Numerical study of particulate turbulent flow to investigate recovery period in cleanrooms

Ali Pourfarzaneh¹, Ali Jafarian²*, Hamidreza Kharinezhad Arani³

¹,²,³- Faculty of Mechanical Engineering, Tarbiat Modares University, Tehran, Iran
* P.O. Box 14115-143, Tehran, Iran, jafarian@modares.ac.ir
1-a.pourfarzaneh@modares.ac.ir
2-jafarian@modares.ac.ir
3-h.kharinejad@modares.ac.ir

Abstract

The Clean room is a controlled space and is used in various industries such as electronics, medical and military industries. One of the most important tests to evaluate the performance of the cleanroom is recovery test. Recovery test determines the time period during which a cleanroom returns to its designated cleanliness level after an instant or a period of deliberate or unintentional contamination. In this paper, a thorough investigation of recovery period has been implemented. In this study, air change rate and its pattern were studied using the Eulerian and Lagrangian approaches and LES, DES and k-ω SST turbulent models. Simulation results were evaluated against control volume analysis. Parameters such as the air change rate, the number of particles, and pressure and energy consumption in various radial and tangential angles of diffusers were studied. Results showed that radial angle had little positive and occasionally negative effect on recovery period. On the contrary, tangential angle improved decontamination rate, at maximum performance (β=45°), it could reduce recovery period as much as 25% which in turn reduces energy consumption. In addition, the DES model provides the best and most coinciding answers between all turbulence models.

Keywords

Cleanroom, Recovery period, Swirl diffuser, Computational Fluid Dynamics (CFD), Lagrangian approach, Eulerian approach

1. Introduction

The recent growth in high-tech industries, especially electronics and medical, resulted in an increased demand of what is known as a “cleanroom”. To put it simply, a clean room is an environment within which concentration of aerosols, temperature and humidity are controlled accurately according to predefined standards.

In a cleanroom, the number of particles larger than a specified size, should be less than a specific number per unit of volume (numeric concentration). This specified particle size is between 0.1 and 5 microns. Number of aerosols of any size is determined by the type of activity implemented in the room, and it’s called the “Cleanliness Level”. Since equipment and personnel in the room are
continuously producing and spreading particles, a number of methods are used to maintain this Designated Cleanliness Level (DCL) throughout the room. Introducing aerosol-free air into the room through HEPA filters and creating a pressure difference is a common method of inhibiting particle diffusion from more contaminated areas to the cleaner ones.

Several different situations could force the cleanroom to lose its DCL which could disturb or even halt the production or activity. These situations and respective recovery scenarios categorized are shortly as below:

**Unsteady flow of particle and air:** This scenario is mostly associated with *Power Outage*. When power supply is interrupted, ventilation system stops functioning and the differential pressure between different sections is lost. Due to particle generation, mostly by the personnel, DCL rapidly falls below the designated value. Recovery period is defined as time period during which DCL is reached after restoration of power.

**Unsteady flow of particle and steady airflow:** This scenario, also known as *Field Test Scenario*, mostly occurs when a deliberate contamination is introduced in a specified period of time when there is a steady airflow throughout the room. In this case, recovery is defined as time period during which cleanroom recovers its DCL after contamination process ceased.

**Steady flow of particle and air:** Also known as *Incident Scenario*, occurs when an equipment (like a filter or a glove) fails to maintain satisfactory performance and a constant flow of particles is introduced into the airflow. In this scenario, recovery could be defined as the period of time during which a specified fraction of particle generation rate are exhausted through the outlet.

In the absence of a classified definition of recovery period and in order to keep a certain amount of applicability, this research has been implemented based on *Power Outage Scenario* as it is the most frequent scenario.

Multiple researches have been carried out on cleanrooms, but heretofore, few studies [1, 2] have completely and comprehensively investigated duration of recovery and transient removal of contamination in clean rooms. Lage et al. via a two dimensional study of contamination removal (Eulerian), have shown that relocation of intake and exhaust vents can improve decontamination rate. In a steady flow study, Mendez et al. [3] considered the effects of intake and exhaust vent configuration in a hospital room. The
effect of moving objects on particle distribution in a clean room was investigated via Eulerian method by Saeidi et al. [4] In a numerical and experimental study Chen et al. [5] used the Eulerian method to investigate particle distribution and removal process. Khoo et al. [6] used an experimental study in a steady state flow to inspect rate and level of effective ventilation in particle concentration in a clean room. In a numerical analysis, Wang et al. [7] conducted a three-dimensional investigation in both Eulerian and Lagrange methods; using two specified points to compare and inspect turbulent models.

In this paper, a comprehensive investigation has been conducted to predict the recovery time in a cleanroom using Eulerian and Lagrangian approaches. Results have been compared against Control Volume Analysis as a conventional method. To simulate the flow field, commonly used turbulence models, namely large eddy simulation (LES), detached eddy simulation (DES), k-ω SST as well as Descrete Random Walk (DRW) model for the discrete phase were employed. Parameters such as the air change rate and energy consumption in various radial and tangential angles of diffusers were studied.

2. Case Study Definition

The space simulated in this study, is a cleanroom of mixed flow type, whose characteristics are accurately described.

This positively-pressurized room is part of an industrial complex and consists of two sections. The main part [3m×2m×2.5m], is a unidirectional laminar hood certified as ISO 5 cleanliness class. The second and smaller section [3.8 m² area, 11.4 m³ volume] is certified as ISO 6 cleanliness class and forms the multidirectional conventional flow section.

The nominal air change rate, while unidirectional hood is switched off, is 47 times an hour. The minimum required pressure in the room is 12.5 Pa. Two swirl diffusers [0.7m×0.7m] supply the air. The exhaust, of rectangular shape [1.4m×0.7m], is located on one of the side walls. Room’s dimensions and different parts and section are illustrated in Figure 1.

Before entering the room, the incoming air passes through H13 class filters. With an efficiency of 99.75%.

In order to study the effects of equipment in the recovery period, two different layouts were considered. First one is As-Built layout which contains a working desk located in the center of the unidirectional hood.
This table is 1.5m long, 0.6m wide and 0.9m high. The second layout, known as At-Rest, which is exactly the same as As-Built mode but lacks the desk.

According to standards, in order to evaluate room’s cleanliness level, air samples of specified volumes are to be collected from specific spots in the room and particle concentration are to be calculated. Mandatory number and volume of sampling units are calculated from equations Error! Reference source not found. and Error! Reference source not found., respectively [8].

\[ N_s = \sqrt{A} \]  
\[ V_s = \frac{20}{C_r} \]  \hspace{1cm} (1)  
\hspace{1cm} (2)

Where \( A \) is the area of the room in square meters and \( C_r \) is the maximum allowable count of the largest particle in DCL. Act of sampling shall be done in the height of the activity and shall be uniformly spread throughout the room with a volume not less than 2 liters for each sampling[9].

For a more precise investigation of recovery in our cleanroom, a total number of 32 samples units were considered. 24 of these sampling units were taken as three rows each of which contains 8 sampling unit, uniformly spaced throughout the room in three different height. The remaining 8 units were located in the height of activity.

In order to be able to use a structured mesh, sampling volumes have not been created in the model. Instead, an ASCII format file was exported from Fluent® and used in a Matlab® program to calculate mass concentration in both Lagrangian and Eulerian approaches for each unit. The geometry of these volumes was assumed to be cubic.

To validate our code, its results were compared with a sample Fluent® analysis by creating a sampling volume in the grid. Then two different reports for average concentration in the sampling unit were extracted from converged solution; First one with Fluent® itself and the second one through ASCII data export and running the Matlab code. Results were exactly the same to the order of 10\(^{-4}\).

3. Control Volume Analysis:

As the simplest and most comprehensible method, control volume analysis is widely used in order to predict a cleanroom’s recovery period. This analysis does not concern airflow pattern or state inside the room, so it can be applied to all three scenarios mentioned before.
The general case for this analysis is shown in Figure 2 Error! Reference source not found.. Particle instant dispersion is the core assumption of this analysis which presumes uniform particle concentration throughout the room, including exhaust vent. Applying continuity and mass conservation equations will lead to\([10, 11]\):

\[
\frac{dC(t)}{dt} = S + \eta_f \frac{\dot{m}_i}{\rho_f V_f} \left( \frac{1 - \dot{m}_m}{\dot{m}_i} \right) C_t + \frac{\dot{m}_m}{\dot{m}_i} C_a - \frac{\dot{m}_i}{\rho_f V_f} C(t)
\]

\(C(0) = C_0, ACH = \frac{m_0}{\rho_f V_f}\)

\(C(t) = C_0 e^{-ACH \cdot \xi t} + \frac{ACH \cdot F \cdot C_a \left(1 - \eta_f\right)}{ACH \cdot \xi} \left(1 - e^{-ACH \cdot \xi t}\right)\) \(\text{(4)}\)

In this equation \(\xi\) is:

\(\xi = 1 - \left[\left(1 - F\right) \times \left(1 - \eta_f\right)\right]\) \(\text{(5)}\)

\(F\) is make-up air fraction to total recirculated mass flow of air and is defined as:

\(F = \frac{\dot{m}_m}{\dot{m}_i}\) \(\text{(6)}\)

The first and second part of Equation (4) are known as decontamination and contamination parts respectively. If Recovery is defined as the time period required for particle concentration decreases two order of magnitude, we will have:

Solving the equation will result:

\(t_{0.01} = -\frac{1}{ACH \cdot \xi} \ln \left[\left(\frac{C_0}{100} - \frac{ACH \cdot F \cdot C_a \left(1 - \eta_f\right)}{ACH \cdot \xi}\right) \times \frac{ACH \cdot \xi}{ACH \cdot F \cdot C_a \left(1 - \eta_f\right) + S} \left(\eta_f\right)\right]\) \(\text{(8)}\)

Supposing 100% efficiency for HEPA filters, recovery time is reduced to:

\(t_{0.01} = -\frac{1}{ACH} \ln \left[\left(\frac{C_0}{100} - \frac{S}{ACH}\right) \times \left(\frac{ACH}{ACH \cdot C_0 + S}\right)\right]\) \(\text{(9)}\)

This equation indicates that when HEPA filters performance is 100%, recovery period is independent of recirculated and make-up air fractions.

Several protocols for clean rooms O&M, clearly mandate evacuation of the cleanroom in case of a power failure, while others have associated it to the power outage duration. In our case of study, due to absence of emergency or uninterruptable power supplies, its protocol stressed evacuation in case of a power failure. Therefore, particle source term is eliminated and Equation (9) will be solved into:
\[ t_{0.01} = \frac{16578.6}{ACH} \]  

Also, fractional concentration profile equation will be:

\[ \frac{C(t)}{C_0} = e^{-ACH.t} \]  

The simplicity of the volume control analysis is the greatest strength and weakness at the same time; although it makes analysis easier, in addition to the possibility of deviation from real case, the effects of parameters other than air change rate are not considered.

**3.1. Assumptions, Equations**

The first governing equation of fluid’s dynamics is continuity. Regarding the limit of air velocity to amounts much lower than the speed of sound, the incompressibility assumption is valid and after averaging, the continuity equation is simplified to the form of equation (12)[12]:

\[ \nabla \cdot \bar{\mathbf{u}} = 0 \]  

Solving the continuity equation is not meaningful on its own. Therefore it will be enforced through correction on pressure field. In this study, SIPMILE correction with a first order upwind scheme has been utilized to modify pressure filed in each time step.

The second most important equation governing fluid’s dynamic, is the linear momentum equation, also known as the “Navier-Stokes” equation. Considering the stream incompressible, after averaging, the equation is simplified in the form of equation (13).

\[
\begin{align*}
\rho_f \left( \frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} \right) &= \left( \rho_f g_x - \frac{\partial \bar{p}}{\partial x} + \mu_f \left( \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) \right) + \frac{\partial}{\partial x} (-\rho_f \bar{w}') + \frac{\partial}{\partial y} (-\rho_f \bar{u}') \\ \\
&+ \frac{\partial}{\partial z} (-\rho_f \bar{u}')
\end{align*}
\]  

Similarly, it can be done for the other two directions.

Regarding the absence of spillage as the boundary condition, all the components of velocity on the walls are equal to zero.

\[ \bar{u} = 0; \bar{v} = 0; \bar{w} = 0 \]
3.2. Turbulent flow equations

To replace averaged product of two fluctuating term in Equation (13) (known as Reynolds stress), Boussinesq approximation is used which assumes isotropic turbulent filed. Reynolds stresses, then, can be approximated to mean velocity as Equation (15). For this, Boussinesq approximation is used.

\[ (-\rho_f \bar{u}_i u_j) = \mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \rho_f (\rho_k \delta_{ij} + \mu_t \frac{\partial \bar{u}_k}{\partial x_k}) \] (15)

With substitution in Equation (13), with arrive at Equation (16).

\[ \rho_f \left( \frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} \right) = \left( \frac{\partial \rho}{\partial x} + \mu_{eff} \left( \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) \right) \] (16)

\[ \mu_{eff} \] is the effective diffusion coefficient.

So far, several studies have been conducted on different methods of turbulent flows modelling. Ruaud et al. while comparing k-\(\varepsilon\) and k-\(\varepsilon\) RNG model concluded the latter is more accurate for simulating particle motion. Zhang and Chen [13] used k-\(\varepsilon\) model in their study with an acceptable accuracy; although it demonstrates deviation with experimental results in several situations. In a similar study, Wang et al. [7] used k-\(\varepsilon\) RNG methods, LES (Lilly-Smagorinsky sub-grid) and DES models and deduced RANS/URANS methods can’t predict correct particle concentration; but other two methods present more suitable results.

In this study, LES turbulence with Lilly-Smagorinsky sub-grid scale, DES with k-\(\omega\) SST sub-grid scale, and k-\(\omega\) SST as URNAS method, are used. In the following aforementioned models are explained.

**k-\(\omega\) SST:** This method is based on transport equations of turbulent kinetic energy and specific dissipation rate of turbulent energy. Both k-\(\omega\) and modified k-\(\varepsilon\) methods are combined which allows k-\(\omega\) method to be used in regions close to walls, and k-\(\varepsilon\) for areas far from it [14]. This method uses transversal dispersion in \(\omega\) equation; also, the definition of turbulent viscosity is changed to include turbulent tension transfer.

These characteristics have caused this method to be widely used in problems ranging from flows with adverse pressure gradient, airfoils and shock waves. K and \(\omega\) equations are illustrated in Equations (17) and (18).

\[ \frac{\partial (\rho_f k)}{\partial t} + \frac{\partial (\rho_f \bar{u}_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \Gamma_k \frac{\partial k}{\partial x_i} \right] + \bar{\omega}_k - Y_k + S_k \] (17)
\[
\frac{\partial (\rho f \omega)}{\partial t} + \frac{\partial (\rho f \bar{u}_i \omega)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \Gamma_\omega \frac{\partial \omega}{\partial x_i} \right] + \tilde{\omega} - Y_\omega + S_k + D_\omega
\]  

(18)

Where \( G \), \( Y \) and \( S \) represent production, dissipation and source terms respectively. Also, \( D_\omega \) is cross-diffusion[15, 16].

**LES:** One of the most widely used models of turbulent flow, is Large Eddy Scale. In LES method, unlike the DNS method in which the entire field is solved accurately, large structures of the flow field are calculated directly. Using LES allows larger time steps and coarser grid in comparison to DNS, although both of these quantities are still smaller than URNAS methods. In this method, subgrid filters omit flow field scales of smaller than a specific time and length. This filter appears as in Equation (19)[17].

\[
\tilde{\phi}(x, t) = \int \phi(r, t)G(x - r,t)dr
\]  

(19)

In this research, Smagorinsky subgrid model has been used. Therefore, turbulent stress term is defined as Equation (21).

\[
(\tau_{\text{SGS}})_{ji} = 2(\nu + \nu_s)\tilde{S}_{ij}
\]  

(21)

\( \tilde{S}_{ij} \) is the rate of strain and is calculated from Equation (22).

\[
\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]  

(22)

The turbulent viscosity is calculated from Equation (23).

\[
\nu_s = L_s^2(\bar{S}_{ij}\bar{S}_{ij})^\frac{1}{2}
\]  

(23)

\( L_s \), the mixing length for subgrid in three dimensional flow, is calculated from Equation (24).

\[
L_s = C_0(\Delta x \Delta y \Delta z)^\frac{1}{3}
\]  

(24)

\( C_0 \) is a coefficient valued between 0.094 and 0.2. This coefficient is constant throughout the solution.

**DES:** Also known as hybrid LES/RANS method, was created for internal flows with high Reynolds number. Using LES around the walls in these types of flow fields, increases the computing cost. In fact, the only difference between this method and LES is the use of RANS in boundary layers. For calculation of
turbulent viscosity, LES equations should be used. But in the K-ω SST based DES method, in the boundary layers, the turbulent kinetic energy expression (K-ω SST) is corrected[18].

\[ Y_k = \rho_f \beta^* k \omega F_{DES} \]  
(25)

\[ F_{DES} = \max \left( \frac{L_t}{C_{DES} \Delta_{max}}, 1 \right) \]  
(26)

\( C_{DES} \) is a calibration coefficient and valued as 0.65 and \( \Delta_{max} \) is the maximum size of the local grid.

3.3. Lagrangian approach

Since a particle is a discrete phase, its equations should be analyzed separately and in a reference coordinate system. Particle’s equation of motion is Newton’s second law.

The forces acting on the particle are drag, gravity and buoyancy forces. These are the only effective forces in the present work. Therefore, the final particle’s equation of motion is transformed [7, 19] to the following form in Equation (28):

\[ \frac{d\mathbf{u}_p}{dt} = \frac{1}{\tau} (\mathbf{u}_f - \mathbf{u}_p) + \mathbf{g} \left( 1 - \frac{\rho_f}{\rho_p} \right) \]  
(28)

\[ \tau = \frac{\rho_p d_p^2 C_c}{18 \mu_f} \]  
(29)

3.4. Effects of turbulent field on particles

The Discrete Random Walk method is used to apply the effects of turbulence field on particle’s equation of motion. In this method, the turbulence is assumed isotropic; as a result, its three components are equal. Therefore, velocity of fluid in the equation of motion is formed as Equation (30) demonstrates [20].

\[ \mathbf{u}_f = \left( \bar{u} + \zeta \sqrt{\frac{2k}{3}} \right) \hat{i} + \left( \bar{v} + \zeta \sqrt{\frac{2k}{3}} \right) \hat{j} + \left( \bar{w} + \zeta \sqrt{\frac{2k}{3}} \right) \hat{k} \]  
(30)

\( k \) is turbulence kinetic energy and \( \zeta \) is a random number of Gaussian distribution with zero mean value and standard deviation of 1. During the analysis, the discussed random number would change in accordance with the turbulence field.
In this analysis, both large and small turbulent length scales were compared to particle radius. Since neither of the large nor small scales in the whole field are smaller than particle radius in the most severe turbulence, the effects of particles on turbulent field considered to be negligible.

In order to create a realistic field for Lagrangian approach (as the initial condition), first a unidirectional velocity field is defined in the entire solution geometry with a zero gravity field and zero turbulent kinetic energy. Then, particles are released into the room forming a uniform but not randomly distributed field of particles. Afterwards, the particles are allowed to be dispersed in a zero-velocity and gravity field and a turbulent kinetic energy and dissipation rate of 1, so a physical and realistic field will be formed which is randomly uniform. At this point, the decontamination process is initiated (ventilation system starts up) to a point which number of particles is decreased to 1/200 to 1/150 of its initial count.

3.5. Eulerian approach

Mass transfer equations are used in Eulerian approach. By applying the transport equation for each species, Equation (31) is achieved [21].

\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \nabla \cdot (\mathbf{J}) + S
\]  

(31)

\(C\) is the concentration (mass fraction) of the intended species and \(J\) is its flux vector which can be obtained from Fick’s law.

\[J_i = -D \frac{\partial C}{\partial x_i}\]  

(32)

\(D\) is Fick’s coefficient or the diffusion coefficient for the intended particle. Through averaging and Boussinesq approximation, Equation (31) will change into:

\[
\frac{\partial \bar{C}}{\partial t} + u_i \frac{\partial \bar{C}}{\partial x_i} = (D + \Gamma_t) \left( \frac{\partial^2 \bar{C}}{\partial x_i \partial x_i} \right)
\]  

(33)

\[\Gamma_t = \frac{\mu_t}{\text{Sc}_t}\]  

(34)

\(\text{Sc}_t\) is turbulent Schmidt number which must be considered 0.7 to achieve realistic solutions[22].
Mixture of air and carbon monoxide is used for Eulerian analysis to minimize change of carrier fluid’s characteristics due to similarity of carbon monoxide’s property (molecular mass, density and viscosity) to those of air.

### 3.6. Conformity Analysis

In order to quantify how close numerical results are to that of experiments, correlation factor according to Pearson’s R-squared method was applied. If X and Y are two vector of the same size (e.g. data of numerical analysis and experimentation obtained in specified intervals of time), then Pearson’s correlation factor is defined as Equation (35):

\[
CF = \frac{Cov(X, Y)}{\psi_X \psi_Y}
\]  

(Numerator is covariance of the given vectors and is defined as:

\[
Cov(X, Y) = \frac{\sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y})}{n - 1}
\]  

(Denominator of Equation (36) is product of each vector’s standard deviation and for vector X is defined as:

\[
\psi_X = \sqrt{\frac{\sum_{i=1}^{m} (x_i - \bar{x})^2}{n - 1}}
\]  

### 3.7. Model validation

Before starting the analysis of our studied case, it’s necessary to verify the chosen models. Lou et al. [23] experimental results were used for this. The space used in their study includes two similar enclosures, each 2.5m in length, 3m in width, and 2.4m in height, joined together with a sliding door of 0.9m in height and 0.7m width. Both air diffusers are one meter wide and half a meter high, but are located in different levels and sections on the room. It’s worth noting that the results of this experimental study was obtained from Wang et al. [7] experiments.

The particles used in this experiment, had diameters between 0.5 and 5 microns. At first, the sliding door between the two sections is closed, while the particles are released into first section of the room, in order for them to reach a uniform dispersion. Then, ventilation devices with air change rate of 10.26 start working while the sliding door opens at the same time. Particle concentrations reading in each section is done 1 minute intervals.
3.7.1. Turbulent models

In this study, 3 turbulent models of LES, DES and URANS were investigated. Regarding the use of swirl diffusers and presence of high-speed flow fields and high curvature of the stream, this model benefited from K-ω SST method. K-ω SST was also used in boundary layers of the DES method, while Lily-Smagorinsky sub-grid model was employed in LES.

Result show that although k-ω SST predictions are not entirely consistent with experiments in the both Eulerian and Lagrangian methods, but compared to k-ε RNG results (used in previous studies), they’ve been improved significantly. Besides, although LES and DES methods have predicted concentration variations better in the Lagrangian method, Eulerian method provided better overall results. Figure 3 shows a comparison of both numerical Eulerian and Lagrangian methods.

By comparing correlation coefficients obtained from the results of these three methods with experimental values in both sections and both approaches, it was apparent that DES method provides the best and most accurate results.

3.7.2. Particles Boundary Conditions

Studying the effects of boundary conditions on the results showed that trap boundary condition doesn’t provide correct results. In reflect boundary condition, results have little dependency on coefficient of restitution; though results obtained with 1 as coefficient of restitution, present a greater correlation with experimental and Eulerian approach results.

3.7.3. Sampling Unit Volume

As described in section 2, sampling volumes are not formed inside our grid and mean concentrations are calculated inside a Matlab code. Therefore, it is highly likely for sampling units to have close but not exact same volumes. So, it demands to perform a sensitivity analysis on sampling unit volumes. To measure the effects of change in the volume of sampling unit, in the result extracted in DES model and unity coefficient of restitution, 3 different volumes in shape of cube were considered. The results, as presented in Figure 4, showed that in the Eulerian analysis, the outcome is not very dependent on sampling unit size; however, with volume increasing, it converges to a specific amount. On the contrary, volume in the Lagrangian approach has a more pronounced effect on results. Although little difference was observed
between 82 and 340 liter volumes, but with volume decreased to 3 liters, the results show a noticeable fluctuation which is the result of sampling unit size being comparable to mean particle distance. Thus, as long as the sampling unit volume is not comparable with the room volume, and mean particle distance incomparable to sampling unit characteristic length, the result is more dependent to the location of the sampling unit, rather than its size.

4. Grid, Time Step and Number of Particles Study

After the models and boundary conditions were investigated, a proper grid independency to the results should be obtained. In addition similar procedure should be carried out for time step. Grid and time step independency was studied simultaneously in this research; meaning since grid independency was not achieved with large time steps, in smaller time steps, all the studied grids over the 24 sampling volumes were graphed over time and compared in their basic analysis and concentration reduction process mode. The grids studied had 15457, 25920, 62080, 122500, 207360, 496640 cells. Time steps also started with 0.2 seconds and were halved in 4 stages, reaching 0.01 in the fifth stage. Results showed that 0.025 seconds is suitable time step and no perceivable change is observed in results by changing the grid from 207360 to 496640. Therefore, grid number of 207360 and 0.02 time step were chosen for analysis.

Calculation cost of Lagrangian analysis is directly proportional to the number of particles present in the field of solution. Minimum number of particles for reaching an independent solution, is highly dependent to the number of computational cells in the field. Previously and in other researches, proper ratio of particle count to grid cells for achieving this independency has been stated. Inspired by previous studies, this ratio was regarded as 0.5 and results were compared by increasing the number of particles, (107246, 165240, 364715 and 563547, respectively). The results show that by increasing the number of particles, the analysis results converge to a specific value; so that an increase from 364715 to 563547, no significant change occurs. Therefore, the aforementioned ratio was approximately determined to be 1.8.

4.1. Investigated parameters

To study recovery time in the intended case of study, three parameters were changed. These three parameters, namely, are ventilation rate of the room (ACH), tangential entry angle ($\alpha$) and radial entry angle ($\beta$). Separately, both tangential and radial angle set to be 15, 30, 45, 60, 75 degrees.
5. The results of the studied room

5.1. Control volume Interpretation

One of the aspects concerned in this research is the deviation of control volume analysis from real results, described in section 2. In the first encounter, instead of observing each sampling unit, it was preferred to study the behavior of the case of study as a whole. Therefore, we performed a control volume interpretation which made it possible to compare results in large scale with control volume analysis.

In each parameter of study, namely air change rate per hour, radial angle and tangential angle on the inlet, fractional particle count plotted against time in a semi-logarithmic scale are shown in Figure 5. On all pictures, control volume analyses are also plotted in order to perform a better comparison. Intersection of each curve with horizontal axis, indicates recovery period.

First picture indicates in case of increase in air change rate, recovery period will decrease as expected; though it does not demonstrate much deviation from control volume analysis. This deviation even decrease to zero when air change is doubled.

On the middle picture, when increasing radial angle of inlet flow to 45° recovery period will increase by 12%; but it will decrease and even reaches the same amount as vertical flow when α=75°. Though changing radial angle might have effects on recovery period, it will not help the room to recover faster than control volume analysis.

As for the third picture, increasing swirl angle of the inlet flow to 45°, recovery period experience descend of 28%, although it increases once more when β=75°. Unlike radial angle which has negligible effect, tangential angle not only cause noticeable drop on recovery period, it will make the whole system to recover faster than control volume analysis.

5.2. Change in pressure and energy consumption

Since pressurizing is one of the necessary factors of clean room design, change in pressure in accordance to other parameters becomes of utmost importance. On the other hand, discussions on reducing energy consumption is necessary in today’s industry. Therefore, change in pressure and energy consumption was investigated in this section.
In most modern clean rooms, adjustable outlet vents are used to create minimum required pressure; these diffusers are opened just far enough to create required pressure in the room.

In order to consider the required pressure and energy, the pressure at room inlet diffusers and mean pressure at the room entrance was calculated in every particle concentration reading. Mean pressure till recovery and energy requirements were calculated by control volume criterion [Equation (1)].

\[ W = (\bar{p}_{in} - \bar{p}_{out})V_a \]  

(1)

Energy and pressure ratio are obtained through Equations (2) and (41). Since exhaust pressure equals to zero, and air volume is equal to intake flow rate times the recovery time, we arrive at:

\[ \text{Energy ratio} = \frac{W}{W_{ref.}} \]  

(2)

\[ \text{pressure ratio} = \frac{\bar{p}_{in} - \bar{p}_{out}}{\bar{p}_{in,ref.} - \bar{p}_{out,ref.}} \]  

(3)

which ref. subscript refers to value of each quantity in reference state, i.e. air change rate at 47 and both radial and tangential angles at zero. Results of both quantities are illustrated in Figure 6.

Results clearly indicates pressure ratio follows a quadratic pattern with change in ventilation rate which physically sounds. Unlike air change rate, change in both radial and tangential of inlet flow does not have a noticeable effect on pressure ratio, tough they might slightly weaken pressure field inside the room.

Like Pressure ratio, energy ratio follows relatively the same quadratic dependence with change in ventilation rate, meaning increasing ventilation rate by n times, roughly increases fan filter unit absorbed power n^3 times, while reducing the recovery time by about n time. Though air change rate might have a direct and noticeable effect on energy consumed, it does not happen with radial and tangential angles. As change in pressure is negligible and air change is kept constant at 47, energy is mainly influenced by a change in recovery time.

5.3. Sampling units Analysis

In previous section, only a control volume approach was considered to monitor recovery period, pressure and energy consumption. Though it gave an overall perspective of what happens in clean room when changing ventilation parameters, it does not conclude if cleanroom has recovered based on all sampling units. Therefore, in this section and as a more precise analysis, sampling units’ behavior is investigated to verify cleanroom recovery.
To this point, results have definitely indicated, when considering the whole room, decontamination process might not coincide with control volume analysis closely, but still follows a control volume pattern, creating a straight line on semi-logarithmic diagram against time. On the other hand, data acquired through time for all sampling unit and all rate of air change or inlet flow pattern is too vast; so we need a proper and compact way to present and interpret results. Therefore, in order to prevent observing each sampling unit during recovery, its behavior is fitted with a function. Since the behavior of the room is largely corresponding with control volume analysis, the exponential function of control volume analysis was considered. The fitting as seen in Equation (4) will give the best results.

\[
\frac{C_{SU}}{C_0} = e^{\frac{a(t-b)}{3600}} \quad (4)
\]

which means the behavior of sampling volume was regarded as a control volume with a ventilation rate of \(a\); but a delay or early offset time of \(b\) was considered to compensate the probable deviation.

5.4. Recovery Performance, Recovery period

The recovery period in each sampling unit, is the required time for fractional concentration to reach 0.01. At first glance, obtaining recovery period for each sampling unit necessitates observation of unit’s behavior in a specified interval of time; but calculating the recovery period with this method is not possible because of the following reasons:

First, because collected data is discrete, and calculating accurate recovery period time requires suitable interpolation and extra mathematical operations.

Second, indistinguishable recovery which means, in some sampling units, especially in Lagrangian approach, fractional particle concentration might exceed 0.01 long after it has been recovered. Though these volumes may recover in a short while, but this behavior makes exact instant of recovery indefinite.

The amount of data in this study is quite high and therefore practical calculation of recovery time with this method for all sampling unit in each approach, geometry and parameter, is time consuming.

Thus, recovery time can be calculated after fitting a proper function on the results of each sampling unit. For assessing the recovery time in each unit, the left side of the Equation (4) is equal to 0.01 and it’s solved for \(t\), giving us Equation (5) which presents recovery time in seconds.
In order to compare sampling unit recovery with control volume analysis, recovery Performance was defined as Equation (6).

\[ \eta_v = \frac{a}{ACH} \]

This equation simply indicates whether a sampling unit overtakes or falls behind control volume analysis. If recovery performance is greater than 1, it means sampling unit recovery is faster than what CVA has predicted; the opposite is also true if Recovery Performance is less than 1.

5.5. Mean and variance of Recovery Performance

Mean value and variance of recovery performance among 32 sampling units is conducted for both Eulerian and Lagrangian analysis methods and both geometries, namely As-Built (no table) and At-Rest, with variance in all three parameters. Covariance, and standard deviation were calculated according to Equation (38) for each case.

Results are shown on Figure 7. Specifically, geometry has little effect on both quantities. When air change rate is elevated, recovery performance calculation for sampling units shows that about half of these units during the entire or most of recovery time, are behind control volume analysis. By increasing ventilation rate, mean recovery performance increases; meaning that performance of ventilation increased in the entire room, which is a result of increased mixing and naturally a more turbulent field; however, standard deviation also follows a similar pattern, which shows the reason of increased overall performance, is an increase in performance in a limited number of sampling units and not all of them.

A rise in radial angle, reduces average and standard deviation; i.e. with radial angle increasing, mean value converges towards 1. Angle increase also has a declining effect in dispersion (except one occasion) reaching about 0.1 at 75°. These diagrams show that radial pattern is significantly effective in keeping uniformity and homogeneity of the air flow inside the clean room.

Similar to results obtained from radial angles, changes in tangential angle is accompanied by reduced mean and dispersion recovery performance; however, in comparison to radial angle, it demonstrates slightly worse performance in homogenizing room air.
5.6. Minimum Recovery Performance and Recovery time

Importance of minimum recovery rate lies in the fact that it specifies the recovery time frame. Minimum recovery rate is shown in Figure 8. In addition to analysis results and control volume interpretation, the first and sixth lowest recovery rate values calculated by Eulerian and Lagrangian analysis are shown. Lagrangian analysis results sometimes showed erratic and even contradictory behavior.

Unlike Figure 4, on which control volume interpretation sometime outpaced control volume analysis, in the first diagram, control volume interpretation is always behind; which is a result of curve fitting and has to be accepted to simplify the results.

The results show that an increase in radial angle causes reduction in minimum efficiency; but demonstrates improvement in angles above 30 degrees in Lagrangian analysis and 45 degrees in Eulerian analysis. However, it never catches up control volume analysis while being higher than base state (0 degree angle) in some angles. Thus, although mixing resulted from radial pattern is useful, it has little positive effect in minimum recovery efficiency.

As evident, in almost every scenario and in both approaches, recovery time decreases with growing ventilation rate. The general trend of change in recovery time is very similar to control volume analysis and interpretation; meaning recovery time can be fitted to a function seen in Equation (4).

Tangential angle has significant positive effects on minimum recovery efficiency. Increasing the angle to 15 degrees results in reduced minimum recovery efficiency, but with further angle increase to 45 degrees, the value increases, surpassing even control volume analysis values. Then with even further increase, the value decreases but it is still higher than base state (0 degree angle). We also learn from results that change in ventilation rate is unable to provide a noticeable change in minimum recovery efficiency. A similar diagram for recovery time versus these three parameters is shown in Figure 7.

Therefore, it’s possible to say that although ventilation rate has little influence on minimum recovery rate, none of the other parameters has a notable influence either, so ventilation rate should be regarded as the most important quantity in recovery time determination.

By a more precise investigation on diagrams regarding variation in tangential and radial angles, it was clear that by mirroring the diagram regarding minimum recovery rate horizontally, a diagram similar to recovery time can be obtained. Meaning each minimum in a diagram in Figure 8 is corresponding to a
maximum in the equivalent diagram in Figure 8. Results also show that the two approaches have high correlation, and recovery predictions of the Eulerian method is between 4% and 17% faster than Lagrangian method.

An important conclusion from these diagrams, is the higher amount of this value in Eulerian analysis compared to Lagrangian to an extent that the worst Eulerian results (rank 1) are comparable to the best Lagrangian results (rank 6). In addition to that, best Eulerian analysis results (rank 6) are comparable to control volume interpretation result. Also, Eulerian analysis results follow a similar trend to those of control volume interpretation.

6. Conclusion

In the present work, a thorough investigation of recovery period was conducted. The air change rate and air inflow patterns were studied using the Eulerian and Lagrangian approaches and LES, DES and k-ω SST turbulent models. Simulation results were evaluated against control volume analysis as well.

Results showed that k-ω SST predictions are not entirely consistent with experiments in the both Eulerian and Lagrangian methods; but compared to k-ε RNG results, were improved significantly. Besides, although LES and DES methods have predicted concentration variations better in the Lagrangian method, Eulerian method provided better overall results.

According to the results, energy consumption and internal room pressure is directly proportional to rate of ventilation squared. Therefore, ventilation rate increase is suggested when it’s going to replace traditional clean room pressurizing methods. Swirl diffusers can decrease energy consumption by reducing recovery time without any effect on mean room pressure; this can be significant in energy savings.

Use of radial flow pattern in intake diffusers, is significantly influential in homogenizing particle concentration; but it can increase the recovery time in some cases. Using the tangential (rotary) pattern of stream in intake diffusers, greatly decreases recovery time while homogenizing particle concentration.

To study recovery in a clean room, sampling should be moved from below the intake diffusers closer to the exhaust vents. Presence of objects in the room has little effect on recovery.

In clean room recovery analysis, Eulerian and Lagrangian approaches present high correlation; but Eulerian method predict a lower recovery time by 4% to 17%.
### 7. Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Room Area</td>
</tr>
<tr>
<td>ACH</td>
<td>Air Change Rate</td>
</tr>
<tr>
<td>C</td>
<td>Species Concentration</td>
</tr>
<tr>
<td>( C_r )</td>
<td>Largest Particle count</td>
</tr>
<tr>
<td>CF</td>
<td>Correlation Factor</td>
</tr>
<tr>
<td>COV</td>
<td>Covariance</td>
</tr>
<tr>
<td>d</td>
<td>Diameter</td>
</tr>
<tr>
<td>D</td>
<td>Brownian Diffusion</td>
</tr>
<tr>
<td>F</td>
<td>Force Applied on Particle</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational Acceleration</td>
</tr>
<tr>
<td>k</td>
<td>Turbulent Kinetic Energy</td>
</tr>
<tr>
<td>l</td>
<td>Turbulent Length Scale</td>
</tr>
<tr>
<td>m</td>
<td>Mass</td>
</tr>
<tr>
<td>N</td>
<td>Cleanliness Level</td>
</tr>
<tr>
<td>( N_{SU} )</td>
<td>Compulsory Sampling Unit Count #</td>
</tr>
<tr>
<td>( N_{SU} )</td>
<td>Sampling Unit Number</td>
</tr>
<tr>
<td>p</td>
<td>Pressure</td>
</tr>
<tr>
<td>Q</td>
<td>Inlet Flow</td>
</tr>
<tr>
<td>r</td>
<td>Random uniform Number</td>
</tr>
<tr>
<td>S</td>
<td>Particle Generation Rate Per Unit of Volume</td>
</tr>
<tr>
<td>( \bar{S}_{ij} )</td>
<td>Fluid Strain Rate</td>
</tr>
<tr>
<td>u</td>
<td>Velocity X-Component</td>
</tr>
<tr>
<td>( \mathbf{u} )</td>
<td>Velocity Vector</td>
</tr>
<tr>
<td>( \mathbf{u}_r )</td>
<td>Particle-Fluid Relative Velocity</td>
</tr>
<tr>
<td>v</td>
<td>Velocity Y-Component</td>
</tr>
<tr>
<td>V</td>
<td>Volume</td>
</tr>
<tr>
<td>w</td>
<td>Velocity Z-Component</td>
</tr>
<tr>
<td>W</td>
<td>Energy</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>Radial Angle</td>
</tr>
<tr>
<td>( \beta )</td>
<td>tangential Angle</td>
</tr>
<tr>
<td>( \delta_{ij} )</td>
<td>Kronecker Delta</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>Turbulent Energy Dissipation Rate</td>
</tr>
<tr>
<td>( \eta_f )</td>
<td>Filter Efficiency</td>
</tr>
<tr>
<td>( \mu )</td>
<td>Fluid Dynamic Viscosity</td>
</tr>
<tr>
<td>( \mu_t )</td>
<td>Turbulent Dynamic Viscosity</td>
</tr>
<tr>
<td>( \mu_{ef} )</td>
<td>Fluid Effective Dynamic Viscosity</td>
</tr>
<tr>
<td>( \nu )</td>
<td>Fluid Kinematic Viscosity</td>
</tr>
<tr>
<td>( \rho )</td>
<td>Density</td>
</tr>
<tr>
<td>( \tau )</td>
<td>Particle Relaxation Time</td>
</tr>
<tr>
<td>( \tau_{sgs} )</td>
<td>Sub-grid Scale Stress in LES</td>
</tr>
<tr>
<td>( u )</td>
<td>Swirl Diffuser Outlet Velocity</td>
</tr>
<tr>
<td>( \omega )</td>
<td>Turbulent Energy Specific Dissipation Rate</td>
</tr>
<tr>
<td>( \Psi )</td>
<td>Standard Deviation</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>Gaussian Random Number</td>
</tr>
</tbody>
</table>
8. References


**Figure caption:**

Figure 1 – Case of study in As-Built mode - Plan (left), side view (right)

1: working desk, 2: inlet diffuser, 3: Exhaust Vent, 4: Sampling Unit Centroids

Figure 2 - General case for control volume analysis and schematic of diffuser flow angles

Figure 3 - Comparison of numerical and experimental analysis results for turbulent models, Eulerian approach (left) and Lagrangian approach (right)

Figure 4 - Comparison of numerical and experimental analysis results for sampling unit volume, Eulerian approach (left) and Lagrangian approach (right)

Figure 5 - Control volume interpretation results against ventilation rate (upper left), radial angle (upper right), tangential angle (lower left) and comparison to control volume analysis

Figure 6 - Change in pressure ratio and consumed energy ratio for recovery against air change rate (upper left), radial angle (upper right) and tangential angle (lower left)

Figure 7 – Change in Average (Left) and Standard Deviation (Right) of All Sampling Units’ Recovery Performance with Air Change Rate (Top), Radial Angle (Middle) and Tangential Angle (Bottom)

Figure 8 – Change in Minimum Recovery Performance (Left) and Recovery Time Deviation (Right) with Air Change Rate (Top), Radial Angle (Middle) and Tangential Angle (Bottom) in As-Built Mode
Figure 5
Figure 6
Figure 7
Figure 8
9. Biographies

**Ali Pourfarzaneh** received his BS degree from the Isfahan University of Technology, Iran, and his MS degree from Tarbiat Modares University, Tehran, Iran, in Mechanical Engineering (Energy Conversion), in 2010 and 2014, respectively. His research interests include: numerical modeling, computational fluid dynamics, and Cleanroom.

**Ali Jafarian** received BS, MS and PhD degrees from Sharif University of Technology, Tehran, Iran, in 2000, 2002 and 2008, respectively, all in Mechanical Engineering (Energy Conversion). He is currently Professor of Mechanical Engineering at Tarbiat Modares University, Tehran, Iran.

**Hamidreza Kharinezhad Arani** received his BS degree from the Isfahan University of Technology, Iran, and his MS degree from Tarbiat Modares University, Tehran, Iran, in Mechanical Engineering (Energy Conversion), in 2014 and 2017, respectively. His research interests include: computational fluid dynamics, numerical modeling, Cleanroom, and turbulent dispersion of particle.