 10 inches in the horizontal plane, by 5 inches in the vertical plane. Higher grid density (smaller cells) must be used close to heat sources and ventilation intakes and returns. Contour plots were made for temperature (Figure 6) and mean-age air (Figure 7). Temperature is an occupant comfort criterion and mean-age air correlates to ACH (600 sec = 6 ACH, 300 sec = 12 ACH). The temperature contour shows the effect of heat sources in the room. Mean-age air data can be used for occupancy criteria and also to determine areas with less circulation and lower velocities. Species contours are shown in Figure 8. In this example, a large amount of contaminant is released for visualization pur-

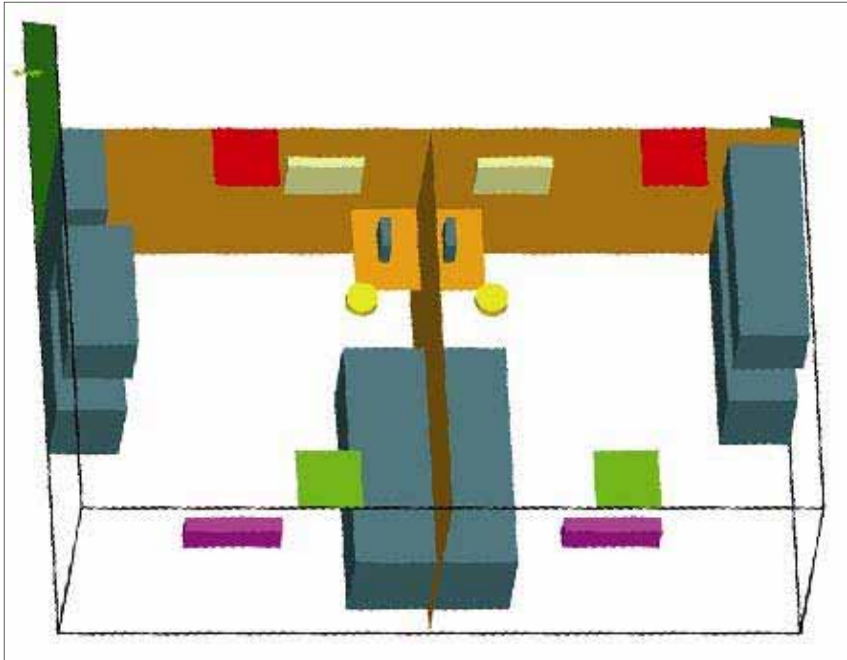
**Figure 4**

**Figure 4a:** Contour plot of velocity. **Figure 4b:** Contour plot of velocity with the 670-cell grid superimposed showing how little is actually “known.” **Figure 4c:** Velocity contours from a 57,518 cell grid for the same problem. Note the improvements the wake region (arrow) and the overall quality. **Figure 4d:** Example of streamlines colored by velocity magnitude showing how the flow enters the domain on the left and travels over the block.



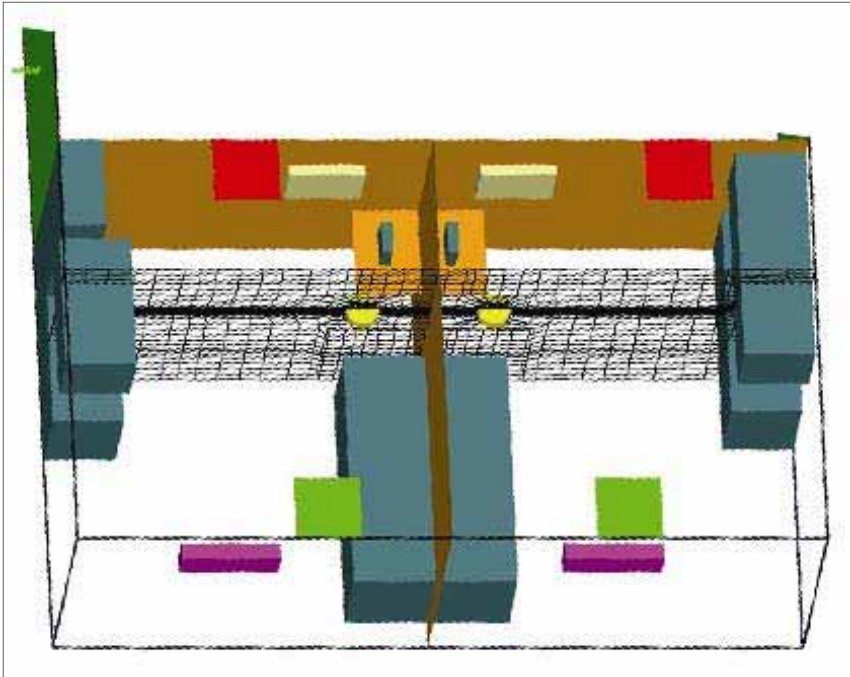
**Figure 3**

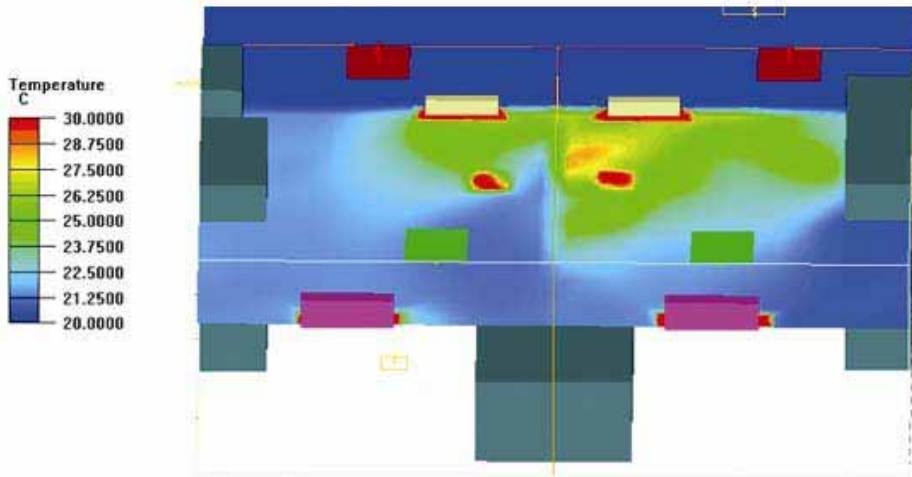
Hospital room showing heat sources (patient light; dark yellow, illuminator panel; light yellow, and diagnostic set; purple), ventilation system (green inflow, red return) and room furnishings (teal).



**Figure 5**

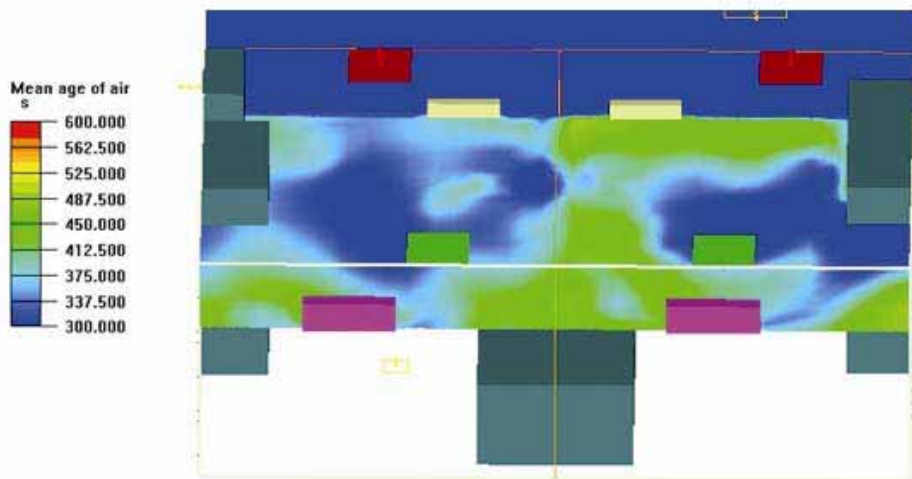
Grid cross-section for the hospital room.





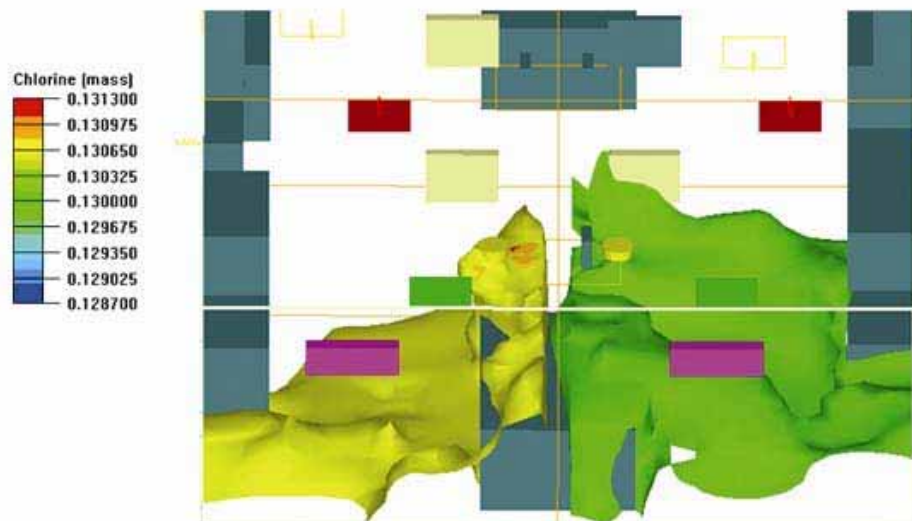
**Figure 6**

Hospital showing a horizontal cross-section colored by temperature. Note that air is warmer near the illuminator panel, diagnostic panel, and over the patient light.



**Figure 7**

Hospital showing a horizontal cross-section colored by mean-age-air (600 sec = 6 ACH). Note that air is circulating less in the corners and that small changes in room design can result in some significant difference in contours.



**Figure 8**

Hospital showing iso-lines of contaminant. In the left room the release point is on the floor near the center of the room, in the right room the release point is at the head of the patient bed.

poses. The contaminant is moved by the air currents and is also diffused from the high concentration where it is added to the low concentration in the room.

An overview of the BSL-3 space being modeled is provided in Figure 9. The space is very complicated containing equipment heat sources, recirculating biosafety cabinets, furniture, and even door undercuts so air can move between the spaces. For the BSL-3 facility, velocity vectors (Figure 10) show the magnitude and direction of air movement. Note that the high inflow vent in the middle “dumps” air in the room, creating vortices on either side. The space was also designed to have negative pressure so air moves between the rooms through the door undercuts. The mean-age air in the laboratory space is provided in Figure 11. The lowest ACH in the space is 12, with most areas seeing many more air changes per hour. Temperature contours in a vertical plane are shown in Figure 12. Note that the presence of high wattage equipment can result in relatively warm air spaces even with a high air-exchange rate.

If the spaces were being reviewed for construction or modification, many more pictures would be provided. Often there are specific objectives such as attaining a minimum ACH everywhere in a space or ensuring occupant comfort near external windows. This detailed discussion can have great value in the design phase, but generally overwhelms someone not familiar with the details of the space.

### Costs

Some explanation of the costs involved in CFD is warranted for budget planning purposes. The costs can be broken down into three main categories: fixed, recurring,

and personnel. The fixed costs include the computer hardware and configuration, initial software purchasing, and construction of an area to house the system (these computers can be noisy and generate a lot of heat). The yearly maintenance fees on the software dominate the recurring costs. One also has to consider routine maintenance on the hardware. There is quite a bit of variance from different vendors for both the software and hardware. Table 1 provides a rough estimate of the costs associated with setting up and maintaining a small system.

Personnel costs are most difficult to assess because of the variances in expertise and information provided to clients. Some companies have one person who does CAD (Computer-Aided Drafting/Design), grid-generation, and CFD; others have people assigned to each task. Engineering rates are researchable, keeping in mind that most CFD personnel and resources are applied in the Aerospace industry. The engineering costs should be compared relative to the services being provided.

Rather than setting up a computing facility for a short-term project, CFD is often subcontracted to firms who have invested significantly in specialized personnel and computing resources. Costs for CFD projects vary depending on simulation requirements. Small projects can often be completed for less than \$10,000. Very large, complex projects can approach the hundreds of thousands of dollars associated with typical Aerospace projects.

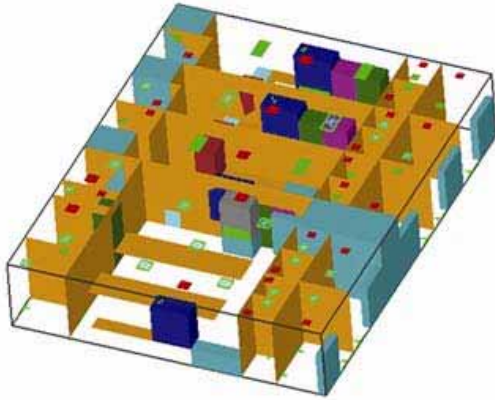
### Value-Added

CFD in a pure dollars view is not inexpensive, but from the perspective of the cost of a multi-million dollar facility and the cost of individual components of a facil-

**Table 1**

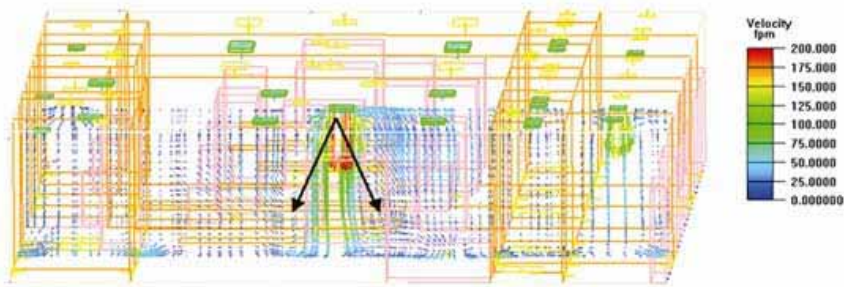
Estimate of costs for a small CFD facility.

Software costs (per seat)	
CFD fluid dynamic solver	\$ 22,000.00
Parallel licenses	\$ 3,000.00
Advanced grid generator	\$ 20,000.00
CAD solid modeling	\$ 5,000.00
Computer costs (per processor)	\$ 4,500.00
10 CPU system, 2 solvers, 8 parallel licenses, 1 grid generator, 1 CAD	\$ 138,000.00
Yearly maintenance costs (30 % of system)	\$ 41,400.00



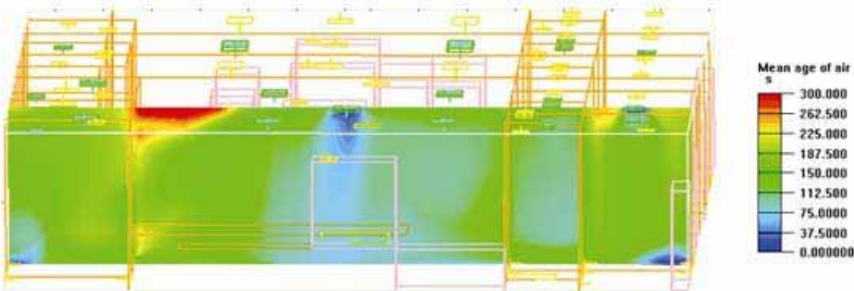
**Figure 9**

BSL-3 laboratory overview where inlets are green and outlets are red. Door undercuts allow for negative pressure flow effects. Various recirculation and externally venting laboratory devices are included. Thermal effects are also considered for heat generating pieces of equipment.



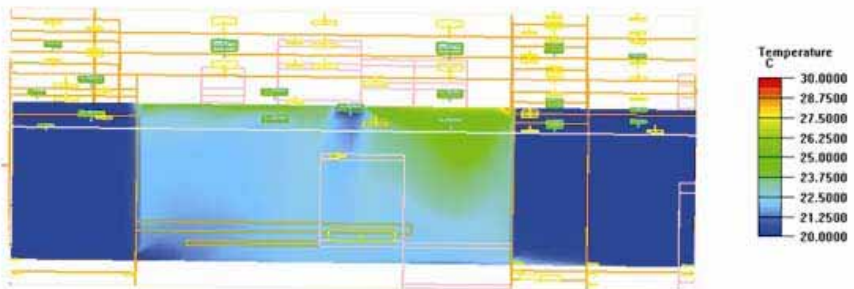
**Figure 10**

BSL-3 velocity vectors. Note the high velocities near the inlets and under the doors. The high velocity vent “dumps” to the floor creating vortices (arrows) to the left and right.



**Figure 11**

BSL-3 vertical plane showing mean-age-air. In this facility the air is rapidly exchanged, the lowest ACH is 12.



**Figure 12**

BSL-3 showing temperature contours. Note the presence of high wattage equipment can create warm zones even with a low mean-age-air.

ity, it can be a good investment. A very valuable aspect of CFD is that it can help identify potential problems in the design phase of a facility. CFD can be used to identify short-circuiting and dead-air regions that can affect the operation of ventilation equipment in a room. Additionally, it can sometimes identify savings in airflow while still meeting ACH requirements. The value of CFD is in a facility that operates better and safer from the start, without costly retrofitting, and protects the most valuable asset in the room, the employees. The cost of the failure of a design to operate as suggested by simple analytical calculations is difficult to estimate. The results could be higher operational costs, a less efficient workspace, or even safety threats to occupants and potential litigation.

### Information Needed

When communicating with an applied CFD engineer, it helps to have a basic understanding of the information needed to develop a CFD model. A short list includes:

- Floor and ventilation plans
- Characteristics of objects in the room
  - Dimensions
  - Location
    - ◆ Fixed or mobile
  - Heat sources in watts
  - Device inflow/outflow
    - ◆ Is it just air or are other chemicals/species being released?
- Ventilation
  - Location
  - Type (flow area)
  - Flow rates (inflow/outflow)
  - Temperature

When presenting data, it is very important to clarify the units of measurement being used. Most CFD codes default to metric units, which may not be consistent with the units used by the architects, developers, and HVAC designers for a project. In addition, be sure to communicate the design priorities to the CFD engineer since this will often affect how the computer model is built.

### Conclusions

The objective of this paper is to provide the practicing biological safety professional a context for applied CFD. This background includes a discussion of the basic considerations of grids and their relationship to solution quality. The two modes of contaminant transport, flow pattern and Fickian Diffusion, are explained in lay-terms. The importance of having a skilled CFD expert interpret results is explained and an example is provided with a focus on ACH criterion. Results from a simulation of a hospital and a BSL-3 environment are provided. The costs associated with CFD and the potential value-added is explained. Finally, a list of key information needed to develop a CFD solution is provided to facilitate communication between the biological safety professional and the applied CFD engineer. For an indoor environment, CFD can provide more detailed information than analytical calculations and is the next best option to building a scale model to test a facility design.

### Suggested Further Reading

In lieu of References, a Suggested Further Reading list in order of increasing technical complexity is provided.

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