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PRACTICAL APPLICATION OF THE LES METHOD TO MIXING IN LARGE INDOOR SPACES

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ABSTRACT

The scope of protecting public venues in the U.S. is staggering in the areas of money, time and experience at doing this sort of thing. Derivation of protection strategies for the building infrastructure will necessarily involve a combination of experiments and computer simulations to provide confidence in building design or retrofit before the needed dollars and time are committed. Computer simulation can be less costly and be performed in shorter times than experiments even when the building of interest is quite large and thus, will be used extensively now and in the future for building protection design. This paper specifically targets the accuracy and application of computational fluid dynamic (CFD) codes for prediction of mixing behavior. The ability to determine the nature, make correct identification and quantify the amount of a release from a chemical or biological weapon (CBW) relies in part on understanding the underlying physics of air propagation throughout the domain. Specifically, we must understand the rates at which a contaminant may mix throughout the domain. Turbulent mixing is a function of the range of spatial and temporal scales found in the domain, i.e., the large scale eddies (on the size of the domain) advecting the contaminant, the small scale eddies (inertial range) "mixing" the contaminant as it is being advected and the time scales corresponding to these eddy sizes. The widely used Reynolds Averaged Navier-Stokes (RANS) numerical modeling methods cannot capture the time dependent motions which are responsible for a significant amount of mixing. The Large Eddy Simulation (LES) method is based on simulating the turbulent fluctuations that can be resolved by the mesh while the smaller eddies are modeled. The LES method can produce more information about the nature of the flow field than RANS. This paper discusses the application of the LES method, specifically an LES/DES (Detached Eddy Simulation) coupled method, to simulate mixing in a realistically scaled fictitious airport. Application of the LES method such as determination of what eddy size to resolve, transient startup effects, determination of eddy turnover time and others are discussed.

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Keywords: LES, large eddy simulation, turbulent flow, scalar mixing, chemical and biological protection

INTRODUCTION

Analysis of protection from CBW attacks involves asking 'micro' sized questions of concentration for 'macro' sized domains such as office buildings and airports. A example question is: 'How many particles will reach a location for a sensor in that location to trigger?' The large eddy behavior is dependent upon the geometry of the domain in question forming the macro scale problems and the small eddy mixing accounts for most mixing effects which form the micro scale of the problem.

Questions pertaining to building protection contain macro- and micro-sized questions that are based on the physics and computational constraints. Large scale issues entail: There are large domains to be protected. Large eddies are that advect the contaminant are geometry dependent. Long time scales for flow evolution and for the contaminant to decay. Small scale issues entail: Small contaminant release amounts. Particle diameters are on the order of one micron. Release amounts are suspected to be near 1 g. There will be small eddy mixing in the large eddies. This will account for the anisotropic propagation of the contaminant as it is being advected by the large eddies.

Accounting for the large and small scale issues will eventually help us determine what concentration amounts will arrive at the sensors. The non-homogeneity of the concentration plume may be an issue at the small scales versus using Gaussian plume models.

In light of the state of world terrorist attacks, protection agencies need to act quickly. They must evaluate:

- ◊ many attack scenarios
- ◊ many protective responses
- ◊ costs versus effectiveness for many attack/protection combinations
- ◊ attack/protection combinations for varied public building architectural layouts

Conducting experiments is the most preferred way of evaluating what-if scenarios for fluid flow. However, there is a low tolerance for experiments in public venues; simply too much cost and liability. Therefore, computer simulations provide an opportunity to gain insight into attack results and protection measures with a smaller amount of capital investment and within shorter times than experiment.

Computers are now capable of calculating LES simulations in time frames similar to RANS calculations. This allows engineers to simulate fluid flows that require accurate representation of the large scales of the flow. For this study, 'large scales' was considered to be approximately 0.3 m to 15 m. This range encompassed the mixing eddies near 0.3 m up to the large advective eddies of 15 m.

Analysis of attacks will be transient in nature following a timeline after the attack. Therefore, steady state solution methods cannot be employed. The RANS method is an averaging method and can incorrectly average out a transient flow to a steady state flow. Therefore, a more accurate transient solution method must be employed.

This paper contains an assessment of the use of LES as the tool for choice for CFD analysis of CBW attacks in an airport check-in terminal. The assessment tools that are recommended for assessment on all CFD models. For security purposes, some plots and graphs do not contain axes or legends.

NOMENCLATURE

1D	one dimensional
2D	two dimensional
3D	three dimensional
CBW	chemical and biological weapons
cfm	cubic feet per minute
D	diameter
DES	detached eddy simulation
DNS	direct numerical simulation
HVAC	heating, ventilation and air conditioning
k-ε	RANS turbulent model
$k(l)$	kinetic energy of turbulent eddies
l	length scale of an eddy
l_0	length scale of a characteristic eddy
LES	large eddy simulation
RANS	Reynolds Averaged Navier-Stokes
Re	Reynolds number
St	Stokes number
u'	deviation of the x-component of velocity from its mean, u
v'	deviation of the y-component of velocity from its mean, v
w'	deviation of the x-component of velocity from its mean, w
η	Kolmogorov length scale
ϕ	scalar or contaminant

FLOW IN LARGE SPACES

Advection by air currents within a terminal is the primary transportation method of airborne particles. Accurate predictions of the flow patterns are required to analyze detection and mitigation responses. A discussion of general fluid flow principles below will delineate the flow features that need to be captured in order to have confidence in the solutions and understand the mechanisms that account for the mixing.

Understanding types of flow regimes begins with the calculation of the Re = vl/ν, where v is the velocity magnitude, l is a characteristic length and ν is the kinematic viscosity of the fluid, in this case, air. The Re for the flow in the terminal based on a characteristic length of nine meters and the velocities of the supplies of 0.472 m/s is 380,000. Therefore, the flow is turbulent.

Experiments in turbulent flows have shown that there are eddy sizes that range from a characteristic size in the domain down to sizes that are dissipated by viscous shear [1]. Based on the Re for this flow, the smallest sized eddy in the flow, η, is approximately 0.00078 m. The shapes of the large eddies created by the HVAC are a function of the geometry of the domain, in this case the islands, vendors and the shape of the outer boundaries of the terminal. The size of the large eddies can be on the order of nine to fifteen meters using a terminal's general dimensions, particularly the height of the ceiling. The large eddies are responsible for transporting a contaminant large distances within the domain. Anecdotal evidence using flow visualization show that there are eddies on the order of 0.3 m that are responsible for mixing the contaminant while it is being transported by the large eddies.

There are many different flow regimes in a large space that must be captured by a simulation code. There is free shear coming from the jet flow at the supplies. Jets enhance mixing and exhibit fast momentum diffusion in a short distance.

Boundary layers in the terminal are probably 3D with adverse pressure gradients. Common models use the Law of the Wall which is valid for 2D flows in equilibrium with favorable pressure gradients.

Buoyancy plays a large part in adding momentum to the flow. Large areas of south facing windows in a terminal will be major heat sources or sinks depending on the time of year. The effects of buoyancy was not studied for this project.

The large and small eddies will need to simulated with a code that has robust treatment of streamline curvature.

The flow may or may not be statistically steady, non-stationary flow

The large scale flow will be anisotropic due to the irregular geometry of the domain. It is unknown whether the small scale eddies (inertial range) are anisotropic but it is equally unknown whether the isotropic nature will have an effect. The focus here is to have the small eddies actually resolved for their overall mixing effect.

SIMULATION OF FLOW AND MIXING

Below is a possible ranking of fluid simulation codes based on the ability to predict turbulent mixing at the scales needed for prediction of contaminant mixing. Other methods may be more accurate at the smaller scales needed for combustion and other physics [2].

DNS is the most accurate method for simulating fluid flows. With the advancements of computer speeds, there have been many discoveries of fluid characteristics using this method. However, DNS is still computationally intractable for many industrial flows of Re > 10^3.

LES is the one of the next most accurate methods and now becoming computationally tractable for large Re. As stated before, the eddies that need to be resolved for mixing in the terminal is on the order of 0.3 m.

The RANS method contains many assumptions that average the solution in some way. A discussion of these assumptions is in the next section. RANS can be accurate for steady state flows and ball park answers. It is computationally tractable for many Re. The RANS method is a good approach for insight and many flows are steady state. However, closure models are frequently misused in attempts to 'just get a converged solution.'

Lumped parameter models such as CONTAM, COMIS and DEGADUS are 1D descriptions of flow and mixing. They are not designed to capture the Kolmogorov range of eddy sizes, assume instantaneous mixing and are not considered for use for this class of problem.

A more detailed description of all three methods can be found in the textbooks of Pope [4] and Wilcox [5].

REYNOLDS AVERAGED NAVIER-STOKES

The RANS is a time averaging method. As such, transient features such as small eddy mixing will be averaged.

RANS was developed based on the assumption of turbulent intensities of 10% or less. Flows inside offices and large spaces possess flows that have turbulent intensities of 10% or higher.

The results of RANS simulations are sensitive to closure methods such as k-ε and the Reynolds Stress models.

Transient runs may not stay transient and eventually reach a steady state – the averaging helps the solution to "relax" to a steady state that may not exist in the real flow. The transfer of energy to the large scales is thought to explain the tendency of numerical simulations to evolve from random velocity fields toward states consisting of a few large scale regions of like-signed vorticity [6].

Three dimensional fluctuations at any scale are averaged to a one dimensional direction as shown in Figure 1. The averaging will produce 'smooth' flow fields.

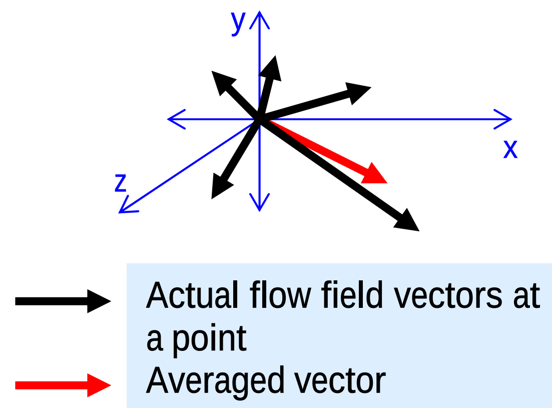

Figure 1. Eddies centered at a point in the flow will fluctuate in many directions (black vector). Time averaging will average this behavior into one direction (red vector).

EQUILIBRIUM TURBULENT FLOW MODEL

The k-e model has some assumptions that are not applicable to flows in large spaces when trying to assess mixing behavior. It was developed to predict wall bounded flows in equilibrium.

Jet spreading requires adjustments of the coefficients to balance the dissipation of energy with its production. Experiments must be used to obtain these new coefficients for each flow that a jet is in.

The k-e model was developed to predict conditions with a favorable pressure gradient, assumes isotropic turbulence and thus has weak treatment of streamline curvature.

Because of these assumptions, turbulent particle tracking models must be used with the RANS/k-ε method to attempt to predict the paths of particles from a release. These models use information from Gaussian sampling from the local velocity vector plus the sqrt(k) The Gaussian sampling is done because the sqrt(k) does not give information on u', v' and w'.

LARGE EDDY SIMULATION

The LES method is an attempt to directly represent the larger three dimensional unsteady turbulent motions. The smaller eddies are modeled using sub-grid models. The Smagorinsky Sub-grid Scale Model is one such model.

The LES method can an accurately simulate strongly non-equilibrium flows, separated flows (law of the wall is not valid) and unsteady, anisotropic turbulent flows.

LES has a more rigorous treatment of vorticity. The energy transfer from large to smaller eddies and from small to larger eddies is still an area of research. However, LES model methods of capturing the energy transfer has been more accurate than that of the RANS method.

FLOW SOLVER

LES cannot be used to calculate flows in the near-wall region. The DES method is more accurate in the near wall region than the more commonly used Smagorinsky model.

AcuSolve was chosen as the flow solver because of its high accuracy and speed. AcuSolve is a finite element method that is fully coupled for greater accuracy

A proprietary iterative linear solver plus preconditioner allows the code to execute faster and thus, makes a fully coupled solution more attainable.

AcuSolve is directly coded for parallel application thus increasing its speed – there are no legacy code issues.

AIRPORT ARCHITECTURE, MESH AND RELEASE PARAMETERS

A generic airport check-in terminal model was created and is shown in Figure 2.

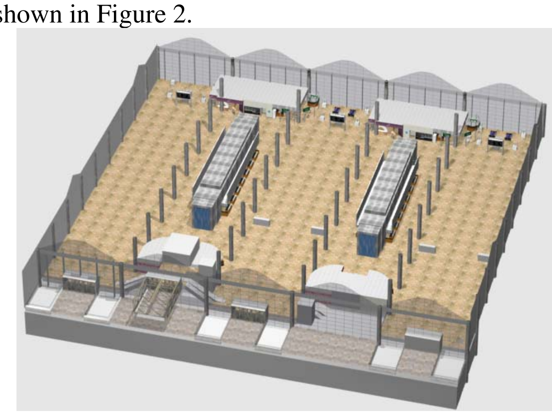

Figure 2. A view of the check-in terminal model without the roof.

Release parameters include location, amounts and speed. Locations can include: w alls, chairs, phone booths, etc.

Amounts will be dictated by what can be realistically manufactured which will be in grams.

The speed of a release would depend upon the release mechanism. A slow release or an explosive release. For this study, the contaminant was released at the same speed as the surrounding fluid.

MODEL SETUP

Computational constraints did not allow the modeling of the whole check-in terminal using CFD. The project ended before we were able to finish our study of modeling different portions of the terminal. If the mixing rate is dictated by eddies on the order of a meter then the partial domain models should still compute the correct mixing rate of the contaminant. However, the contaminant is also advected by large eddies that could possibly span the length or width of the terminal and so would not be captured by a partial domain model.

The corner of the terminal is shown in Figure 3. It is about 1/16th the size of the whole domain. The next sized mesh is shown in Figure 4 which is approximately 1/8th of the terminal. The last CFD model attempt was a 1/4th sized model shown in Figure 5.

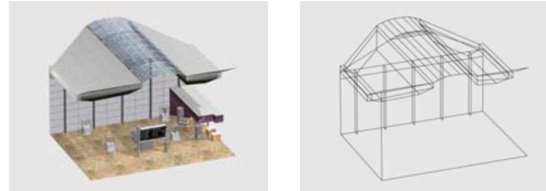

Figure 3. A textured and wireframe representation of the 1/16th portion of the terminal used for the CFD simulations.

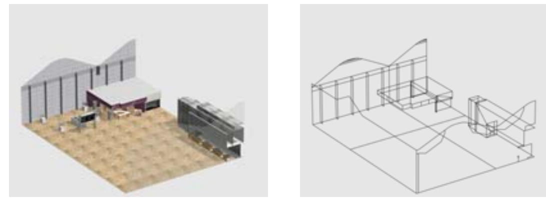

Figure 4. A textured and wireframe representation of the 1/8th portion of the terminal used for the CFD simulations.

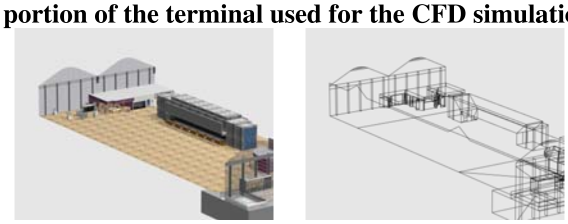

Figure 5. A textured and wireframe representation of the 1/4th portion of the terminal used for the CFD simulations.

There are three choices to model the boundaries that cut though the interior of the domain. They are outlet flow, a pressure boundary or symmetry. On both cases of the outlet flow and the pressure boundary, the code will not know the conditions on the other side (outside of the model domain) to compute incoming flow. In order to get a solution, most CFD codes simply mirror nearby outgoing velocity magnitudes and reflect the vector 180° to make it enter the domain. Therefore, the conditions at the boundary can start to drive the flow which can result in a flow field that is not representative. In the 1/16th and 1/8th models two walls were specified as symmetry. It was assumed that the flow inside the whole terminal would exhibit to quantitative behaviors: advection throughout the domain due to the large eddies and mixing at the two meter scale and below. By using the symmetry boundaries, the small scale mixing is still accurately calculated while the large eddy advection through out the terminal is omitted. This assumption then makes the mixing results an upper bound in that the concentration amounts will be higher in the models than the respective portion in a real terminal.

The airflow rates in each model were specified per building code of 1000 cfm per 600 ft^2. Supplies and returns were placed per building code used for airports. Long thin supplies are usually placed on the floor near the base of south facing windows. This is done to reduce condensation in the cooler seasons and to control the heat produced in the hotter seasons. Supplies are generally placed four to five meters above the floor on walls or above check-in counters and vendor stores. They are oriented such that the horizontal direction of the supply air enhances the flow at the south facing windows.

MESH SENSITIVITY STUDY

The mesh size for the CFD models was based on anecdotal visualization of previous experiments and Kolmogorov's Energy Cascade. To capture 80% of the energy, the smallest grid distance l/l_0 ~ 0.42 as shown in Figure 6.

	ℓ/ℓ_0
$k(\ell)=0.1k$	6.10
$k(\ell)=0.5k$	1.6
$k(\ell)=0.8k$	0.42
$k(\ell)=0.9k$	0.16

Figure 6. The energy cascade based on length scales.

A characteristic length scale of the CFD model domain can be anywhere from 3 m to 15 m. If 3 m is the limiting scale then 42% of that length is 1.26 m. Anecdotal visual evidence directed us to go even smaller. The distance between nodes was targeted to be approximately 0.3 m. We were able to achieve this density with a mesh that was computationally tractable.

A mesh sensitivity study (using the 1/16th mesh) was conducted to examine whether results changed with mesh density. Four different mesh densities were examined.

- ◊ 70,000 nodes
- ◊ 170,000 nodes
- ◊ 457,000 nodes
- ◊ 1,150,000 nodes

It was found that the solution did not change by an appreciable amount between the 170,000 node solution and the 457,000 node solution. The 475,000 node mesh was chosen as an extra measure of accuracy.

CFD MODEL SENSITIVITY STUDY

All fluid models must be checked for boundary condition, initial condition and model assumption sensitivities. There will be velocity gradients of high and low speed flow. A time step sensitivity study was completed to determine when to let AcuSolve use adaptive time stepping and when to force the time step size. During the contaminant release was the only time that the time step had to be lowered to retain transient resolution.

The implementation of the dynamic Smagorinsky model in AcuSolve was compared to the DES method. There were no dramatic differences in the flow but the Dynamic Smagorinsky method in AcuSolve did not have a robust treatment near the wall and so it was dropped from consideration. Therefore, the LES-DES method was chosen.

VORTICITY

Figure 7 and Figure 8 show the vorticity field in a few cut planes of a portion of the terminal. Note the smoothing of the field by the RANS/k-ε method.

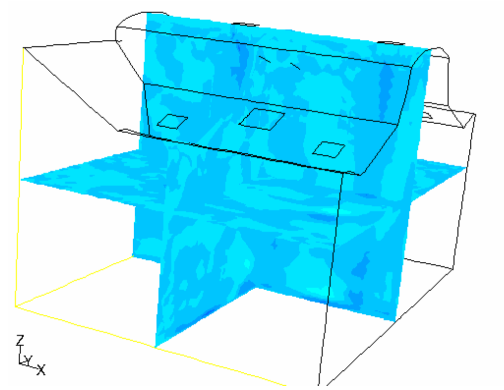

Figure 7. The vorticity field in centered x-, y- and z-planes in the 1/16th portion of the terminal using LES.

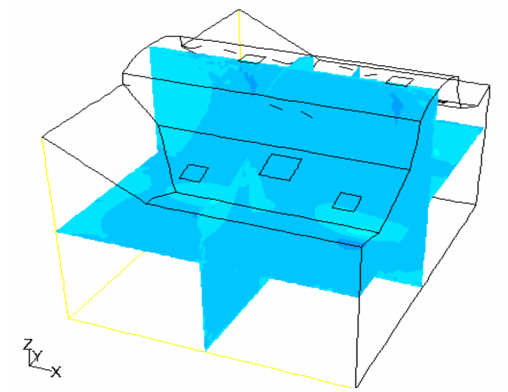

Figure 8. The vorticity field in centered x-, y- and z-planes in the1/16th portion of the terminal using RANS/k-ε.

TRANSIENT EFFECTS

Transient simulations have two places where error could be introduced: during simulation startup and letting the simulation run for enough characteristic eddy turnover time. Eddy turnover time is a characteristic timescale for the domain = l_0/v_{jet} or l_0/v where l is the largest length scale of the domain and v is the smallest vector which gives a bounding estimate. CFD manuals recommend at least 5 to 15 characteristic eddy turnover times from time = 0 to put the flow field beyond startup effects. For the flow in the 1/16th model l_0/v_{jet} = 40 s, therefore startup effects could persist until 600 s. Figure 9 shows that the startup effects went to ~500 s.

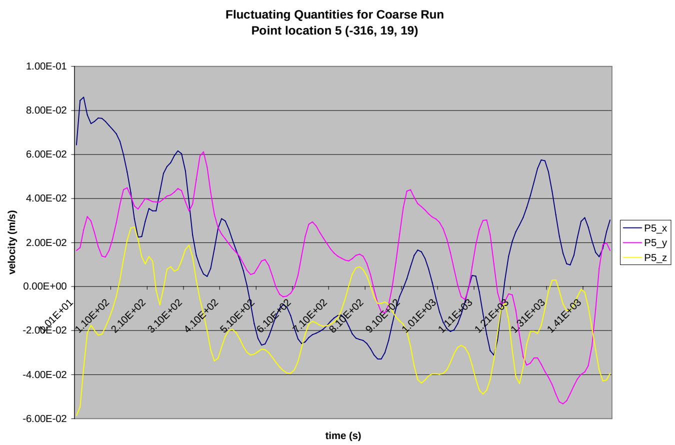

Figure 9. Transient profiles of the x-, y- and z-velocity at a point in the flow.

SCALAR MODELING

Contaminants are either particles or chemicals for CBW analysis. Chemicals can be released in large amounts but are quickly mixed into small concentrations at the leading edges of the plume and can still do damage to humans and facilities at such small amounts. This illustrates the range of scales that will be needed to be resolved in a simulation. Biological threats cannot be manufactured in large amounts. Usually simulations are run for biological releases on the order of grams and the particle size is around 3e-6 m < d < 10e-6 m. The small concentrations of CBW must be accurately calculated on a finite mesh in a large domain. The finite mesh size will cause some numerical error. Dispersing large or small amounts in large domains will cause the concentration amounts to become very small such that simulations should be completed in double precision. A single precision byte has one bit for the plus or minus sign and the other 7 bits are juggled between the fraction and base exponent bias. This strains the computer's capacity for accuracy.

Particles of the size of one micron have a very low Stokes number, St. The St is a measure of settling velocity or inertia and is equal to $(\beta/18)(\sigma/\eta)^2$ where β is the particle to fluid density ratio, σ is the diameter of the particle and η is the Kolmogorov length scale as calculated in a previous section. Particles with high Stokes numbers will settle out of the flow quickly due to gravity. The Stokes number of micron sized particles in air range from 10^{-4} to 10^{-2}. The St for this study is 8.2e-5. When the St is within this range it can be assumed that particle inertia can be ignored and the assumption can be made that the particles will follow the pathlines in the flow.

Resolving actual particles in the flow cannot be done with the computing power available today. The grid would have to have node spacing of D/2 to resolve a particle. Pathlines can be used to trace the paths of where particles would go if the actual particle does not settle with gravity or exhibit centripetal acceleration with the swirl in the flow. Pathlines, however, cannot give concentration amounts unless extra postprocessing is completed. Therefore, pathlines were only used to determine the times when a particle first enter a zone in the domain as an assessment of when sensors would possibly see the first particle. To determine the number of particles at a point over time, the scalar advection-diffusion equation was used. A scalar is a material contained in the flow that does not possess its own velocity nor does it affect the existing velocity field. A scalar is advected by the underlying flow field and can possess its own diffusive properties. The scalar is a continuum while particles are finite. It is assumed for this study that the since the particles do not settle with gravity nor exhibit centripetal acceleration and the release is of sufficient size (~10^{12} particles per gram of release) that the particles are advected and spread in a manner similar to a continuum.

RESULTS – FLOW BEHAVIOR

LES captures the intermittency and anisotropy in a large open space. Figure 10 shows the changes in direction of the three components of velocity at irregular intervals. Note that there is no pattern to the magnitudes but there may be limit as dictated by the energy balance in that location.

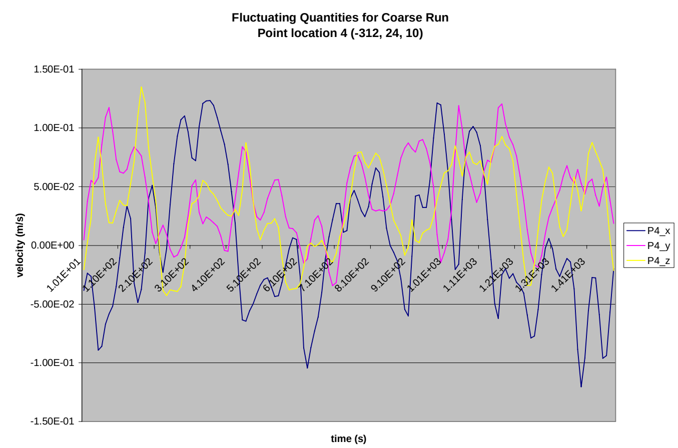

Figure 10. Transient profiles of the x, y and z components of velocity at a point in the flow.

The evolution of the scalar and velocity flow field show a complex morphology [7]. The studies conducted here were not to the scale such that this morphology was examined. The uncertainty in actual prediction of what a real release would produce as far as concentration amounts is larger than what the fine structure of the flow could affect.

PATHLINE EVALUATION

Pathlines allow us to qualitatively assess large flow behaviors. Figure 11, Figure 12 and Figure 13 show the pathlines released from a central location in the domain over time.

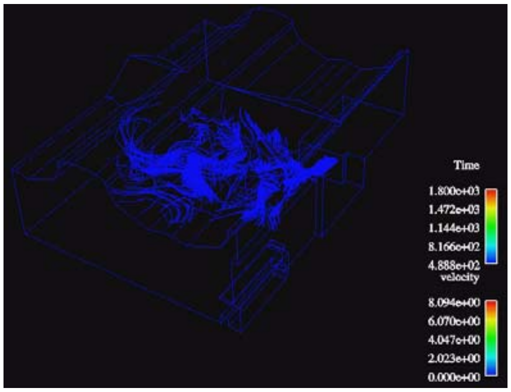

Figure 11. Pathlines extending from a central location in the domain. Time after release is t_1. The pathlines are truncated for easier viewing.

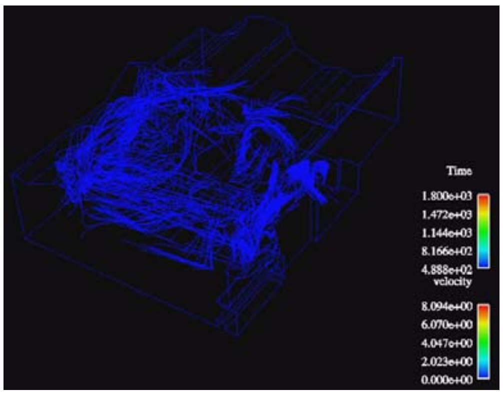

Figure 12. Pathlines extending from a central location in the domain. Time after release is t_2. The pathlines are truncated for easier viewing.

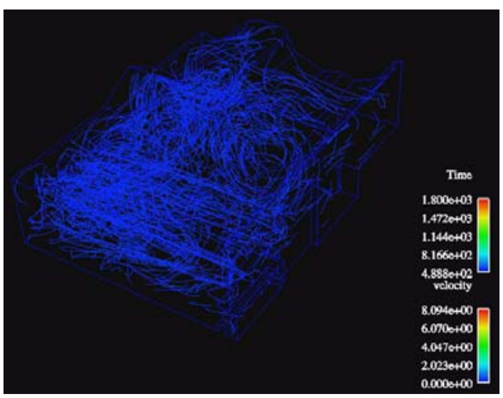

Figure 13. Pathlines extending from a central location in the domain. Time after release is t_3. The pathlines are truncated for easier viewing.

There is no coherent plume shape that an averaging code would predict. Figure 11 shoes that eddies the size of one or 2 meters have great effect on the dispersion of the contaminant.

MICRO RESULTS IN A MACRO DOMAIN

Most models show a single peak leading to an immediate well mixed condition with exponential decay, $Q = e^{rt}$.

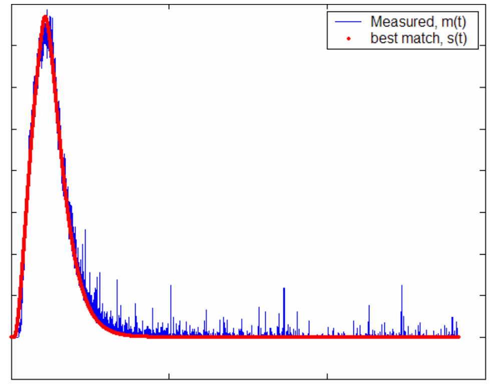

Figure 14. Experimental data showing near instantaneous mixing with exponential decay.

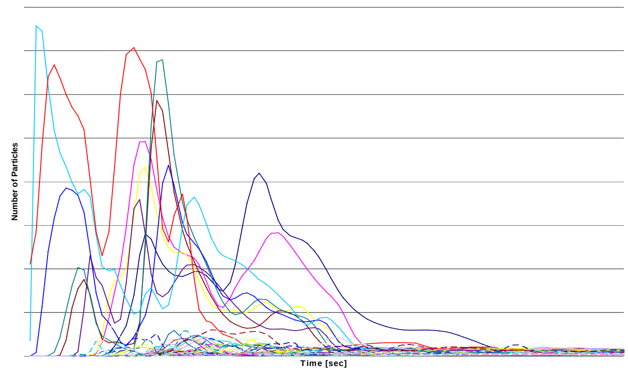

Figure 15. Plume behavior subject to small eddy mixing.

The unsteady, anisotropic motions cause intermittent gradients to appear in the plume which drives sensor development.

CONCLUSIONS

Computer advancements in computational speed is allowing the LES method to replace the RANS method as the CFD method of choice.

Adding LES to the suite of tools used for CFD analysis will require up front learning of the different aspects of the LES approach. Assumptions are different and because the flow accuracy is greater, engineers will need to be more careful in applying boundary and initial conditions to achieve a correct flow solution.

Protection agencies will need tools to evaluate many differing domains (office buildings, airports, train stations, etc.) in a timely manner. LES is a more accurate tool for analysis due to its accurate representation of small eddy mixing and large eddy advection.

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