Improving air quality in classrooms using ART and using ML to expedite simulation results

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Abstract

The objective of this case study is to study air flow patterns that exist in a classroom environment consisting of two adjacent split air conditioners and two exhaust fans. One of the exhaust fans has a fixed location and the other one is moved around the room. Further, these flow simulations will be used to find out the maximum air residence time for a given case with the aim to minimize it. To ease the process of estimating air quality, a machine learning neural network model will be trained to predict the maximum air residence time for a particular configuration of exhausts in a classroom environment. Lastly, an intervention which can modify the flow pattern and hence the air quality is proposed to further minimize the maximum air residence time in that configuration of exhausts that produced the minima. The project aims to make classroom ventilation design easier and standardized for any given room with similar air inlet and outlet conditions. The simulator used for all simulations in OpenFOAM 9.

1. Introduction

Air quality in an important factor determining the health and development of the human race. With ever increasing industrial activities of human beings, the amount of pollutants released in the environment continue to rise. Degradation in air quality can cause diseases like asthma, infections and even cancer.

Apart from man-made pollutants, air is also a carrier of dust particles and infectious micro-organisms. Dust allergy is a common problem especially affecting those with weaker immune systems. Airborne micro-organisms include several types of fungi, bacteria, algae etc. Air being one of the fastest mediums for these micro-organisms to travel, posses a real danger. Numerous pandemics in human history have been caused by bacteria and fungi being able to travel through air and infecting the respiratory system of human beings. One such recent case is the COVID-19 pandemic which caused millions of deaths and large amount of financial and mental strain. Hence, it is important that we track our air quality, especially for these airborne disease-causing pollutants.

Humans are spending more time than ever indoors. Most of the office and educational activities are carried out in closed rooms spending large amounts of time indoors, at a continual stretch. This posses an important issue. With closed spaces being more and more common, the chances of interacting with airborne pollutants increases largely. Hence, it is important to design our buildings, meeting rooms and classrooms with proper ventilation. These posses a challenge to ventilation designers to ensure air replenishment in such spaces at a pace fast enough to keep up with fast and infectious pollutants and large amount of time spent indoors at a stretch. One of the measures used to track this is called the Air Residence Time (ART).

United States Environmental Protection Agency defines ART as the amount of time that it takes for a sample of ambient air to travel from the opening of the inlet probe (or cane), through the manifold, to the inlet of the instrument. Here, ART has been defined as the time taken by a fluid particle to travel from the inlet of a room to any given position. To provide best air quality management, it is important that we tract the maximum ART that could exist in a room and try to minimize this to an extent that our classrooms and meeting rooms become safer and healthier places and do not promote diseases caused by air pollution.

With technology in ventilation systems approaching saturation, the major question is to optimally place such systems provide the best possible air quality. Commonly used ventilation systems in classrooms are air conditioners, exhaust fans and table fans. The goal of this project is to understand, evaluate and conclude the various effects in air flow and air residence time due to varying location of exhaust fans in a classroom environment. To achieve this, computational fluid dynamics (CFD) solvers in OpenFOAM 9 have been used.

CFD simulations for large domains take up lots of computational resources. Due to the scale of importance of the problem at hand, running CFD simulations for all possible configurations of all rooms is a very tedious, time consuming and expensive task. With rise in machine learning to replace complicated systems into simpler models for faster results, the application in predicting air quality is an interesting domain to explore. Using ML, fewer CFD simulations can be used to extract results for new and innovative ventilation location configurations without spending a lot of resources.

The further parts of the report are divided into the following sections. Section 2 discusses the exact problem statement. Section 3 defines the governing equations to be solved. Section 4 presents the geometry, meshing conditions, boundary conditions, solver configurations for airflow and ART simulations. Section 5 summarises the various findings from these simulations. Section 6 proposes an intervention to further improve the results. Section 7 formulates the machine learning model for the simulations. Section 8 summarises all the conclusions including the interventions and ML model.

2. Problem Statement

A classroom in Chemical Engineering Department, IIT Bombay has been consider as a test subject. The room is defined as a cuboidal fluid domain. One wall has a door and two air conditioners. The opposite wall has an exhaust near the corner. A second exhaust is tested for different locations at the same height as the first exhaust on all three walls. Fig 1 shows the room with an exhaust to scale. However, the position of the exhaust is only for demonstration.

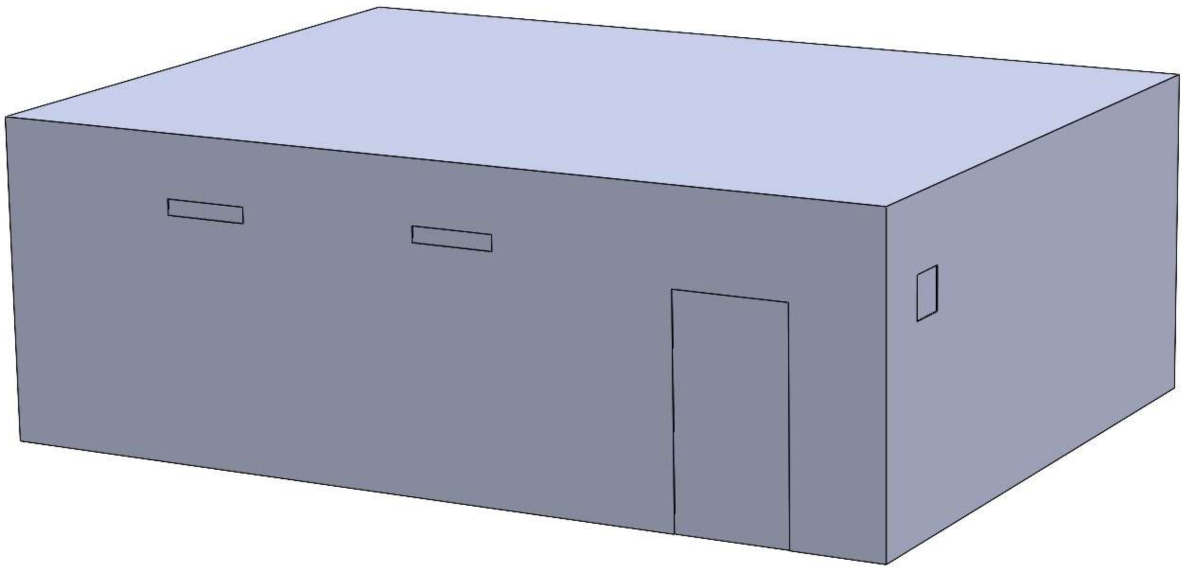


Figure 1: A pictorial depiction of the classroom model. Note that the exhaust location is only representative but may actually shift at that same height.

Hereafter left, right and front walls will be mentioned in reference to the door. The left wall is the wall with cases 17 to 23. The right wall is the wall with cases 10 to 16. The left wall is the wall with cases 1 to 9 and default. The origin is defined at the bottom left corner of Fig 2 and at ground level.

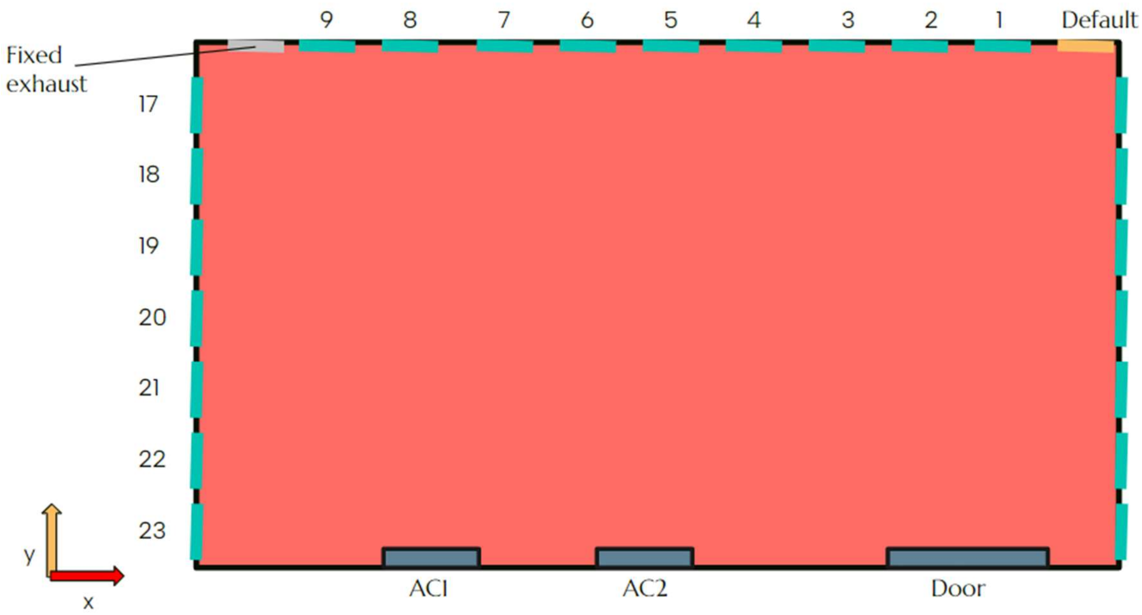


Figure 2: Top view showing all the positions of the exhaust for which CFD simulation in OpenFOAM 9 will be run for

For the left and right wall, the centre of the moving exhaust lies at steps of *80cm* beginning from $y = 80cm$. For the front wall, the same lies at steps of *75cm* beginning from $x = 150cm$ for case 9. The fixed exhaust has its centre at $x = 80cm$.

3. Governing Equations

There are two things to be solved for. The airflow velocity and the ART. For the air velocity simulation, the N-S equation is solved for along with continuity.

$$\nabla . \bar{U} = 0 \tag{1}$$

$$\rho \frac{\partial \bar{U}}{\partial t} + \rho(\bar{U} . \nabla)\bar{U} = -\nabla p + \mu \nabla^2 \bar{U} \tag{2}$$

The effect of turbulence is taken into account by solving the Reynolds averaged N-S equation for the $k - \varepsilon$ model for turbulent viscosity.

$$\rho \frac{Dk}{Dt} = \rho \nabla . (D_k \nabla k) + P - \rho\varepsilon \tag{3}$$

Here, k is the turbulent kinetic energy at a given location and D_k is its diffusivity. P is the rate of generation of the turbulent kinetic energy.

$$\rho \frac{D\varepsilon}{Dt} = \rho \nabla . (D_\varepsilon \nabla \varepsilon) + \frac{C_1 \varepsilon}{k}\left(P + C_3 \frac{2}{3} k \nabla . \bar{U}\right) - C_2 \rho \varepsilon^2 / k \tag{4}$$

Here, ε is the turbulent kinetic energy dissipation rate at a given location and D_ε is its diffusivity. C_1, C_2, C_3 are some constants.

$$\vartheta_t = C_\mu \frac{k^2}{\varepsilon} \tag{5}$$

The turbulent viscosity is calculated form the above expression with the constant being equal to 0.09.

For the air residence time, a Reynolds transport theorem for a scalar variable *S* is taken with an implicit source of 1.

$$\frac{\partial S}{\partial t} + \nabla.(\bar{U}S) = 1 \tag{6}$$

S stands for air residence time. $\bar{U}$ is the velocity vector.

4. Simulation Procedure

4.1 Geometry and Mesh

The geometry as shown above has the following dimensions. The location for the moving exhaust has been given above.

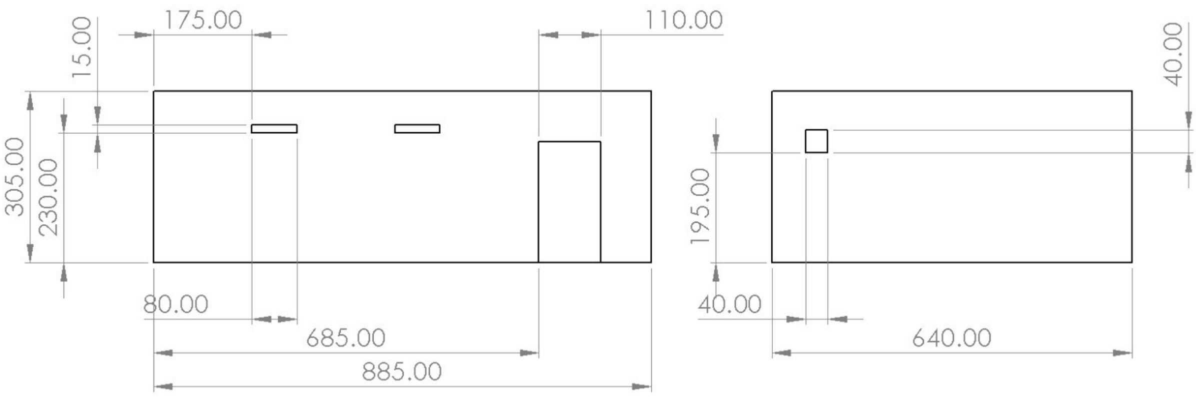


Figure 3: Front view and side view of the domain. Note that the exhaust can move around the room at the given height and size.

All dimensions in cm

The geometry has been made using the blockMeshDict feature in OpenFOAM 9. The patches for air conditioners, door and exhausts were made using the topoSetDict and createPatchDict features in OpenFOAM 9. The meshing for the domain was again done in blockMeshDict. For all 3 directions, *20cm* of domain from each wall was refined with a gradient of 10 with the mesh becoming finer near the external faces. The rest of the domain had uniform meshing. There were 189 cells in x direction, 140 in y direction and 73 in the z direction. A total of 1931580 cells were constructed in the entire domain. Further details of meshing are mentioned below.

Max cell openness = 1.734723476e-16

Max aspect ratio = 10.21738153

Minimum face area = 2.394753336e-05

Maximum face area = 0.0025

Min volume = 1.17190169e-07

Max volume = 0.000125

Total volume = 172.752

Mesh non-orthogonality Max: 0 average: 0

Max skewness = 1.451977157e-12

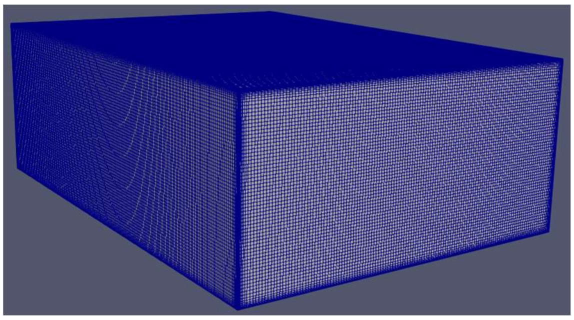


Figure 4: Meshed Geometry

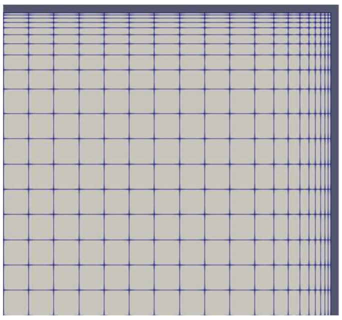


Figure 5: Refinement of 10X in 20cm from edges

The domain was divided into four blocks. A shell *30cm* thick from all 6 faces was formed, hereafter referred as the outer zone. The rest of the domain was further divided into three blocks which were sliced horizontally from the remaining block. These will be referred as the lower inner zone, middle inner zone and upper inner zone. These zones were *60cm* high, *25cm* high and *60cm* high respectively. The domain which is of interest to us the most is the inner middle zone. This zone is at least *30cm (~1 feet)* away from all the walls and ranges from *90cm* to *115cm* in height which is a good representation of the sitting height of a human being. The quality of air in this zone would affect any person sitting in the room the most. Similarly, the inner upper zone lies in the range of human standing height and is also of certain importance.

4.2 Initial and Boundary Conditions

Due to the turbulent nature of the flow, the $k-\varepsilon$ turbulent model was used to simulate the turbulent properties as well. The initial and boundary conditions have been summarised in the table below.

	U	p	k	ε	nut	S(ART)
AC	2m/s @ 60º with vertical	Fixed flux pressure	inlet		Calculated with uniform 6.83e-3	Fixed zero
Door	Pressure Inlet Outlet Velocity	Total pressure 101325Pa	inletOutlet		calculated	
Exhaust	2m/s outside	Fixed flux pressure	inlet		Calculated with uniform 3.43e-3	Zero gradient
Wall	No Slip		Default wall function			
Initial field	Uniform 0	Uniform 101325Pa	Uniform 3.37e-5	Uniform 1.17e-7	Uniform 8.74e-4	Uniform zero

Table 1: All boundary and initial conditions for the simulation

The following equations were used to calculate the initial and boundary values of turbulent kinetic energy, turbulent kinetic energy dissipation rate and turbulent viscosity. An online calculator was further used to verify all the above calculations.

$$k = \frac{3}{2}(U_{\infty}I)^2 \tag{7}$$

$$\varepsilon = \frac{C_{\mu}k^{1.5}}{0.07L} \tag{8}$$

Here U_{∞} is free stream velocity taken as $2m/s$ for both outlet and AC and I is turbulent intensity taken as 5%. L is the characteristic length. This is the longest length of the patch (inlet or outlet) in question.

4.3 Solver

For flow simulations, simpleFoam solver was used with $k-\varepsilon$ turbulent model. simpleFoam is a steady state solver which solves for flow simulation using the SIMPLE algorithm. Here SIMPLE stands for Semi-Implicit Method for Pressure Linked Equations. The time step was taken as 1s and the simulation ran for 15000s for simulation time. The schemes used for various operators are summarized in the table below.

Total time derivative	Steady state
Gradient	Gauss linear
Divergence	Gauss limited linear 1
Laplacian	Gauss linear corrected
Interpolation	Linear
Sn Gradient	Corrected
Wall distance	meshWave

Table 2: Set of schemes chosen for simpleFoam to solve for the velocity field

For ART simulation, a custom ART solver was configured by discretising equation (6) with finite volume methods. This solver was given the solved velocity and φ fields as inputs and it solved for the ART field. The following schemes were found to the most helpful for the ART solver.

Total time derivative	Steady state
Gradient	Gauss linear
Divergence	Gauss limited linear 1
Laplacian	Gauss linear corrected
Interpolation	Linear
Sn Gradient	Corrected

Table 3: Set of schemes chosen for the custom ARTFoam solver for the ART field

The schemes for the above solvers were found to provide the best set of residuals.

5. Results and Discussions on Flow and ART Simulation

Along with running OpenFOAM flow simulation using the simpleFoam solver, several functions were included. Firstly, the default yPlus function was included to ensure turbulent model is accurate. A default function called age was included as well as it could give possibly provide with ART values by running OpenFOAM's built in functions. This function provided an age field for the entire domain. Further functions were included to get maxima and volume average of this field across all four zones/domains (outer, inner bottom, inner middle, inner upper). As suspected, the values of the maximum age and maximum ART after running another ART simulation had an average error of ~0.02%. Hence, hereafter the simulation results of

ART solver and age function have been used interchangeably due to its negligible error. The Fig shows age and ART results for the front wall.

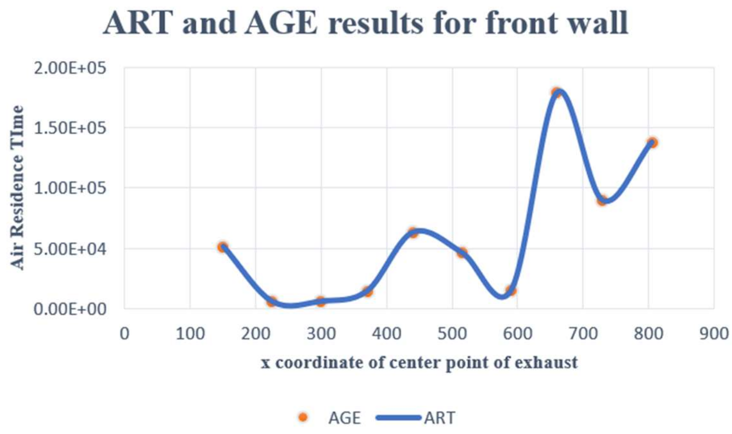


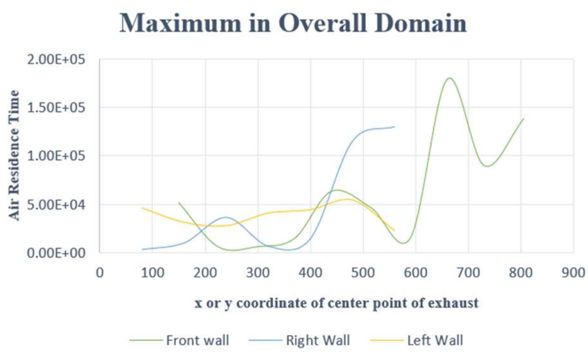
Figure 6: Results of AGE and ART solvers on front wall

A total of 24 cases were simulated each having various positions of the moving exhaust as shown in Fig 2. A summary of the maximum and volume averaged ART in each of the four regions were tabulated. A detailed look at the data can be found here. The plots for these parameters for each of the walls can be found in Fig 7.

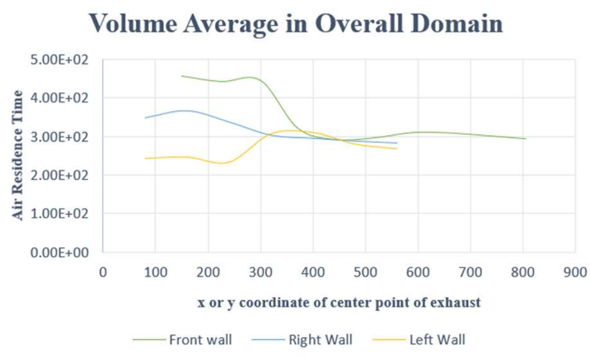
It was found that in a few cases, maximum ART occurred somewhere near the edges or corners of the room. These are usually very small areas restricted to a few centimetres. Since these areas are not of importance to human application, we will not be commenting on the applicability of results of the complete domain. Fig 7(a) and 7(b) confirm this hypothesis with no major trend seen and is characterized by several peaks and valleys.

After iterating through several cases, it was found that such isolated regions do no extend beyond *20-25cms* of distance from the wall and hence the domains had been created excluding *30cms* from each wall to create the inner zones. Of the inner zones we will only comment on the middle and upper zone which are of importance to us.

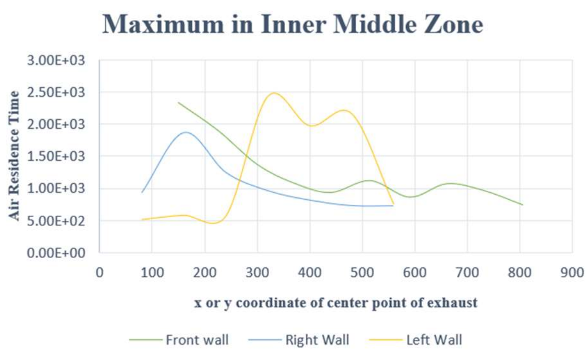
It is seen that the trends followed for maximum and volume averaged ART for each of the walls are similar in the inner middle and upper zones and hence, results for one extend for the other as well.



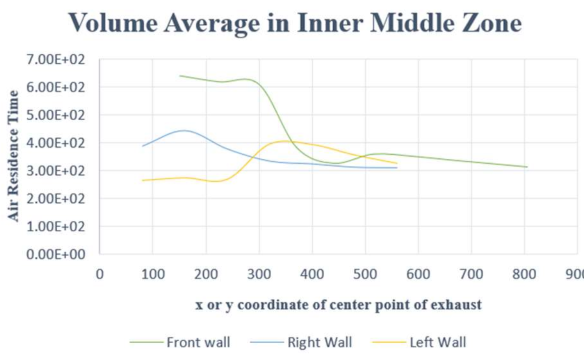
(a)



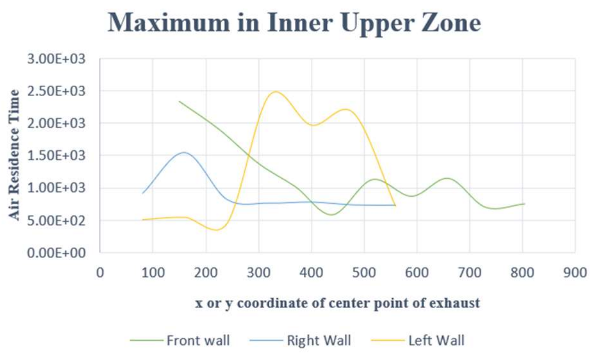
(b)



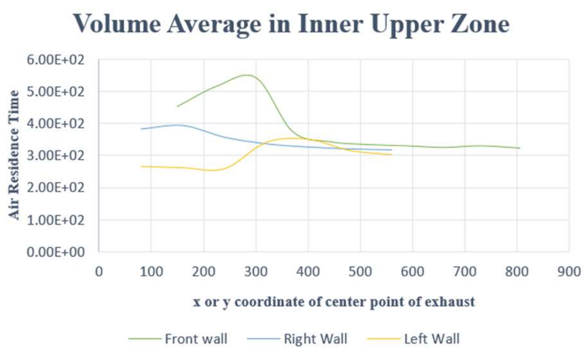
(c)



(d)



(e)



(f)

Figure 7: Plots of volume average or maximum ART from complete domain, inner middle zone and inner upper zone.

For the front wall, it is seen that there is almost a steady decrease in maximum ART as the exhaust is moved from the fixed exhaust to the default case, with the default case giving a minimum at 744s. The volume average ART from the front wall is almost same near the left and right edges showing that moving the exhaust from the left to the centre that diminished the effect of the maxima is actually a small isolated zone. This can be seen and verified in Fig 8.

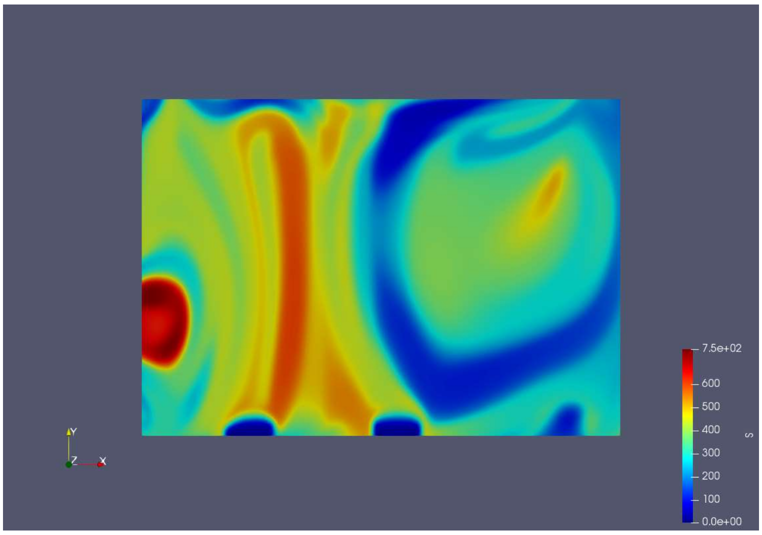


Figure 8: ART contour for default case sliced at z=1.7m

For the right wall, the maximum and volume average ART follow the same trend indicating that regions with high ART are more spread out that in the case of front wall. It is seen from ART contours that the region between the 2 ACs have seen an increase in ART when the exhaust moved to the right wall. This can be seen as an increase in redness from Fig 9. It is also seen that the recirculation zone near top right has also increased in area giving a more distributed ART.

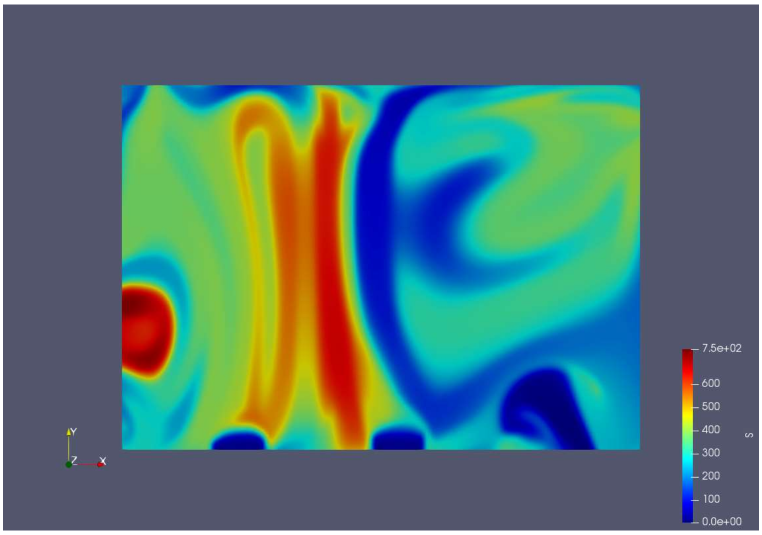


Figure 9: ART contour for case 10 sliced at z=1.7m

For the left wall, there is a maximum when the exhaust is around midway from either edge of the wall. Again, since maximum and volume averaged ART follow similar trends, the ART is seen to be more distributed. Another important observation was that while case 23 provided minimum of the maximum ART when the exhaust was on the left wall, case 20 provided minimum of the volume average ART for the same comparison set. At the same time, case 20 had almost 4 times the maximum ART as case 23. This means that case 20 is characterised with pools of very high and very low ART values.

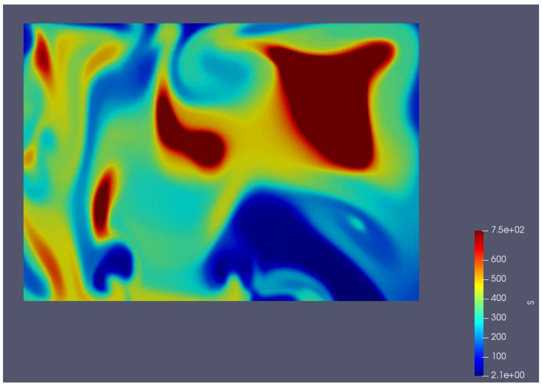


Figure 10: ART contour for case 20 sliced at z=1.7m

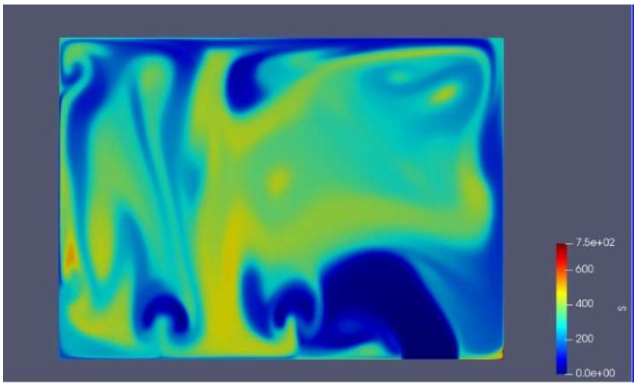


Figure 11: ART contour for case 23 sliced at z=1.7m

The overall best and worst performing cases have been summarized in the Table 4. From flow simulations and streamline tracking, it was seen that for most of the cases, the streamlines generally started from the ACs, moved down to hit the floor, rise up against the front wall, trace back from the ceiling, and keep circulating in a planar circulation zone normal to the x axis. This led to longer times for the streamlines to actually find an outlet to exit the domain. Hence, the exhausts present the front wall could not disrupt the flow to a lot of extent is the flow was largely tangential near such exhausts. This is also noticed by velocity contours near these exhausts. Where the exhausts were shifted to left or right wall, they were able to pull more streamlines out of the domain and cause a better impact to the ART values. Hence, the maximum and volume averaged ART is lower in the case of left and right wall compared to the front wall.

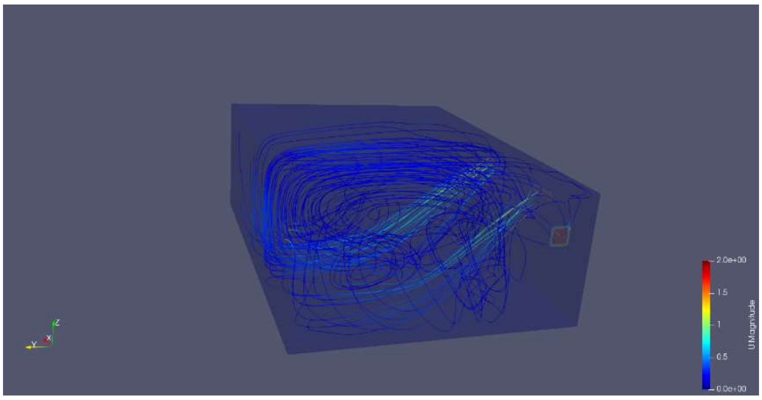


Figure 12: Velocity streamlines for case 23

Taking into account the best overall case giving the best-looking ART contour (uniformly distributed ART) with the minimum maximum ART, similar flow field patter was observed.

Case	Maximum ART (s)	Volume Averaged ART (s)
Default	744	313
10	731	308
23	510	264
20	2431	396
9	2334	640

Table 4: Results of ART for minimum and maximum parameters among all the cases for inner middle zone

5. Proposed Intervention

To further improve the air quality of the room by decreasing both the maximum and volume averaged ART, case 23, which was the best performing case earlier, was chose for performing further improvements. Since the flow field pattern was largely recirculation zones in planes normal to the x axis, to break the recirculation zone and redirect more the streamlines to the exhausts, it was considered to install a ceiling air conditioner in the centre of the room.

The AC was designed to have five parts, four on the periphery and one in the middle. The peripheral edges of the central AC pushed air at 2m/s @ 60º with vertical and the central part pushed air at 2m/s vertically inside. Characteristic length for turbulent kinetic energy dissipation rate was taken to be the diagonal of the AC.

The simulation ran for 23000s with a time step of 1s following the same schemes as the earlier simulations. The streamlines now flow towards all corners of the room and circle back with the central AC as seen in Fig 14. This allows for efficient mixing. The results of this simulation have been tabulated in Table 5.

Maximum ART	Volume Averaged ART
328	**117**

Table 5: ART results with central AC in inner middle zone

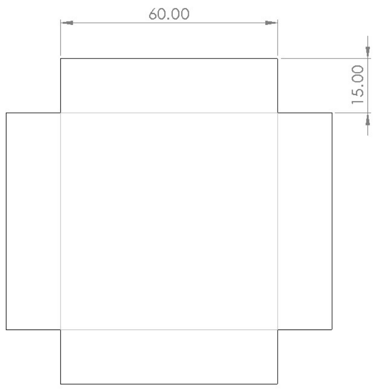


Figure 13: Top view of ceiling air conditioner. All dimensions in cm.

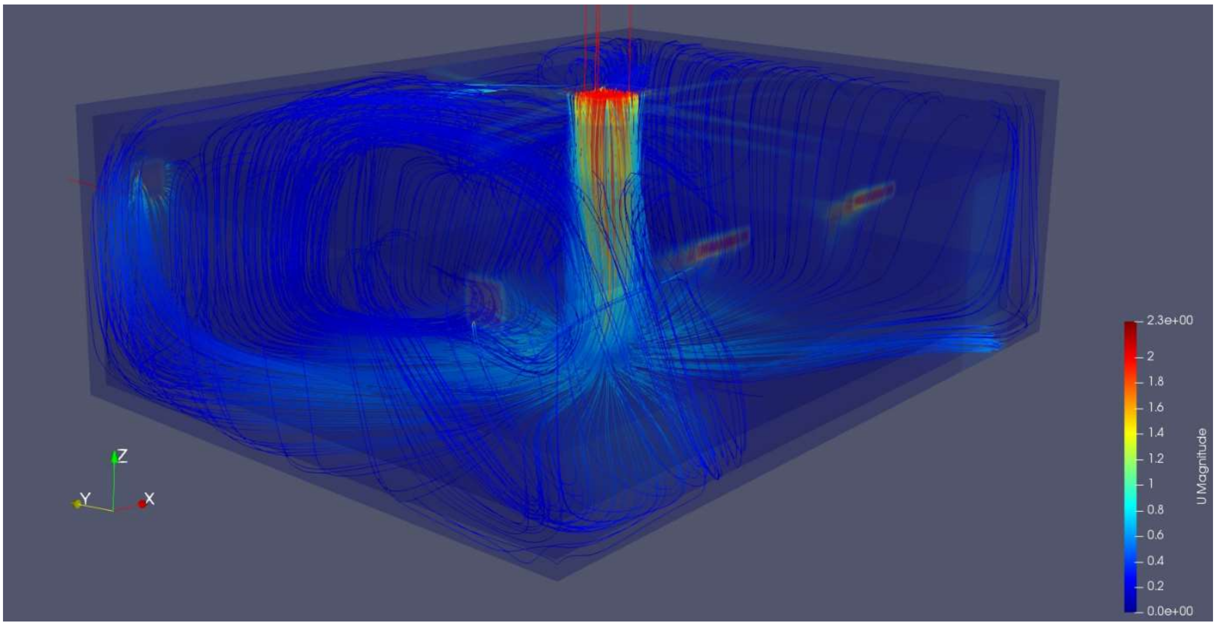


Figure 14: Velocity streamlines with central AC

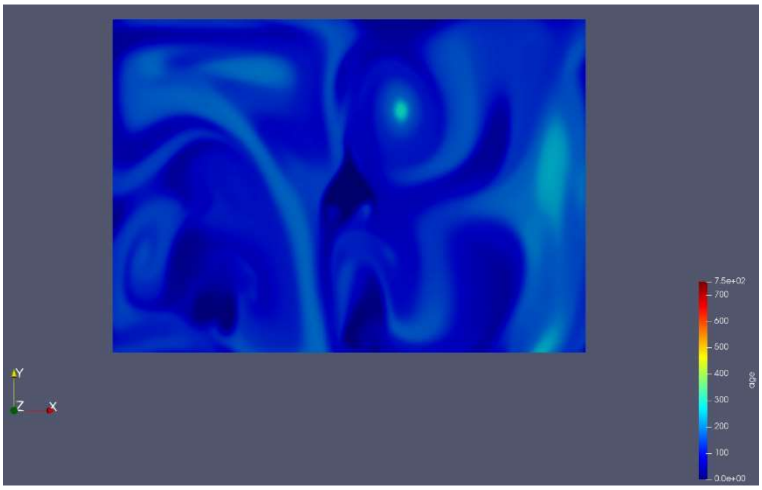


Figure 15: ART contour sliced at z=1.7m with central AC

This has shown a 35.7% decline in Maximum ART and 55.7% decline in volume average ART and shows better results than case 23.

6. Machine Learning Model

Subsequent to performing 24 CFD simulations, machine learning was utilized to identify trends for maximum and volume averaged ART for the various places of the variable exhaust fan. Specifically, a neural network model was used.

The air residence time in various zones was set as a target variable, and the initial input to the model was the x and y coordinates of the variable exhaust fan's centre. The ML model was run in all four zones for both the maximum and volume averaged ART in that zone. As a result, the model needed to be run eight times to obtain all the predictions' accuracies. Additional features generated from the polynomial features transformation from Scikit-learn (a Python library) improved performance of the model.

The linear regressor model from scikit-learn was used to train and test the data after the data had been appropriately scaled. One-fourth of the data was used for testing, while three-fourths was used for training. However, for almost all of the zones, large mean absolute percentage errors were approximately 60% and were caused by a lack of sufficient data.

Following this, the machine learning algorithm was run separately for each wall, taking only one input variable (x or y coordinate) and one target variable (air residence time) to address this issue. The data from each of the three walls where the exhaust fan was present was first isolated. The accuracy of simple linear regression was improved, and the mean absolute percentage errors decreased to around 20% in all eight columns (one column corresponds to either the maximum or volume averaged residence time for a specific zone), with the exception of a few columns, which can also be explained by a lack of data because no particular trend was observed.

Using a simple linear regression model for one variable per wall and one output variable, the ML algorithm performed better. This is because simple models give better results for lesser data compared to more complex models. If there had been sufficient training data, more complex models like artificial neural networks and convolutional neural networks could have been used to predict the air residence time.

7. Conclusions

The ventilation study in Chemical Engineering Classroom at IIT Bombay was carried out varying the location of one of the exhausts while keeping the other one fixed at a constant height. Air residence time was the parameter chose for measure of air quality and replenishment. A total of 24 cases were put through CFD simulation comprising exhausts of several walls. ART was found to be minimum when the exhaust was near the ACs on the adjacent wall. This was further improved by adding a central air conditioner to the room which modified the air flow and caused significant reduction in ART. An ML model was trained which could predict the ART values given the location of an exhaust. Two models were tried, one where both x and y coordinate of centre of moving exhaust was given as input variable and one where either x or y (whichever is changing) was given to 3 models, one for each wall. The latter showed a 3 times reduction in error, with the former giving about 60% error and the latter giving 20%.

For further study, it is recommended to increase number of simulations to train the ML model to expect better accuracies. Results of our analysis show that central AC contributes highly to improving air quality. The parameters of the room can be nondimensionalized to increase the impact of simulations and extending results to any room with ACs and exhausts.

References

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