SECTION III

METHODOLOGY

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3. METHODOLOGY

Airflow and heat transfer within a fluid are governed by the principles of conservation of mass, momentum, and thermal energy. As the equations describing the conservation laws are coupled set of second order partial differential equations, there is no analytical solution available. Therefore, in order to predict the airflow and temperature, at any given point in the isolation room space, CFD techniques are used.

Further, while an Eulerian approach is required for CFD technology, particle tracking is more readily implemented using a Lagrangian approach.

This section describes both the CFD technology, and the simulation of the bacteria particles.

3.1 Airflow Modeling

Airflow and heat transfer within a fluid are governed by the principles of conservation of mass, momentum, and thermal energy. As these conservation equations are coupled set of second order partial differential equations, there is no analytical solution available. In order to predict the airflow and temperature at any given point in the isolation room space, CFD techniques are used.

3.1.1 What is CFD?

Computational Fluid Dynamics can be summarized by the following definitions:

Computational

The computational part of CFD means using computers to solve problems in fluid dynamics. This can be compared to the other main areas of fluid dynamics, such as theoretical and experimental.

Fluid

When most people hear the term fluid they think of a liquid such as water. In technical fields, fluid actually means anything that is not solid, so that both air and water are fluids. More precisely, any substance that cannot remain at rest under a sliding or shearing stress is regarded as a fluid.

Dynamics

Dynamics is the study of objects in motion and the forces involved. The field of fluid mechanics is similar to fluid dynamics, but usually is considered to be the motion through a fluid of constant density.

This shows that CFD is the science of computing the motion of air, water, or any other gas or liquid.

3.1.2 Overview of CFD

The science of computational fluid dynamics is made up of many different disciplines from the fields of aeronautics, mathematics, and computer science. A scientist or engineer working in the CFD field is likely to be concerned with topics such as stability analysis, graphic design, and aerodynamic optimization. CFD may be structured into two parts, generating or creating a solution, and analyzing or visualizing the solution. Often the two parts overlap, and a solution is analyzed while it is in the process of being generated in order to ensure no mistakes have been made. This is often referred to as validating a CFD simulation.

3.1.3 CFD Solutions

When scientists or engineers try to solve problems using computational fluid dynamics, they usually have a specific outcome in mind. For instance, an engineer might want to find out the amount of lift a particular airfoil generates. In order to determine this lift, the engineer must create a CFD solution, or a simulation, for the space surrounding the airfoil. At every point in space around the airfoil, called the grid points, enough information must be known about the state of a fluid particle to determine exactly what direction it would travel and with what velocity. This information is called flow variables.

3.1.4 Governing Equations of Fluid Dynamics

The governing equations of fluid dynamics represent the conservation of mass, momentum, and energy for a fluid continuum. The conservation of mass states that mass cannot be created or destroyed, and the conservation of energy is similar. The conservation of momentum is simply Newton's Law of Motion (force = mass x acceleration) that is cast in a form suitable for fluid dynamics. Because the governing equations are the three conservation laws, they are also referred to as the conservation law equations. The governing equations receive their name because they determine the motion of a fluid particle under certain boundary conditions.

The governing equations remain the same, but the boundary conditions will change for each problem. For example, the shape of an object may be different, or the speed of undisturbed air may change, and these changes would be implemented through a different set of boundary conditions. In general, a boundary condition defines the physical problem at specific positions. Fundamental boundary conditions include the no-slip condition at the interface between solid and fluid that leads to the formation of a wall boundary layer. Another is the fixed mass outlet where it is ensured that a constant mass flow is extracted from the solution domain at a specified plane.

The governing equations have actually been known for over 150 years. In the 19th century, two scientists, Navier and Stokes, described the equations for a viscous, compressible fluid, which are now known as the Navier-Stokes equations. These equations form a set of differential equations. The generic form of these relationships follow the advection diffusion equation 3.1:

$$\frac{\partial}{\partial t}(\rho\varphi) + \mathbf{div}\,(\rho\,\vec{V}\,\varphi - \Gamma_\varphi\,\mathbf{grad}\,\varphi) = S_\varphi \qquad (3.1)$$

Transient + Convection - Diffusion = Source

Where :

ρ **= density**
$\vec{V}$ **= velocity vector**
φ **= dependent variable**
Γ_φ **= exchange coefficient (laminar + turbulent)**
S_φ **= source or sink**

The variable phi (φ) represents any of the predicted quantities such as air velocity, temperature, or concentration at any point in the 3-dimensional model. This equation is derived by applying conservation law to a flow system. The left hand side of the equation refers to the change in time of a variable within this volume added to that advected into it, minus the amount diffused out. This is in turn equal to the amount of the variable flux (i.e. momentum, mass, thermal energy) that is added or subtracted within the finite volume. Though deceptively simple, only the emergence of ever faster computers over the past two decades has made it possible to solve the real world problems governed by this equation.

The numerical techniques used to solve these coupled mathematical equations are commonly known as computational fluid dynamics, hence CFD for short. At the present time, CFD is the only means for generating complete solutions.

The Navier-Stokes Equations are a set of partial differential equations that represent the equations of motion governing a fluid continuum. The set contains five equations, mass conservation, three components of momentum conservation, and energy conservation. In addition, certain properties of the fluid being modeled, such as the equation of state, must be specified. The equations themselves can be classified as non-linear, and coupled. Non-linear, for

practical purposes, means that solutions to the equations cannot be added together to get solutions to a different problem (i.e., solutions cannot be superimposed). Coupled means that each equation in the set of five depends upon the others, so that they must all be solved simultaneously. If the fluid can be treated as incompressible and non-buoyant, then the conservation of energy equation can be de-coupled from the others and a set of only four equations must be solved simultaneously, with the energy equation being solved separately, if required.

The majority of fluid dynamics flows are modeled by the Navier-Stokes equations. The Navier-Stokes equations also describe the behavior of turbulent flows. Many scales of motion that turbulence contains, especially its micro-scales, cause the modeling of turbulent processes to require an extremely large number of grid points. These simulations are performed today, and fall into the realm of what is termed Direct Numerical Simulations (DNS). These DNS simulations are currently only able to model a very small region, in the range of 1 cu. ft., using current supercomputers. Differential equations represent differences, or changes, of quantities. These changes can be with respect to time, or with respect to spatial locations. For example, in Newton's Law of Motion (F = ma), the time rate of change of velocity, or acceleration, is equal to the force/unit mass. If the quantities depend on both time and space, the equations are written to take this into account, and are known as partial differential equations, or PDE's. In most general formulations, the governing equations for physical phenomena are written in terms of rates of change with respect to time and space, or as partial differential equations.

3.1.5 Flow Variables

The flow variables contain the information about the fluid state at a point in space. Enough information must be maintained in order to specify a valid fluid state; i.e., two thermodynamic variables, such as pressure and temperature and one kinematic variable, such as velocity (note that a velocity will usually have more than one component, i.e., in three dimensions it will have three components).

In this research the variables under consideration are the three components of velocity, pressure, temperature, concentration, and two variables characterizing turbulent levels: turbulent kinetic energy and its rate of dissipation.

Over the past 25 years, CFD techniques have been used extensively and successfully in the mainly high-end sectors, such as the nuclear and the aerospace industries. In its raw and general form, CFD has always been the forte of fluids experts. However, recently the concept of tailoring CFD software, combined with the appropriate expertise in the market segment being addressed, specifically building heating and ventilation, has made it possible to apply these powerful methods to provide fast and accurate results to designers under severe time and

budgetary constraints. In fact, this project would not have been practical without these new elements in place.

3.1.6 How Does it Work?

In order to generate a CFD solution, two processes must be accomplished, namely;

- geometry definition and grid generation
- numerical simulation

In broad terms, grid generation is the act of specifying the physical configuration to be simulated and dividing it up into a three dimensional grid containing a sufficient number of small regions known as control volume cells so that the Navier-Stokes partial differential equations can be solved iteratively. Numerical simulation is the process of applying a mathematical model to that configuration and then computing a solution. These two stages are sequential, the grid generation being performed before any numerical simulation work can be done.

3.1.6.1 Grid generation

Grid generation is the process of specifying the position of all of the control volume cells that will define both the physical configuration to be simulated, and the space surrounding it. Grid generation is one of the more challenging and time consuming aspects of CFD because it involves creating a description of the entire configuration that the computer can understand. The model thus defined must include the relationship with the space surrounding the chosen model as well as the surfaces and processes contained within it. In both cases the most important factor is to maintain a suitable number of control volume cells in areas where there will be large or rapid changes occurring. These changes may be changes in geometry, such as a sharp corner of an object, or they may be sharp changes occurring in the flow field about the object, such as the edge of jet issuing from the diffuser. This is called maintaining a suitable grid resolution. Without a suitable grid resolution, valuable information can be lost in the numerical simulation process, and the resulting solution can be misleading. Determining what exactly constitutes enough grid resolution is one of the most important jobs a CFD scientist or engineer must perform. While too few control volume cells can lead to useless simulations, too many control volume cells can lead to computer requirements that can't be fulfilled (example: trying to run the latest version of Microsoft Word on a 286 chip).

3.1.6.2 Numerical simulation

As with every other aspect of CFD, the numerical simulation process can also be broken into two steps:

1) Modeling the Physics

If the user does nothing else, then the boundary surfaces of the solution domain are "zero flow" (i.e., symmetry surfaces). These have zero mass flow, zero surface friction and zero heat transfer. The interior of the domain contains only fluid as defined by the properties (such as density, viscosity, etc.). Anything else (e.g., inflow or outflow, walls, internal objects, heat gains or losses) must be specified explicitly by the user. These are known as boundary conditions.

The locations of boundary conditions are defined in terms of six spatial coordinates (say, xS, xE, yS, yE, zS, zE), in meters, referenced from the origin located on one corner of the solution domain. In the case of a two dimensional planar (flat) boundary condition (e.g., the shelves), the orientation is specified and the six coordinates degenerate to five. Additionally, some planar boundary conditions should only affect the fluid (e.g., an external boundary wall has only one surface present in the solution domain).

For accurate geometrical representations, the grid lines (surfaces of the control volume cells) can be forced to align with a boundary condition. If this is not done then the boundary condition will "snap" to the nearest grid line in the final model. This type of allowance is often acceptable when setting up room geometries as the exact location of an item need not be clearly defined.

Below is a list, with a brief description, of the boundary conditions relevant to the approach taken in this study, referred to in the sections of this report.

Rectangular Obstructions	Rectangular obstructions are three-dimensional solid rectangular objects, with faces aligned with x, y and z. Friction at all surfaces exposed to fluid is included. There are a number of possible thermal specifications: • Fixed uniform heat flux at all surfaces • Fixed uniform surface temperature • Solve in solid (to investigate conduction through solid)
External Walls	External walls are walls at the edges of the solution domain - or exceptionally internal walls for which solution is required only on one side and "external" conditions can be applied on the other side. Surface friction is evaluated automatically and there are a number of thermal options: • Prescribed heat flux • Prescribed inner wall surface temperature • Prescribed external temperature with detail of the heat transfer through the wall.
Exhausts	Exhausts represent any outflow of air usually when driven using mechanical means. The flow rate is specified as: • Fixed mass flow rate (kg/s) • Linear pressure drop / flow rate fan characteristic • External static pressure
Openings	Openings are any opening through which fluid can enter or leave the domain as a result of pressure differences. The temperature and angle of flow of incoming air can be specified. It is also possible to represent, for example, a grille across the opening by setting a pressure drop (see **Resistances**).

Resistances	Resistances cover any kind of flow resistance (i.e. pressure drops) caused by porous items within the flow domain Two options are available: • **Planar resistances:** These provide for areas where the resistance is thin and can be applied in one plane. The pressure drop is given by the expression: $DP = f \, ½ \, \rho (v/b)^2$ Where DP Pressure drop f loss coefficient ρ density v velocity of fluid b geometrical free area ratio of obstruction • **Volume resistances:** These provide for areas where the resistance occupies a significant thickness in the solution domain and resistance will occur in more than one direction. The pressure drop is the same as for a planar resistance except that it is expressed as pressure drop per meter and the factor and free area ratio is required for each co-ordinate direction. **Loss Coefficient and Free Area Ratio:** The loss coefficient will depend upon the actual geometry of the item causing the pressure drop. This will be obtained from experiment or empirical relationships in textbooks. Care is needed as it may be set with respect to an approach velocity or device velocity. If the latter is chosen then there will be an associated free area ratio so that the program can correctly calculate the pressure drop. The free area ratio is not required if the setting is based upon the approach velocity.

Sources	Planar and volume sources provide regions of defined source of heat or momentum, or fixed values of velocities, concentration, and / or temperature. The following options are available: • Prescribed source of heat, concentration, and / or momentum • Fixed values of velocity, concentration, and / or temperature • Linear source of heat, concentration, and / or momentum given by the expression: *source = coefficient (value – velocity or temperature)* The last option also allows the specification of a pressure drop which varies linearly with (velocity), rather than $(\text{velocity})^2$, which is defined through Planar Resistances. A pressure drop term is seen as a source term in the Conservation of Momentum Equation (Equation 5.3). A linear source of momentum can be arranged to replicate this term as follows: • Source = coefficient(value – velocity) Considering the x-coordinate direction, and setting value = 0, we obtain: • $\text{Source}_x = -\text{coefficient}_x \times \text{velocity}_x$ Which can be seen to be equivalent to: • $DP = -f_x \times \text{velocity}_x$
Supplies	Supplies are to bring air in from outside, normally conditioned air from the main plant. The flow is set using: • Fixed mass flow rate (kg/s) • Linear pressure drop / flow rate fan characteristic The temperature and angle of flow of incoming air can be specified.
Thin Walls	Internal thin walls are thin solid surfaces within the solution domain and aligned with the grid. Solution is carried out on both sides. The walls are impervious to flow but it is possible to specify heat transfer across them. Surface friction (different on each side if required) is evaluated.
Triangular Prisms	Triangular prisms are solid objects with triangular cross section, and with all faces except the sloping face aligned with x, y and z. All surfaces are zero friction and only the sloping surface has heat transfer. This is specified in terms of a temperature and heat transfer coefficient, or, as a fixed heat flux.

2) Numerically Solving the Physical Model

Integration is one of the cornerstones of calculus, the other being differentiation. In order to find the solution domain (area under a solution curve) numerically, the curve would be chopped up into little pieces, and then the area under each little curve would be approximated. The sum of all of the approximate little areas will be close to the actual area under the curve. The difference between the actual and approximate areas is the numerical error and the object is to make this error so small it isn't noticeable. In CFD, rather than integrating a relatively simple function like the equation for a curve, the governing equations of motion for a fluid continuum are integrated. Let us consider a typical room. The objective is to predict airflow and temperature at any point in the room space.

Figure 3.1 shows a set of design parameters such as

- the *geometry and layout of the room*
- the *sources of heat*,
- as well as the position of *exhaust and ventilation systems.*

In order to do this *the 3-dimensional space* of the room is subdivided into a large number of *control volume cells* (Figure 3.2). The size of the cells will influence the detail and accuracy of the final results. In all the isolation room cases, the number of grid cells ran into the hundreds of thousands, and, in some instances, totaled over one million grid cells.

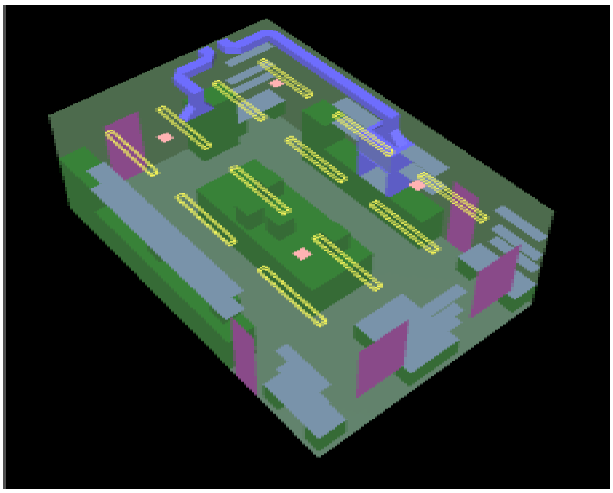

Figure 3.1. *Geometric model of a room*

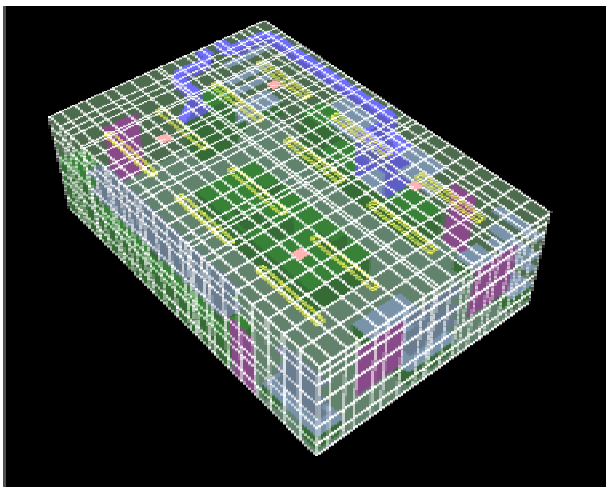

Figure 3.2. *Superimposed grid of cells for calculation*

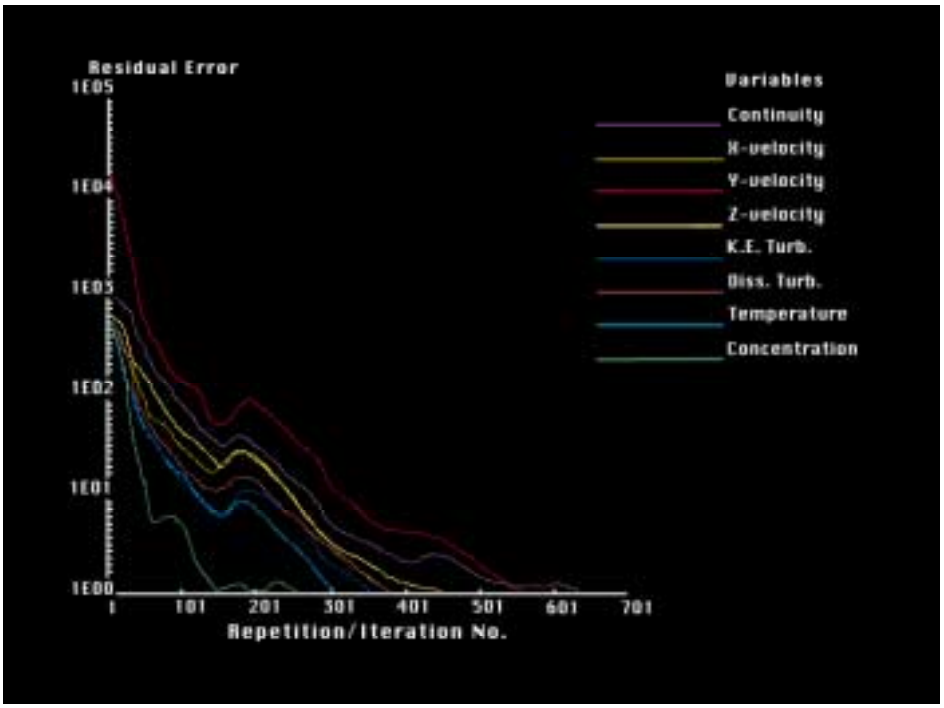

Figure 3.3. *Convergence history of CFD simulation.*

The equations in each cell will subsequently represent the mathematical definition of the equipment and phenomena contained within it. For example, a cell could encompass a volume that envelops :

- *a representation of a group of furniture,*
- *or some heat source,*
- *or just some air.*

The CFD software will then attempt to solve the Navier-Stokes equation for a pre-determined set of variables for each cell. In a typical three-dimensional calculation these variables would represent :

- *velocities in three directions;*
- *temperature;*
- *pressure;*
- *concentration (if required); and the*
- *turbulence quantities.*

Note that the solution for each variable will depend on the solution for each and every variable in the *neighboring cells and vice versa.* The laws of physics based upon the *conservation of mass, conservation of momentum, and conservation of energy* must be preserved at all times. In this approach, turbulence is modeled using the well established and robust two parameter method known as the k-epsilon model where k represents the kinetic energy and epsilon represents the rate of dissipation.

The mathematical solution is highly iterative, with each iteration resulting in a set of errors. At the end of each iteration the errors for each variable are summed, normalized with an acceptable error and plotted against iteration number (Figure 3.3). A solution is reached when the sums of the errors for each and all the variables reaches a pre-determined and acceptable level.

Each cell within the solution domain has 7 equations associated with it (pressure, three velocities, temperature, two turbulence quantities). The isolation room model in this research typically has 100,000 to 600,000 cells. This results in 4,800,00 to 6,400,000 equations that have to be solved iteratively until the convergence criteria is satisfied. This is an extremely computer intensive operation that requires the use of powerful state-of-the-art workstations.

3.2. Description of Mathematical Model

3.2.1 Governing Equations

The generic form of the governing equations, shown by equation 3.1, can be expanded to form the three fundamental conservation laws that comprise the Navier-Stokes equations. These are the conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0 \tag{3.2}$$

the conservation of momentum:

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho U_i U_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial U_i}{\partial x_j}\right) + g_i\left(\rho - \rho_0\right) \tag{3.3}$$

and the conservation of thermal energy:

$$\frac{\partial \rho H}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho U_i H\right) = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \frac{\partial P}{\partial t} \tag{3.4}$$

These equations describe the behavior of fluids under both laminar and turbulent flow conditions. One of the most important physical effects when calculating the flow in the built environment is that of turbulence

3.2.2 Turbulence Modeling

For this project, a well established and reliable approach to turbulence modeling is required to achieve the large number of calculations necessary for analysis of the many configurations. This section provides some background on the different approaches to modeling turbulence.

To model a turbulent flow, the temporal terms of equations 3.2, 3.3, and 3.4 would have to have a time step (*dt*) small enough to capture all turbulent fluctuations on even the smallest time scales. The same applies to all physical dimensions of the control volume cells (dx_i) terms. They would have to be as small as that known as the Kolmogarov scale, which decreases non-linearly with an increase in Reynolds number.

To overcome these limitations, variables are split into a mean and fluctuating component, i.e.:

$$U = \overline{U} + u'$$
$$H = \overline{H} + h' \qquad (3.5)$$

These are then substituted back into the instantaneous momentum equation producing the following:

$$\frac{\partial}{\partial x_j}\left(\rho \overline{U}_i \overline{U}_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \overline{U}_i}{\partial x_j} - \rho \overline{u_i' u_j'}\right) + g_i\left(\rho - \rho_0\right) \qquad (3.6)$$

This is known as the time averaged momentum equation. A similar equation exists for the enthalpy equation:

$$\frac{\partial}{\partial x_i}\left(\rho \overline{U}_i \overline{H}\right) = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial \overline{T}}{\partial x_i} - \rho \overline{u_i' h'}\right) \qquad (3.7)$$

The extra terms are produced by this substitution are:

- Reynolds stress = $\rho \overline{u_i' u_j'}$
- Reynolds flux = $\rho \overline{u_i' h'}$

A turbulent flow is characterized by the dominance of diffusion due to the Reynolds stresses and fluxes over the diffusion due to laminar viscosity or laminar diffusivity of the fluid. The spread of particles in the isolation room, is controlled strongly by the turbulent diffusion. The role of turbulence modeling, to calculate the Reynolds stresses and fluxes, is therefore of vital importance in the prediction of particle trajectories.

The introduction of the Reynolds stresses and fluxes after decomposition of the turbulent fluctuating variables means that the equation set is now not closed. Some form of closure is required to model these fluxes and stresses. There have been a wide range of methods used to do this, varying from the most simple zero-equation models to the much more complex Reynolds stress transport equations. Figure 4 shows how these turbulence models relate to each other.

At the center of the zero-, one-, and two-equation models lies the analogy that where a laminar stress exists, then so can an equivalent turbulent stress (i.e. , Reynolds stress). A laminar shear stress is defined as:

$$\tau = \mu \frac{\partial U_i}{\partial x_j} \tag{3.8}$$

So, if a fluid can have a laminar viscosity, μ, then a turbulent flow should have a turbulent or eddy viscosity, μ_T. By using the eddy viscosity hypothesis, which Boussinesq proposed, we can relate the Reynolds stress to the mean strain by:

$$-\rho\overline{u_i' u_j'} = \mu_T\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) - \tfrac{2}{3}\rho k \partial_{ij} \tag{3.9}$$

A zero equation turbulence model simply sets a constant value of the eddy viscosity, or deduces it as an algebraic function of flow parameters. A one equation model uses a differential equation to predict one part of the eddy viscosity while a two equation model uses two differential equations.

The main limitation imposed at this stage by equation 3.9 is that the eddy viscosity is the same in all directions at any point. Now, where this may be true of laminar viscosity, which is a property of the fluid, it may not be true of turbulent viscosity, which is effectively a property of the flow. Therefore, this eddy viscosity can have differing values in relation to differing Reynolds stresses. This occurs when the turbulence is said to be anisotropic. Conditions that under certain circumstances may cause anisotropy, and thus could invalidate the isotropic assumption of equation 3.9, include extreme streamline curvature, swirl, adverse pressure gradients, and buoyancy.

The two-equation approach including the standard *k*-ε model and the RNG *k*-ε model variant is presented first. Reynolds stress modeling is then discussed and finally the modeling of the Reynolds fluxes is briefly outlined.

$$\frac{\partial}{\partial x_j}\left(\rho\overline{U}_i\overline{U}_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu\frac{\partial\overline{U}_i}{\partial x_j} - \rho\overline{u_i'u_j'}\right) + g_i\left(\rho-\rho_0\right)$$

EDDY VISCOSITY ASSUMPTION

$$-\rho\overline{u_i'u_j'} = \mu_T\left(\frac{\partial\overline{U}_i}{\partial x_j}+\frac{\partial\overline{U}_j}{\partial x_i}\right)-\tfrac{2}{3}\rho k\partial_{ij}$$

from dimensional analysis it is shown that:
$\mu_T = \rho \times$ const. $\times$ velocity scale $\times$ length scale

REYNOLDS STRESS MODELS

the Reynolds stresses are each derived from their own transport equations

ZERO EQUATION

$\mu_T =$ constant *or* an algebraic function of a flow parameter such as Reynolds number

ONE EQUATION MODELS

$$\mu_T = \rho C_\mu \sqrt{k} l$$

the velocity scale, *k,* is derived from its own transport equation and the length scale, *l*, is assumed constant

TWO EQUATION MODELS

both the velocity scale, *k*, as well as a length scale, ε, are derived from their own transport equations

Figure 3.4. *Tree of turbulence modeling*

3.2.2.1 k-ε turbulence model

This turbulence model calculates two variables; the kinetic energy of turbulence (k) and the dissipation rate of k (denoted ε).

The eddy viscosity is defined from dimensional analysis as:

$$\mu_T = \mathrm{C}_\mu \rho \frac{k^2}{\varepsilon} \tag{3.10}$$

The transport equations for *k* and ε are:

$$\frac{\partial \rho \overline{U_i} k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right) + \mathrm{P} + \mathrm{G} - \rho\varepsilon \tag{3.11}$$

$$\frac{\partial \rho \overline{U_i} \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right) + C_1 \frac{\varepsilon}{k}\left(\mathrm{P} + C_3 \mathrm{G}\right) - C_2 \rho \frac{\varepsilon^2}{k} \tag{3.12}$$

where P is the shear production defined as:

$$\mathrm{P} = \mu_{eff} \frac{\partial \overline{U_i}}{\partial x_j}\left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i}\right) \tag{3.13}$$

G is the production of turbulence kinetic energy due to buoyancy, and is given by:

$$\mathrm{G} = \frac{\mu_{\mathrm{eff}}}{\sigma_{\mathrm{T}}} \beta \mathrm{g_i} \frac{\partial \mathrm{T}}{\partial \mathrm{x_i}} \tag{3.14}$$

C_μ	0.09
C_1	1.44
C_2	1.92
C_3	1.0
σ_k	1.0
σ_ε	1.217

This model has been tried and tested for a whole range of engineering applications. It is simple, but more importantly, it is *stable*. Only two extra differential equations are introduced and the convergence process is less prone to divergence than other, higher order turbulence models. This is the approach adopted for the present research.

3.2.2.2 Re-normalized group theory (RNG) kε turbulence model

Essentially, this model has much the same form as the standard model. It is part empirical and part analytical. The only changes are a modified term relating to the production of energy dissipation in the ε equation and a different set of model constants. This RNG model is typical of those offered by some commercial general purpose CFD codes. The new equations for *k* and ε become:

$$\frac{\partial \rho \overline{U_i} k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right) + \mathrm{P} + \mathrm{G} - \rho\varepsilon \tag{3.15}$$

$$\frac{\partial \rho \overline{U_i} \varepsilon}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right) + \left(C_1 - C_{1\mathrm{RNG}}\right)\frac{\varepsilon}{k}\left(\mathrm{P} + C_3\mathrm{G}\right) - C_2\rho\frac{\varepsilon^2}{k} \tag{3.16}$$

The new function C_{1RNG} is given by the equations:

$$C_{1\mathrm{RNG}} = \frac{\eta\left(1 - \eta/\eta_0\right)}{\left(1 + \beta\eta^3\right)} \tag{3.17}$$

and:

$$\eta = \frac{\mathrm{k}}{\varepsilon}\sqrt{\frac{\mathrm{P}}{\mu}} \tag{3.18}$$

In this case η_0 and β are additional model constants, and the latter should not be confused with the coefficient of thermal expansion. The main modification is to the ε equation where the rate of strain of the flow has been incorporated into the model constants. Under conditions of extreme strain the eddy viscosity is reduced. It is this feature of the RNG model that is said to accommodate *strong* anisotropy in regions of large shear, i.e. the treatment of massive separation and anisotropic large-scale eddies. Most validation of this model has been only under these extremely high strain conditions such as internal flow in a 180° bend and flow within a

contracting-expanding duct. Accurate prediction of separation regions seems to be the grail of the validation work. A more realistic range of *softer* type flows (i.e. less extreme strain) has not been studied with the RNG model. It is because of the infancy of this approach that it has not been incorporated at this stage. As and when the model becomes as tried and trusted as the present standard *k*-ε model it will be given greater attention.

3.2.2.3 Reynolds stress models (second order closure models)

Instead of employing the eddy viscosity assumption, which assumes an equal eddy viscosity in all three spatial directions, a Reynolds stress model has an equation for each of the six Reynolds stresses themselves. This allows the modeling of the transport of each of these individual stresses. This is the most complex of all models and suffers accordingly. Instead of two extra equations we now have an extra seven (an equation for ε is still required as it pops up in the stress transport equations). Convergence stability now becomes a serious problem. Even if convergence is achieved, it normally takes considerably longer than with a two-equation model. Prescription of boundary conditions is also tricky. Instead of setting just *k* and ε, we now have to set values at supply boundaries of all stresses, not the easiest of parameters to obtain from experimental measurement. The question has to be asked as to whether the added theoretical capabilities of an RSM are worth the increased solution time and decrease in stability.

3.2.2.4 Modeling of Reynolds fluxes:

The velocity-enthalpy correlations known as the Reynolds fluxes use much the same methodology as the Reynolds stresses. An eddy diffusivity is therefore defined as:

$$-\rho\overline{u_i'h'} = \Gamma_T\left(\frac{\partial\overline{T}}{\partial x_i}\right) \tag{3.19}$$

where this eddy diffusivity is related to the eddy viscosity by:

$$\Gamma_T = \frac{\mu_T}{\sigma_T} \tag{3.20}$$

where σ_T is the turbulent Prandtl number having a fixed value of 0.9. The next step up, as with a second order closure model, is to calculate each of the three fluxes from their own transport equations.

3.2.3. Near Wall Treatment

Fluid velocity at a wall surface is zero, which is known as the no-slip condition. The type of flow between the wall and the bulk flow is known as a shear layer, in this case a wall boundary layer. The boundary layer is a very complex region of high velocity gradient and diffusion dominated development. To model it precisely would necessitate an extremely fine grid. An empirical relationship is therefore used to describe the shape of the boundary layer so that only one grid cell near the wall is required. This empirical relationship describes the shape of the boundary layer in non-dimensional terms. Two non-dimensional terms are formulated. These are the friction velocity:

$$u_\tau = \left(\frac{\tau_w}{\rho} \right)^{1/2} \tag{3.21}$$

and a non-dimensionalized distance from the wall (which can be viewed as a local Reynolds number):

$$y^+ = \frac{u_\tau y \rho}{\mu} \tag{3.22}$$

These formulae are based upon the well-established 'universal' relationships:

$$\text{For } y^+ > 11.5 \text{ (turbulent): } \frac{u}{u_\tau} = \frac{1}{0.435} \ln\left(9 y^+\right) \tag{3.23}$$

$$\text{For } y^+ < 11.5 \text{ (laminar): } \frac{u}{u_\tau} = y^+ \tag{3.24}$$

All that is required to deduce the wall shear stress from the near wall velocity is therefore the distance from the near wall cell center to the wall itself.

3.2.4 Integration of the Governing Equations

The governing PDEs have to be integrated, or discretized, over the solution grid so that the finite values of the flow variables may be predicted at each cell. The discretization process converts the governing PDEs into algebraic equations. The following figure shows the cell notation that is to be used:

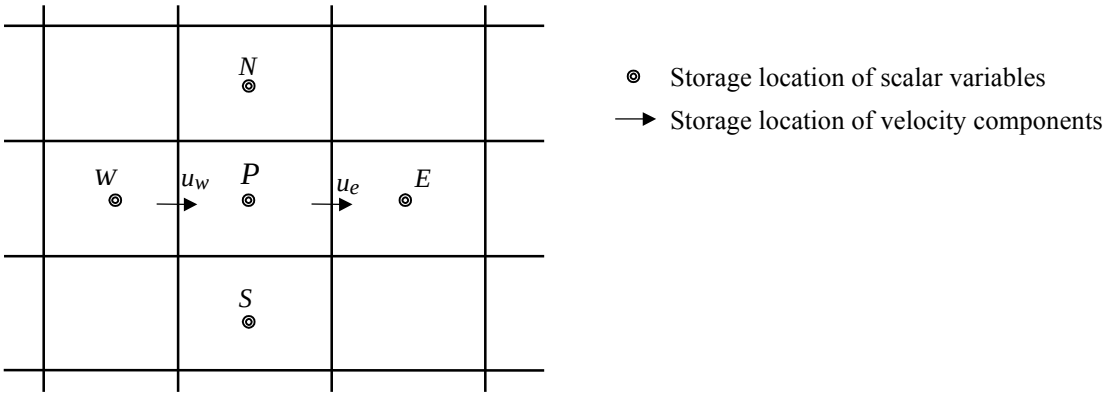

Figure 3.5. *Cell Notation.*

Here, we see that all scalar variables are stored at the center of each cell, or rather the scalar variable has the same value throughout that entire cell. The vector variables are stored on the center of each face of the cell so that fluxes flowing through the cell can be calculated directly.

Once the solution domain has been gridded then each governing equation must be integrated over each cell. Only when the laws of conservation, as well as the turbulent transport equations, are satisfied at each cell (to within a tolerable degree) is the solution complete.

For simplicity of coding, all the governing equations are organized into a similar form. This generic form can be written as:

$$\frac{\partial \rho \overline{U_i} \phi}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\Gamma \frac{\partial \phi}{\partial x_j}\right) = S \qquad (3.25)$$

The first term represents the convection of any variable, ϕ, by the mean fluid velocity, $\overline{U_i}$; the second term represents diffusion where Γ is the diffusion coefficient; and the third term is a source or sink term where ϕ is either created or destroyed. When integrating over a control volume we obtain:

$$\int \rho \phi \overline{U_i} . \mathbf{n} dA - \int \Gamma \frac{\partial \phi}{\partial x_j} . \mathbf{n} dA = \int S dV \qquad (3.26)$$

The calculation of these integrals is the center of the discretization process. Figure 3.5 shows a single orthogonal cell and some of its neighbors. With a non-staggered grid all variables are stored at the center of the cell at point P. Neighboring points include points E, W, WW, etc. In

the schemes that follow a lower case subscript (n, e, s, w) refers to values at the appropriate face whereas an upper case subscript (N, E, S, W) refers to values at the appropriate cell centers.

3.2.4.1 Treatment of the diffusion terms

The diffusion term is the simplest to integrate. By looking at the diffusive flux at the west face of the cell we can write:

$$\int \Gamma \frac{\partial \phi}{\partial x_j} . \mathbf{n} dA = \frac{\Gamma A_w}{h_w} \left(\phi_P - \phi_W \right) \tag{3.27}$$

Where h_w is the distance between cell centers. The above equation can be rewritten as:

$$\frac{\Gamma A_w}{h_w} \left(\phi_P - \phi_W \right) = D_W \left(\phi_P - \phi_W \right) \tag{3.28}$$

Such that D_W is the west-face diffusion coefficient. There is a diffusion coefficient for each face of the cell.

3.2.4.2 Treatment of the convective terms

The integration of the convective (sometimes referred to as advective) term is achieved by employing the upwind differencing scheme. Here, the value of the flow variable at a cell interface is equal to the flow variable on the *upwind* side of the face. Considering convection through the west face of the cell (where the fluid enters from the west neighboring cell):

$$\int \rho \phi \overline{U_i} . \mathbf{n} dA = \rho \overline{U_w} A_w \phi_W \equiv F_W \phi_W \tag{3.29}$$

Such that F_W is the west face convection coefficient. Again, there are convection coefficients for each face of the cell.

By combining the effects of both convection and diffusion the finite volume equation is formulated:

$$a_P \phi_P = \sum_{nn} a_{nn} \phi_{nn} + S \tag{3.30}$$

The coefficients (a_P etc.), that express the contribution of convection and diffusion across the cell boundaries, are called matrix coefficients. Each matrix coefficient is simple the sum of both

diffusion and convection coefficients. The value of the convection coefficient is determined by the direction from which fluid enters the cell.

3.2.4.3 Solution of the Finite Volume Equations

Having covered the derivation of all linearized equations from the governing partial differential equations, the process by which they are solved will now be explained. An iterative process is used, starting from an initial estimate of the values of all variables at each cell through to the converged solution where the final values obey their respective conservation equations to within an acceptable degree of accuracy.

The solution process consists of two loops. An initial guess, or initial condition, is taken for the values of all variables at each cell. The two loops are then iterated in a nested manner. The inner loop solves the linearized equations for each variable in turn at each cell assuming all other fields are fixed. The outer loop involves updating all variable fields with the values calculated in the inner loop. As this process progresses, the flow field approaches its final or converged state. The iterative process stops when the errors in all governing equations reaches an acceptably small value

3.2.4.4 The inner iteration

The inner iteration consists of taking each variable in turn, whilst assuming all the others to be fixed, and passing the relevant equations for each cell to a Gauss Siedel equation solver. All updated variable values are not passed on to the other linearized equations until the completion of the inner loop. It is within the outer loop that this takes place.

At some point the iterative process must be terminated so that the inner iteration can proceed onto the next variable. A criteria must be met before the inner iterations for a given variable stops. Either that the total number of inner iterations are reached or the reduction in the residual error (the amount by which the current governing conservation equation is not satisfied) for the given variable reaches a tenth of the level when the inner iteration began.

3.2.4.5 The outer iteration

Once the inner loop has been completed, i.e. each variable taken in turn and iteratively solved until the stopping criteria has been met, the outer iteration is performed. The main aim of the outer loop is to update all variables in all equations by the values calculated in the inner loop. It is within this outer loop that the velocity–pressure-coupling algorithm, SIMPLE, is implemented.

This predicts the correct value for cell pressure based on the current cell momentum (Patankar 1980).

The outer loop is stopped when the problem is said to have converged. This occurs when the residual errors for all equations are acceptably small (i.e. 0.5% of the inlet flux for each variable).

3.2.5 Validation of Airflow Modeling Methodology

The methodology and most of the results generated in this paper have been or are under peer review by numerous entities such as Harvard University, etc. The methodology was also used extensively in a previous publication by Memarzadeh (1998), which considered ventilation design handbook on animal research facilities using static microisolators. In order to analyze the ventilation performance of different settings, numerical methods based on computational fluid dynamics were used to create computer simulations of more than 160 different room configurations. The performance of this approach was successfully verified by comparison with an extensive set of experimental measurements. A total of 12.9 million experimental data values were collected to confirm the methodology. The average error between the experimental and computational values were 14.36 percent for temperature and velocities, while the equivalent value for concentrations was 14.50 percent.

To forward this research, several progress meetings were held to solicit project input and feedback from the participants. There were more than 55 international experts in all facets of the animal care and use community, including scientists, veterinarians, engineers, animal facility managers, and cage and rack manufacturers. The pre-publication project report underwent peer review by a ten (10) member panel from the participant group, selected for their expertise in pertinent areas. Their comments were adopted and incorporated in the final report.

The publication was reviewed by the American Society of Heating, Refrigeration, and Air Conditioning Engineers (ASHRAE) technical committee and accepted for inclusion in their 1999 handbook.

3.3 Simulation of Bacteria Droplets

3.3.1 Basic Concept

The airborne bacteria in the isolation room can be simulated as particles being generated from several sources surrounding the occupant. These particles then are tracked for a certain period of time in the room. The dose that the particles received when travelling in the room along their trajectories is the summation of the dose received at each time-step calculated as:

$$\text{Dose} = \sum (dt*I) \tag{3.31}$$

Where, dt is the time step and I is the local UV irradiance. Then, based on the dose received, the survival probability of each particle is evaluated.

Since the airflow in a ventilated room is turbulent, the bacteria from coughing or sneezing of the occupants in the room are transported not only by convection of the airflow but also by the turbulent diffusion. The bacteria are light enough, and in small enough quantities, that they can be considered not to exert an influence on airflow. Therefore, from the output of the airflow simulation, the distributions of air velocities and the turbulent parameters can be directly applied to predict the path of the airborne bacteria in convection and diffusion process.

3.3.2 Particle trajectories

The methodology for predicting turbulent particle dispersion used in this study was originally laid out by Gosman and Ioannides (1981), and validated by Ormancey and Martinon (1984), Shuen et al. (1983), Chen and Crowe (1984). Experimental validation data was obtained from Snyder and Lumley (1971). Turbulence was incorporated into the Stochastic model via the κ-ε turbulence model (Alany et al. (1998)).

The airflow simulation described in the previous sections is carried on in Euler System. The particle trajectories, however, needs to be computed in Lagrangian System outside the CFD solving routine. The particle trajectories are obtained by integrating the equation of motion in 3 co-ordinates. Assuming that body forces are negligible with the exception to drag and gravity, these equations can be expressed as,

$$\mathrm{m_p}\frac{du_p}{dt} = \frac{1}{2}C_D A_P \rho(u-u_p)\sqrt{(u-u_p)^2+(v-v_p)^2+(w-w_p)^2} + m_p g_x \tag{3.32}$$

$$\mathrm{m_p}\frac{dv_p}{dt} = \frac{1}{2}C_D A_P \rho(v-v_p)\sqrt{(u-up)^2+(v-vp)^2+(w-wp)^2} + m_p g_y \tag{3.33}$$

$$\mathrm{m_p}\frac{dw_p}{dt} = \frac{1}{2}C_D A_P \rho(w-w_p)\sqrt{(u-u_p)^2+(v-v_p)^2+(w-w_p)^2} + m_p g_z \tag{3.34}$$

$$\frac{dx_p}{dt} = u_p \tag{3.35}$$

$$\frac{dy_p}{dt} = v_p \tag{3.36}$$

$$\frac{dz_p}{dt} = w_p \tag{3.37}$$

Where

u, v, w:	instantaneous velocities of air in x, y and z directions
u_p, v_p, w_p:	particle velocity in x, y and z direction
x_p, y_p, z_p:	particle moving in x, y and z direction
g_x, g_y, g_z:	gravity in x, y and z direction
A_p	cross-section area of the particle
m_p	mass of the particle
ρ	density of the particle
C_D	drag coefficient
dt	time interval

The drag coefficient for a spherical particle, taken from Wallis (1969), is:

$$C_D = \frac{24}{\mathrm{Re}}\left(1+\frac{3}{16}\mathrm{Re}\right)^{0.5} \qquad \text{for Re} \le 1000 \tag{3.38}$$

and $C_D = 0.44$ for Re > 1000 (3.39)

The Reynolds number of the particle is based on the relative velocity between particle and air.

In laminar flow, particles released from a point source with the same weight would initially follow the air stream in the same path and then fall under the effect of gravity. Unlike in laminar flow, the random nature of turbulence indicates that the particles released from the same point source will be randomly effected by turbulent eddies. As a result, they will be diffused away from the steam line at different fluctuating levels. In order to model the turbulent diffusion, the instantaneous fluid velocities in the 3 Cartesian directions, u, v and w are decomposed into the mean velocity component and the turbulent fluctuating component as:

$$u = \bar{u} + u',\ v = \bar{v} + v',\ w = \bar{w} + w'.$$

Where $\bar{u}$ and u' are the mean and fluctuating components in x-direction. The same applied for y-, z- directions. The stochastic approach prescribes the use of a random number generator algorithm which, in this case, is taken from Press et al. (1992) to model the fluctuating velocity. It is achieved through using a random sampling of a Gaussian distribution with a mean of 0 and a

standard deviation of unity. Assuming homogeneous turbulence, the instantaneous velocities of air are then calculated from kinetic energy of turbulence:

$$u = \bar{u} + N\alpha \tag{3.40}$$

$$v = \bar{v} + N\alpha \tag{3.41}$$

$$w = \bar{w} + N\alpha \tag{3.42}$$

Where N is the pseudo -random number, ranging from 0 to1, with

$$\alpha = \left(\frac{2k}{3}\right)^{0.5} \tag{3.43}$$

k is the turbulent kinetic energy.

The mean velocities which is the direct output of CFD determines the convection of the particles along the steam line, while the turbulent fluctuating velocity, $N\alpha$, contributes to the turbulent diffusion of the particle.

3.3.3 Particle Interaction Time

With the velocities known, the only component needed for calculating the trajectory is the time interval (t_{int}) over which the particle interacts with the turbulent flow field. The concept of turbulence being composed of eddies is employed here. Before determining the interaction time, two important time scales need to be introduced: the eddy's time scale and the particle transient time scale.

Eddy's time scale: life time of an eddy, defined as

$$t_e = \left(\frac{l_e}{|N\alpha|}\right) \tag{3.44}$$

where

$$l_e = \frac{C\mu \; k^{\frac{3}{2}}}{\varepsilon} \tag{3.45}$$

l_e is the dissipation length scale of the eddy
k is the turbulent kinetic energy,
ε is the dissipation rate of turbulent kinetic energy,
$C\mu$ is a constant in the turbulence model.

The transient time scale: for the particle to pass through the eddy, $\mathbf{t_r}$, estimated as

$$t_r = -\tau \ln\left\{1.0 - \frac{l_e}{\tau\left|\left(\sqrt{\bar{u}^2+\bar{v}^2+\bar{w}^2}\right)-\left(\sqrt{(u_p)^2+(v_p)^2+(w_p)^2}\right)\right|}\right\} \quad (3.46)$$

and

$$\tau = \frac{\frac{4}{3}\rho_p D}{\left\{\rho C_D\left|\left(\sqrt{\bar{u}^2+\bar{v}^2+\bar{w}^2}\right)-\left(\sqrt{(u_p)^2+(v_p)^2+(w_p)^2}\right)\right|\right\}} \quad (3.47)$$

Where τ is the particle relaxation time, indicating the time required for a particle starting from rest to reach 63% of the flowing stream velocity. D is the diameter of the particle.

The interaction time is determined by the relative importance of the two events. If the particle moves slowly relative to the gas, it will remain in the eddy during the whole lifetime of the eddy, t_e. If the relative velocity between the particle and the gas is appreciable, the particle will transverse the eddy in its transient time, t_r, Therefore, the interaction time is the minimum of the two:

$$t_{int} = \min(t_e, t_r) \quad (3.48)$$

It should be noted that the values of k and ε are assumed constant for the duration of the lifetime of the eddy. This results in a tendency for particles close to wall surfaces to stick to the surfaces, because

In this study, the interaction time is in the order of 1e-5 to 1e-6s. If the particle track time is set to 300s, some 60,000,000 time-steps need to be performed just to calculate the trajectory for one particle.

3.3.4 Testing of Particle Tracking Methodology

A simple test configuration was defined to confirm that the particle tracking methodology was functioning as intended. There are many aspects to be investigated including inertial, gravitational, and slip effects, but in particular the simulations shown here were intended to test that the wall interaction worked correctly. The test was specified to incorporate typical flow and blockage effects present in the isolation room, in particular, an inlet (supply), openings (vents), and a block in the flow path (internal geometry and obstructions).

The geometry of the test configuration is shown in Figure 3.6. The configuration had dimensions of 0.5m (20") x 0.5m (20") x 1.0m (40"). It contained a 0.5m (20") x 0.5m (20") supply at one end through which the flow rate was varied, and an opening of half that size at the other end. An additional opening of dimension 0.1m (4") x 0.5m (20") was also included at approximately halfway along the section. Both openings were defined as representing atmospheric conditions: no flow rate was defined through the openings. The final item in the configuration was a block of dimensions 0.5m (20") x 0.5m (20") x 0.25m (10"), which was included to represent a typical obstruction.

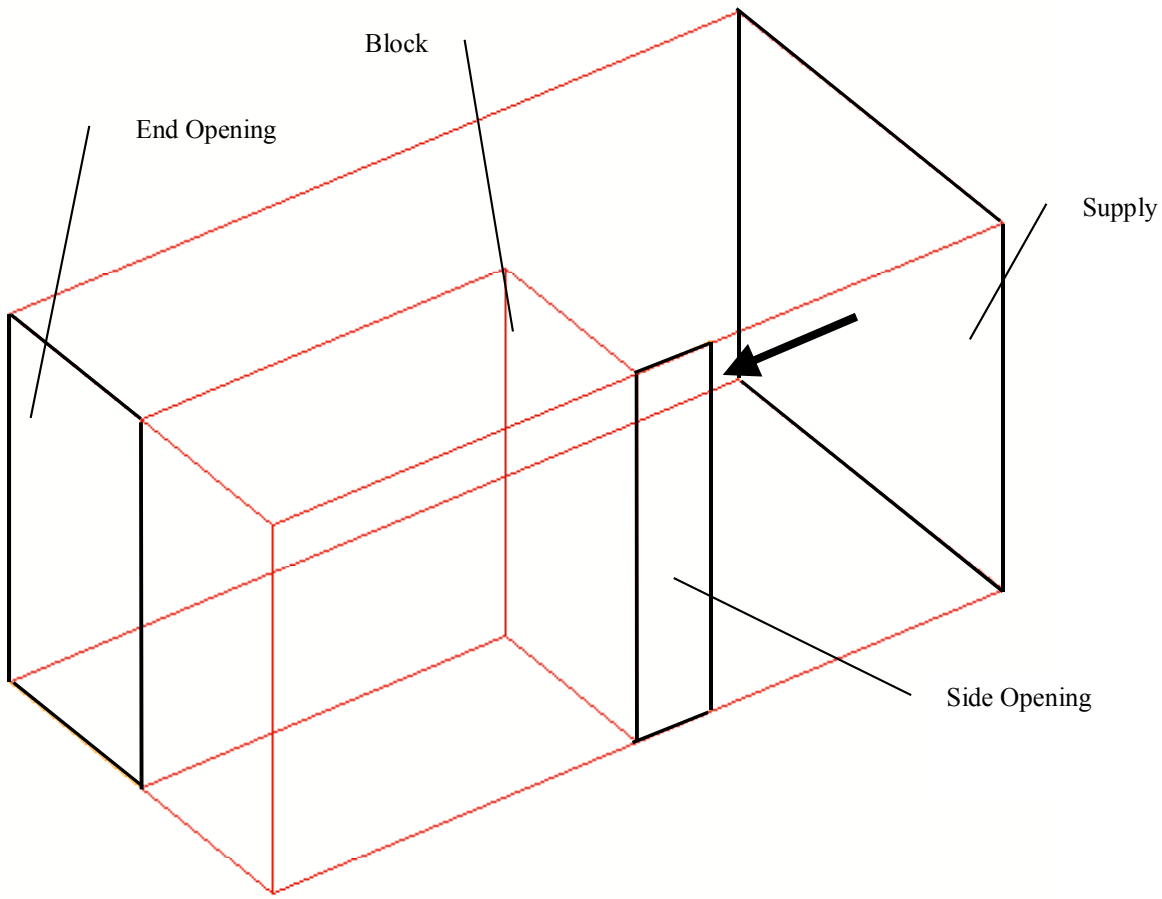

Figure 3.6. *Geometry of test configuration.*

In the tests, 20 particles were released with even spacing across the center of the inlet supply. The test particles were 1 μm in diameter, with a density of 1000 kg/m^3. In terms of supply

conditions, two different flow rates were considered, 0.25 kg/s (445 cfm) and 1.0 kg/s (1780 cfm). Different coordinate orientations were considered to evaluate whether coordinate biasing existed. In particular, the configuration was considered with the supply in the positive and negative x, y and z directions respectively. With the two different flow rates considered, twelve cases were run to test the particle tracking methodology.

The results from three of the cases are shown in figures 3.7 to 3.9, in particular, the positive x orientation at 0.25 kg/s (445 cfm), the negative y orientation at 1.0 kg/s (1780 cfm) and the positive z orientation at 1.0 kg/s (1780 cfm) cases respectively. The blue lines represent the particle tracks. The following can be seen clearly from the figures:

- The majority of the particles exit through the end or side openings.
- Relatively few particles (two or three) impinge on the internal block or side walls.
- There are some (relatively small) differences between the plots. The differences in the tracks can be attributed to the effects of gravity (always defined to act in the negative y direction), turbulence (which is a random effect in the particle tracking) and the flow rate value through the configuration.
- There are no coordinate biasing effects, i.e. the particle tracking routine behaves in the same way in all coordinate directions.

Based on the results from these tests, the particle tracking methodology can be seen to be working correctly.

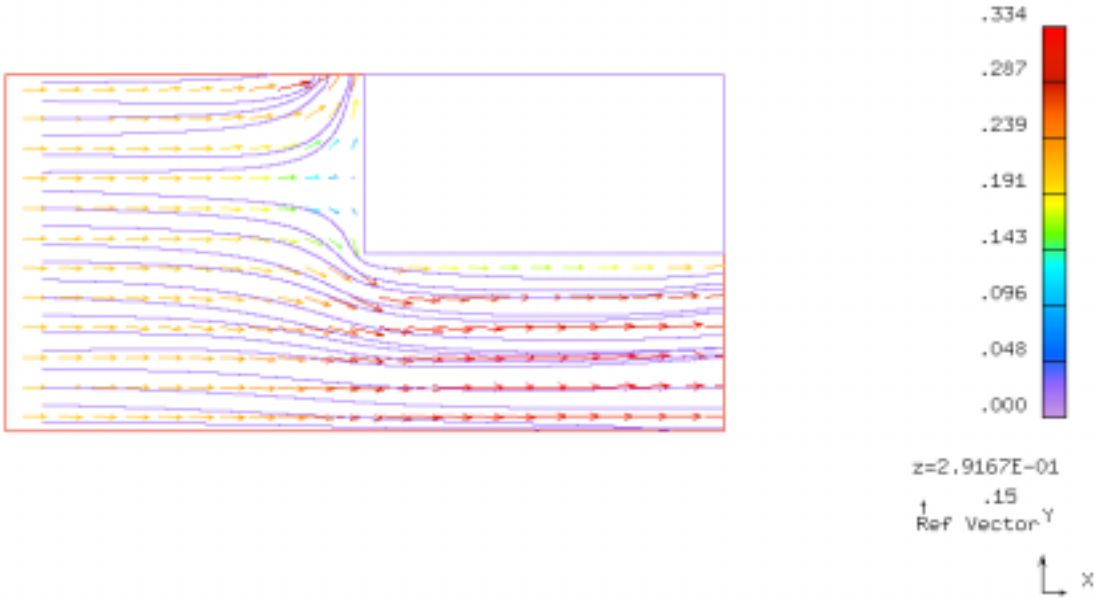

Figure 3.7. *Test Results for Positive x Direction, 0.25kg/s (445 cfm) Case.*

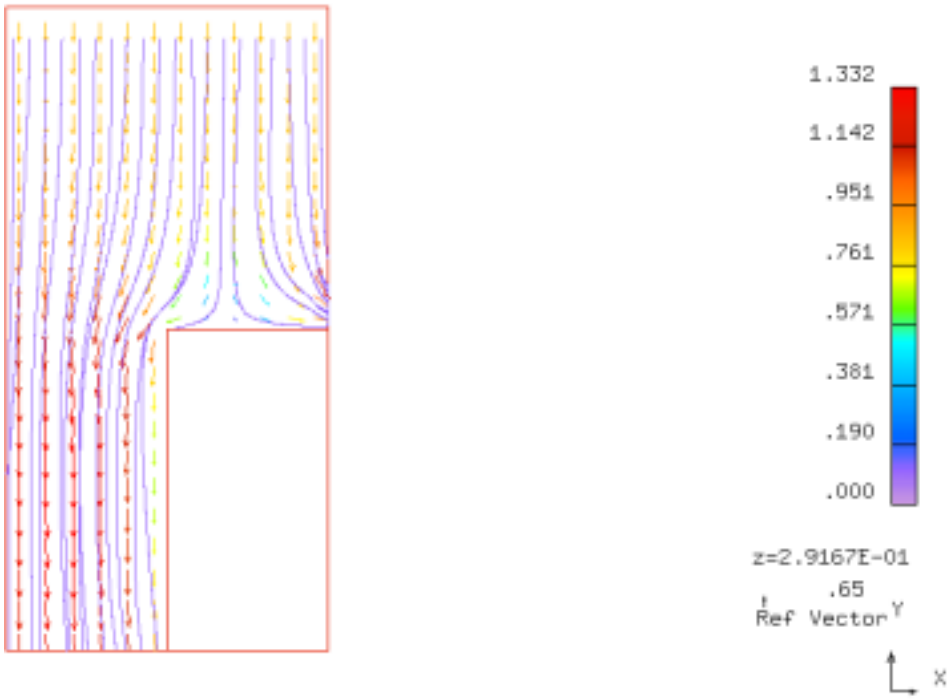

Figure 3.8. *Test Results for Negative y Direction, 1.0 kg/s (1780 cfm) Case.*

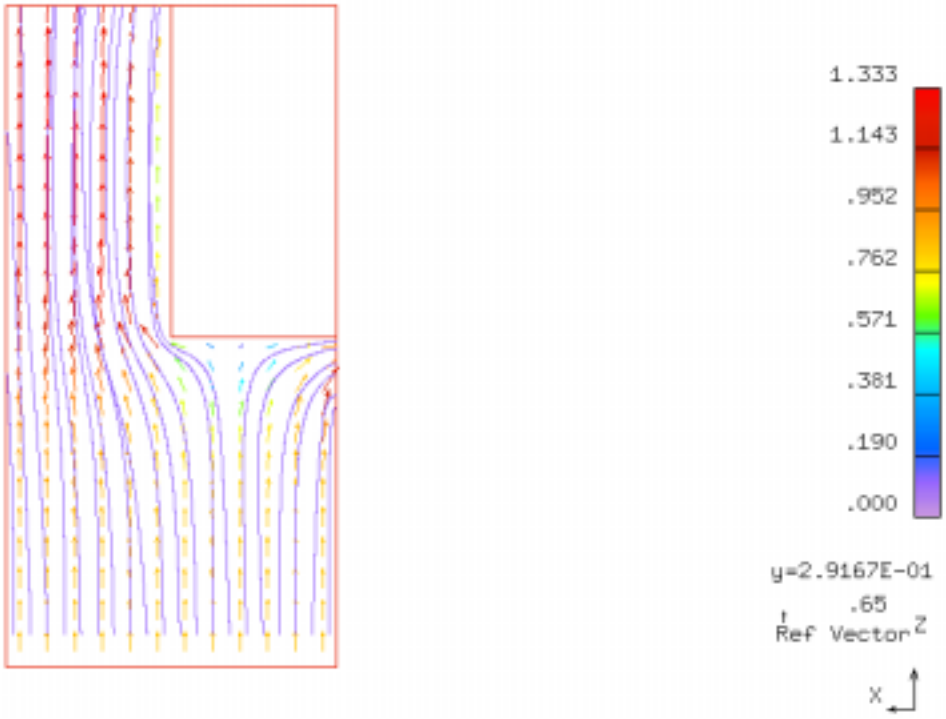

Figure 3.9. *Test Results for Positive z Direction, 1.0 kg/s (1780 cfm) Case.*

3.3.5 Calculation Procedure

The calculation procedure of coupling particle tracking with airflow simulation for each isolation room case consists of 4 steps:

- Computing the field distribution of fluid velocity, temperature and turbulent parameters
- Adding the UV distribution into the result field with the specified fixture location and measurement data of the emissive UV energy distribution.
- Specifying the source locations from where a specified number of particles are released. Note that the particles are not continuously released: they are released from the source locations only at the start of the analysis time period, i.e. t = 0 s.
- Performing computational analysis to calculate trajectory for each particle for up to 300s from initial release.

The flow chart of the particle tracking procedure is presented in Figure 3.10.

The output of the particle tracking analysis is presented as:

- The number of particles being removed by ventilation varying with time (for every 60s)
- The number of viable particles varying with time (for every 60s)
- The number of particles killed by UV dosage varying with time (for every 60s)
- The percentage of surviving particles in the room varying with time (for every 60s
- The number of particles in different dose bands (for every 60s)

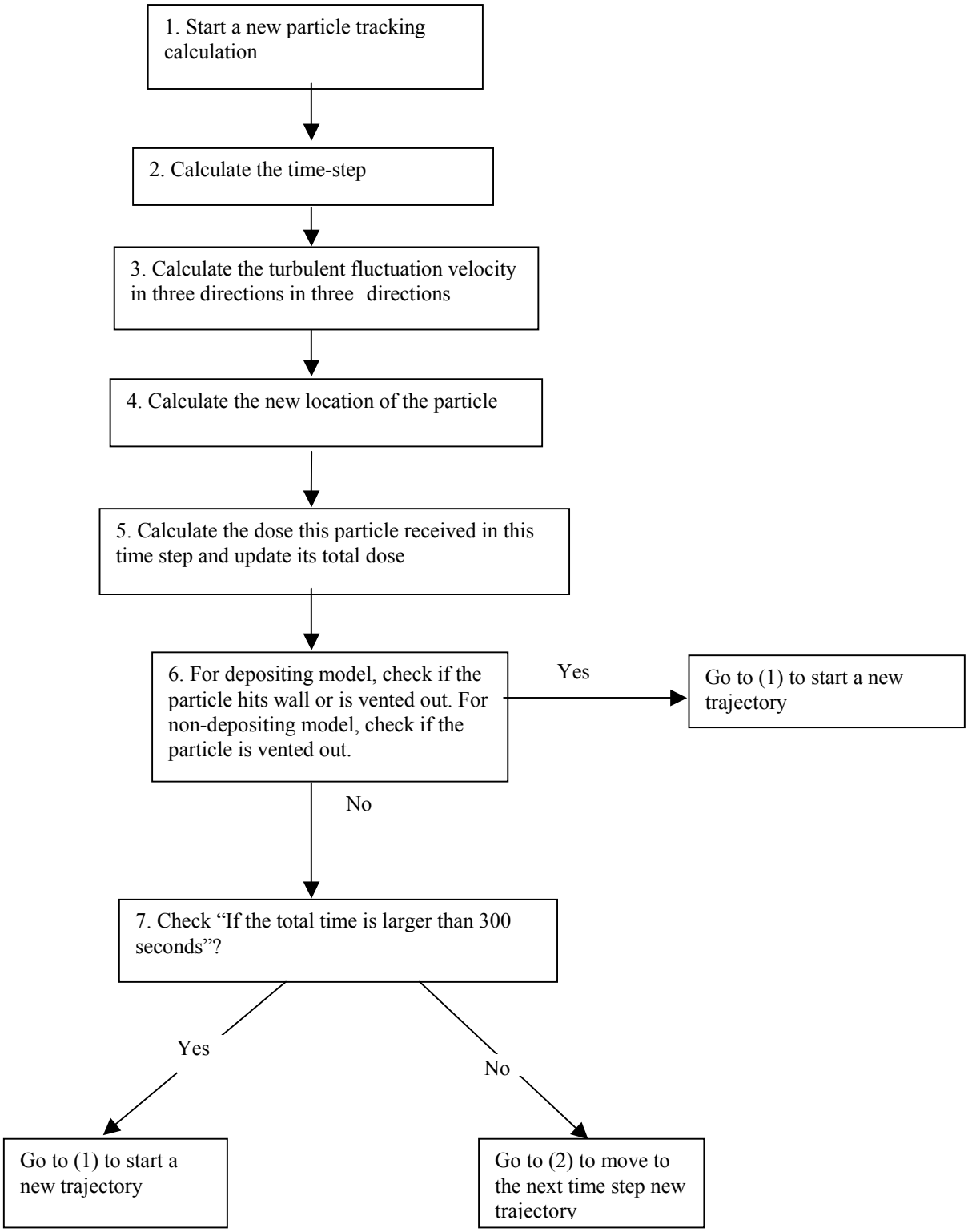

Figure 3.10. *Flow chart of particle tracking procedure*

3.4 Nomenclature

ϕ'	Fluctuating component of variable ϕ
$\bar{\phi}$	Mean component of variable ϕ
∂_{ij}	Kronecker delta (1 if $i = j$ else = 0)
β	Coefficient of thermal expansion
ρ	Density
ε	Rate of dissipation of turbulence energy
τ	Shear stress
λ	Thermal diffusivity
μ	Viscosity
σ_T	Turbulent Prandtl number
μ_{eff}	Effective viscosity ($\mu + \mu_T$)
Γ_T	Eddy diffusivity
μ_T	Eddy viscosity
$C_{1\text{-}3,\mu}$ σ_k σ_ε	Turbulence model constant(s)
g	Acceleration due to gravity
H	Enthalpy
k	Turbulence energy
P	Pressure
T	Temperature
U_i	Velocity tensor
x_i	Distance tensor