TASK SHEET 1E

USE OF COMPUTATIONAL FLUID DYNAMICS (CFD) FOR LABORATORY AIR FLOW

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Introduction

Computational Fluid Dynamics (CFD) is an intensive computer-based method to calculate detailed air flow patterns within a room or air space. CFD modeling can produce results that may otherwise be difficult to observe experimentally. Room temperature, air speed and direction, humidity, static pressure, and contaminant concentration can be calculated over millions of locations within the room and within exhaust devices. The results can then be presented graphically in many ways. However, simply running a CFD simulation program does not provide meaningful results unless well-established guidelines and best practices are followed. This paper presents some guidelines on using CFD for laboratory ventilation given the current state of CFD development. A brief introduction to CFD and the typical steps used in performing CFD are presented in **Appendix A.**

Types of CFD Models

There are two main classifications of CFD models of interest for laboratory ventilation:

1) Turbulent transport models (called RANS)

2) Large Eddy Simulation (LES)

The turbulent transport RANS (Reynolds-averaged Navier Stokes equation) models are less detailed in modeling sophistication, where turbulent fluctuations are fully parameterized. RANS models also typically (but not always) produce only average values of the computed quantities at each grid point. The RANS model is less computer resource intensive and is the more common approach at this time. Within this group there are various types of turbulence closure models that are available through CFD providers. At the present time, the SST k-omega turbulence model is a recommended turbulence model.

The Large Eddy Simulation (LES) model is a more detailed approach with direct simulation of larger turbulent eddy scales and parameterization of smaller scales. LES models are intrinsically transient and produce a time history of computed results at each grid point. The LES model can show important time dependent fluctuations, such as the periodic disruption of fume hood air flow by room currents. The LES model requires finer grids and thus requires much more computer power and computation time than the RANS models. LES models have recently become economically feasible at the engineering design level. At this time LES models do take a significant amount of time, but are definitely worth the cost in some situations where RANS models are weak. Detailed flow modeling within a fume hood and transient modeling of spills are two examples when LES should be used.

Recommendations for Using CFD Modeling

It is important to note that CFD models have a variety of inputs and setups that may not be obvious to the HVAC engineer. Below are presented some recommendations for using CFD models, but it should be stressed that these guidelines cannot substitute for direct experience. Commercial CFD developers should provide guidance and training applicable to their specific products. Users should gain experience first with standard room applications. More detailed guidelines can be obtained from the ASHRAE Handbook of Fundamentals (2005), Chapter 34 “Indoor Environmental Modeling” (or the later version of the handbook due in 2009).

- It is recommended that LES modeling be used for detailed studies of air flow around and within fume hoods rather than using RANS models. Leakage from a fume hood is often a transient phenomenon that is better simulated by a detailed model like LES. In this case, the extra costs of the LES model are justified.

- The grid spacing used in the room is very important for accurate results. Recommended spacing is one inch or less in important areas such as the face of a fume hood and other areas where large variations are expected, and no more than six inches in the general air space far from surfaces and boundaries, where small gradients are expected. The grid spacing should be varied in size (example, by doubling the number of grid points) for some runs to show that the results are independent of grid spacing. As computer speed and memory storage become more economical, grid spacing should be reduced as much as possible.

- For transient calculations, time steps should be appropriately small to ensure convergence of the models. Time steps will decrease as grid spacing decreases, which increase the need for computer resources. Time steps should also be varied to show independence.

- Internal heat sources and sinks should be modeled. These include workers, animals, equipment, lighting, radiant cooling panels, chilled beams, and outdoor sunlight.

- Boundary influences such as walls, windows, people, furniture, supply diffusers, exhausts, and equipment geometry should also be included.

- Correct modeling of supply diffusers is critical to modeling laboratory ventilation. Diffusers are too small compared to the room to accurately model with normal grid spacing. The direction, temperature, and speed of air can vary dramatically depending on the location within the exit of the diffuser. To overcome this problem, several methods have been developed to model the overall effects of the diffuser in terms of momentum and directionality. The 2005 ASHRAE Fundamentals Handbook, Chapter 34, has more information. The particular method should be evaluated in simple room geometries to match the published throw and directions of a diffuser model using manufacturer supplied data or other measurement results.

Two figures are shown below that illustrate the possible differences that can arise in modeling supply diffusers. The first figure shows the exhaust with the correct flow rate but an incorrect velocity, due to exaggeration of the outlet area. The second figure has a correction to better model the supply momentum to better match empirical data from the manufacturer. However, in some cases, the manufacturer data may be suspect. For example, some diffusers will tend to dump colder air downwards rather than distribute the exhaust in many directions as predicted.

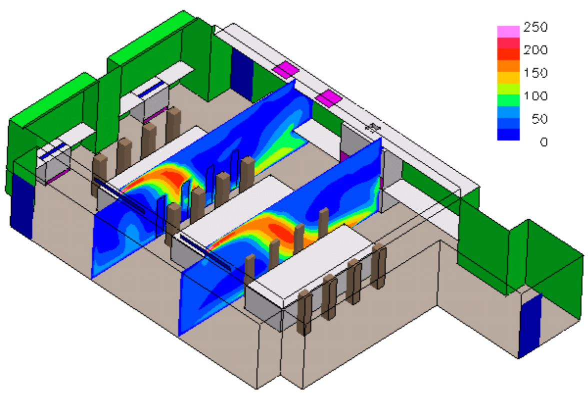

Figure 2 - Incorrect Modeling of Supply Momentum

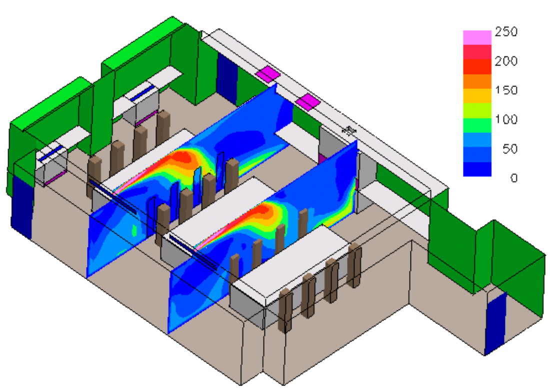

Figure 3 - Corrected Momentum to Match Diffuser Throw Data

When to Use CFD Modeling

Not all laboratory configurations need specialized CFD modeling. Some likely applications for CFD are listed below:

- Rooms with large heat sources from equipment that may challenge thermal comfort and require significant cooling for the equipment itself.

- Rooms where cross contamination from one area to another must be minimized but cannot necessarily be controlled with local exhaust equipment. One example is a specialized room where several human patients are treated in a series of stations. Over-ventilation in one station could push contaminants to other parts of the room.

- Specifying supply diffuser designs where large exhaust flows are concentrated. In this case, supply air may need to travel from other parts of the room towards the concentrated exhaust area. The traveling supply air may create disruptive room currents with higher air speed than desired approaching the fume hoods. A smaller room with a large air change rate and numerous exhausts would also be a good candidate for CFD, where it may be a challenge to provide low velocity supply air due to lack of ceiling area.

  One modeling strategy in selecting a diffuser layout is to compare a proposed design to the "ideal" case of a uniform low velocity supply that covers the entire exposed ceiling (omitting areas over high cabinets). An example is shown in Figures 4 and 5 below with an ideal case compared to two diffuser configurations. Figure 4 shows the room layout, and Figure 5 illustrates the modeling results within the central portion of the room. The results shown are the velocity pattern at four feet above floor level, in plan view. The ideal case (top diagram of Figure 5) shows relatively low velocities near all fume hood entrances at the top and bottom edges of the diagram and at the corridor near the top left corner. The second and third diagrams of Figure 5 show the increased room velocities when real diffusers are used. In this example, the first diffuser configuration (second diagram) appeared to have slightly better performance at the corridor.

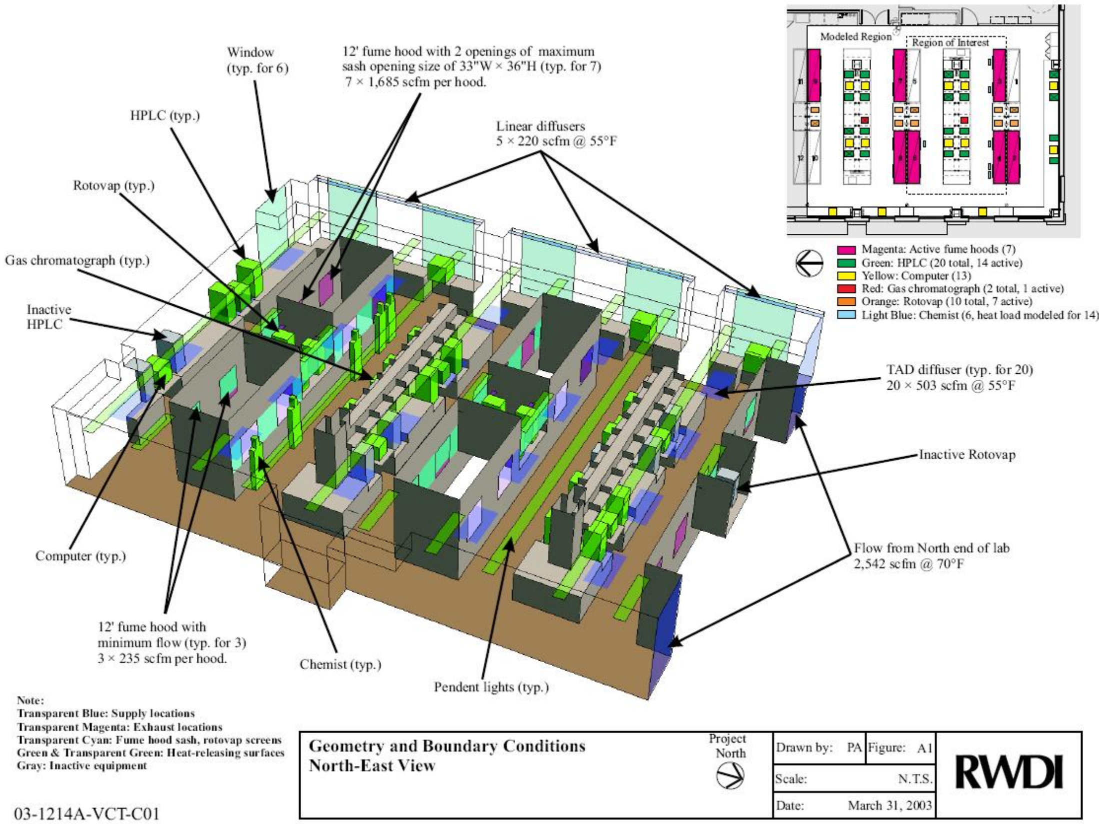

Figure 4 - Room Layout Example

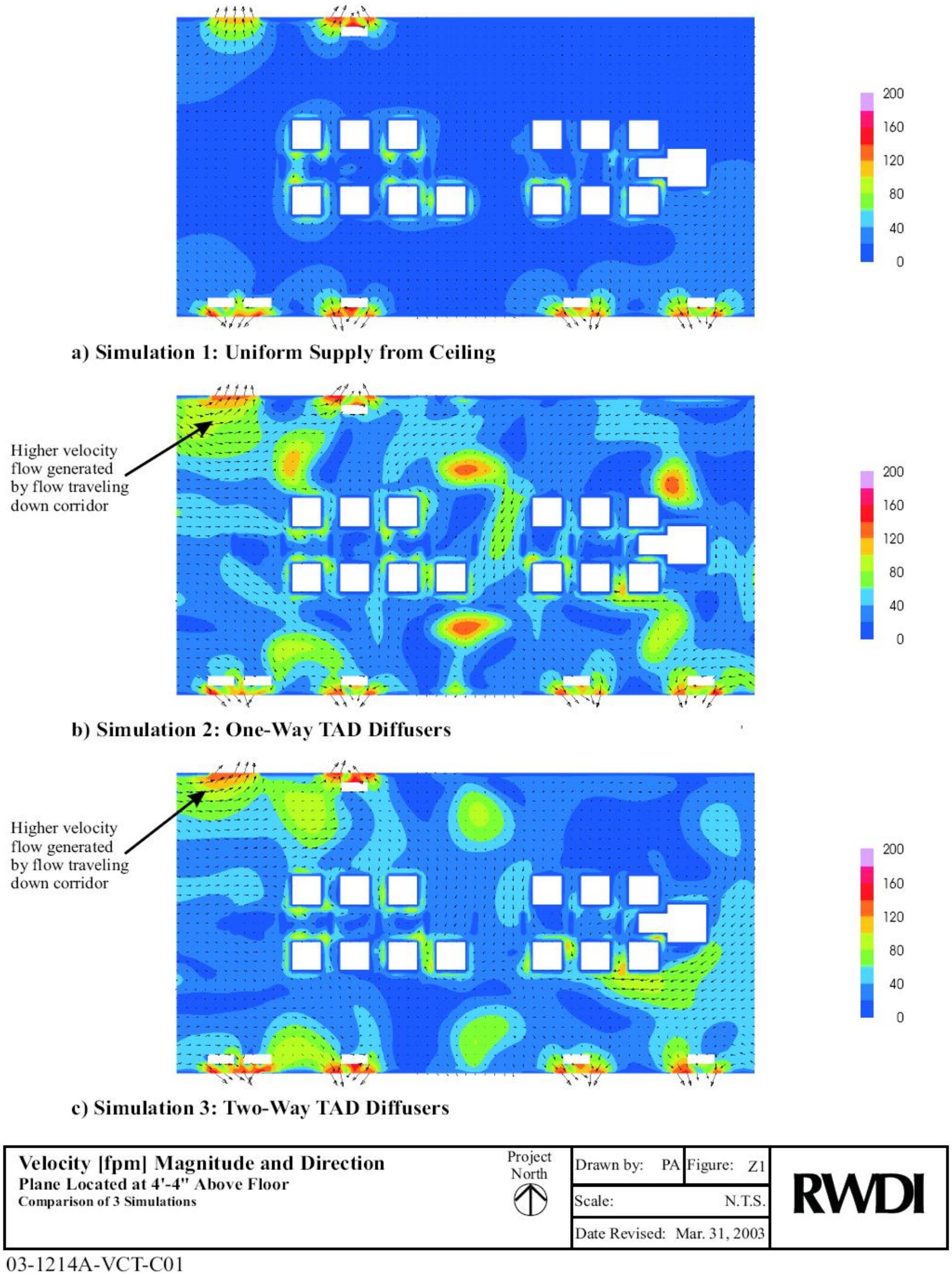

Figure 5 - Comparison of Two Diffuser Configurations to Ideal Uniform Supply

Converting CFD Results to Usable Information: Some Suggested Design Criteria

CFD programs have the ability to produce many types of post-processing and outputs (i.e. “pretty pictures”). It is not always obvious how to interpret these results. The following are some suggestions for evaluating parameters of interest for use in changing and evaluating designs. Quantitative calculated results may be more useful in making decisions than colorful animations or pictures. On the other hand, the colorful visual products can be more useful in understanding flow phenomena.

Thermal Comfort. Thermal comfort is a complicated physiological and psychological reaction to several environmental factors, such as temperature, air velocity, humidity, thermal radiation, activity level, and clothing level. Examining velocity and temperature fields alone may not be able to fully assess comfort. It is recommended that the ASHRAE Standard 55 – 2004 “Thermal Environmental Conditions for Human Occupancy” be used to establish comfort at various fixed points of interest. The 2004 version is a notable change from earlier editions.

Fume Hood Leakage. Fume hood leakage could be reported in several ways. One way would be to simulate a release scenario much like that specified in the ASHRAE Standard 110-1995 for tracer gas testing, by releasing 4 liters per minute of tracer gas in the hood and reporting concentrations at the breathing zone. (Note that the ASHRAE standard does not specify an acceptable concentration). Another method would be examining a cross-section of concentration and velocities at the hood face. Locations of outward moving high concentrations into the room would indicate undesirable leakage. The reporting could be a simple cross section of concentration at the hood face. Alternatively, post-processing could calculate the mass emission rate outward (the product of concentration, outward velocity, and face area over all calculation points along the face).

Room Air Currents. For understanding room ventilation patterns, visualization of room velocities and temperatures is useful. There are a number of ways to achieve visualization. Traditional cross-sections in vertical and horizontal planes are helpful, but cannot easily show the entire room. One way to show more of the room is to use a series of cross sections in an animation. Another way is to have a 3-D surface created that shows velocities (or other values) above a certain amount. For example, a high velocity jet, say above 100 fpm, can be illustrated as a 3-D “tube” that emerges from the diffuser and extends into the room. A cold supply plume, with temperature below a certain level, could also be shown as a 3-D object. Another whole-room approach is an animation by following numerous virtual particles that travel through the room over the calculated velocity field. The particles would tend to travel from the supply diffuser into the exhaust system. These particles can be color coded with travel time, so that the areas of the room with stale air (longer travel times) are more visible.

For evaluating cross drafts, the models can report maximum and average room velocities at specific points in front of fume hoods. The velocities can be compared to typical specifications, such as no larger than 50% of face velocities.

High velocities may not be desired at workbenches with fragile or sensitive experiments. Velocity predictions at specific points in the room are easily generated and could be plotted and compared to a requirement.

Concentration Levels from a Spill or Large Release. For concentration fields where a contaminant is typically released from a small source, the best visualization is with a 3-D smoke plume that shows concentrations above a fixed level. The plume could be fixed in time as with a steady-state RANS calculation, or with a growing plume with a transient LES model. Also, concentrations at specific locations can be reported and graphed, for example at possible ignition points when evaluating LEL (lower explosion limit) situations, or at breathing zones.

Tools Necessary For Evaluating Work Done By The Consultant

This section summarizes how the university or building owner should approach CFD modeling and interacting with a CFD consultant.

The first step is to determine if any modeling is needed, and what the goals of any modeling will be. The previous section on Suggested Design Criteria outlines several possible goals, such as evaluating thermal comfort, fume hood leakage, room air distribution, and concentration levels from a large release. The section When to Use CFD also describes situations where CFD is useful.

For room air distribution, the companion Task Sheet 1-c describes several procedures for designing room air distribution systems. In some cases, not all of the recommendations can be met, for example because of crowding of hoods. CFD could be used to fine-tune the design as much as possible.

Fume hood leakage is a challenging subject; in-place tracer gas testing has shown that even regular fume hoods may have excessive leakage due to unforeseen circumstances in the room. However, there may be some unusual hood designs with multiple openings or using heavy gases, where modeling prior to installation would be useful.

The next step is ensuring that the consultant is using the best type of CFD for the application, i.e. LES versus RANS. This is described in the Section “Recommendations for Using CFD Modeling. In general, LES is more accurate but is not at this time necessary for general room air distribution or for thermal comfort.

Ideally the university or building owner would review the methodology to be used in some detail. Unfortunately, at this time the methodologies are still advancing and are complicated, and there will not be many opportunities for detailed overview. The simulation of diffuser throw, as described in Figures 2 and 3, is an important detail.

Another important detail is that the consultant should demonstrate that grid spacing and time steps are sufficiently small and do not greatly affect the results.

Finally, the results of the modeling should be explained in terms of the original goals and criteria initially developed. The consultant should provide recommendations and insight into the results, as well as computer generated graphics.

Summary

Computational Fluid Dynamics (CFD) modeling is relatively new to laboratory design but has the potential for refining exhaust and supply system design to improve safety and reduce energy costs. An introduction to basic CFD concepts and applications is provided from a management and designer point of view.

References

ASHRAE, 2005. *Handbook of Fundamentals*. Chapter 34, "Indoor Environmental Modeling". American Society of Heating Refrigeration and Air-Conditioning Engineers, Inc.

ASHRAE, 2004. *Standard 55 – Thermal Environmental Conditions for Human Occupancy*. American Society of Heating Refrigeration and Air-Conditioning Engineers, Inc.

ASHRAE, 1995. *Standard 110 – Method of Testing Performance of Laboratory Fume Hoods*. American Society of Heating Refrigeration and Air-Conditioning Engineers, Inc.

APPENDIX A. Brief Introduction to CFD and Typical Methodology

As an example of a CFD simulation, Figure 1 shows a cross-section view of velocity and temperature near two diffuser outlets. The figure shows only a small slice of the calculations actually performed for the entire room.

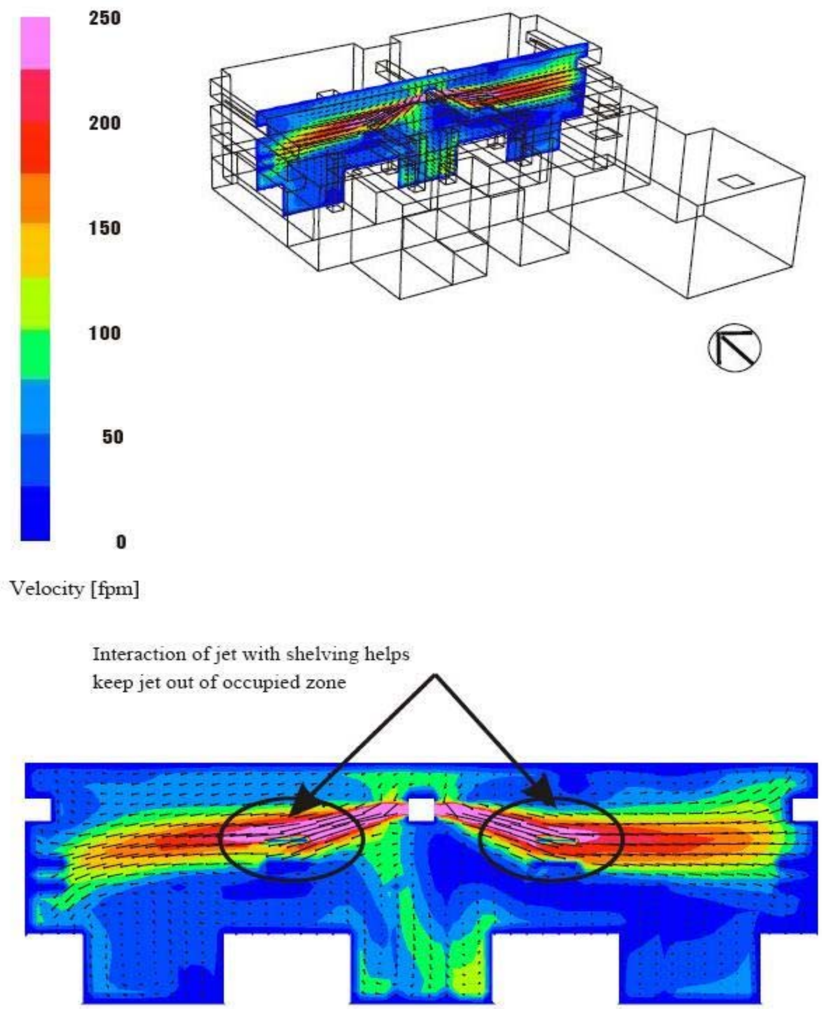

Figure 1 - Example CFD Output – Single Cross-Section of Velocities

Possible Uses for CFD in the Laboratory

CFD could be used to predict several aspects regarding laboratory ventilation:

- The containment ability of fume hoods.
- The best locations and configurations of fume hoods and supply diffusers.
- Whether thermal comfort is achieved, considering temperatures and draft velocities, radiant energy and activity and clothing level of the people.

- Whether low room air velocities are achieved at workbenches and other sensitive areas.

- Where contaminants from releases or spills may be transported within the room.

- Where LEL (Lower Explosion Limits) may be exceeded within a room for various releases.

- How specialty hoods with unusual characteristics behave, such as those with multiple openings.

CFD Methodology

Using CFD involves several steps:

- *Model development* involves the creation of a three-dimensional computer model of the room geometry using a computer-aided design (CAD) package. The model geometry usually includes the interior of the space being modeled and any obstructions to flow present within the space. Supply and exhaust points are identified within the model and are represented to provide similar flow characteristics to actual supply and exhaust points. During the model geometry creation phase, some simplifications are typically made based on experience and an understanding of the flow details of interest. For example, furniture and human shape geometries are often simplified to represent approximate massings. Another important simplification is the modeling of supply diffuser geometries. This simplification requires careful attention to produce correct air flow characteristics and is discussed later.

- *Grid generation* involves the subdivision of the room into often millions of three-dimensional cells within which the equations of motion will be solved.

- *Boundary conditions*, or the factors influencing the flow within the space are assigned to the model. These conditions typically include such things as air supply flow rates and temperatures, exhaust rates, heat flows through surfaces (e.g. walls, roof, floor) and internal sources heat and contaminants (e.g. equipment, humans, animals).

- The *Solution* phase consists of a computer solving a complex and coupled set of equations enforcing the conservation of mass, momentum, energy, and various species of interest between each cell within the space. Within each cell is stored the variables of interest (e.g. temperature, velocity, concentration, turbulence).

- Finally, the *Post-Processing* stage allows the engineer to visualize and probe the resulting flow in both space and time, through colorful stills or animations, providing understanding, including to people unfamiliar with CFD.