FOSSEE, IIT Bombay
OpenFOAM Case Study Project
April 21, 2024

Analysis of ventilation strategies for improved air quality in a classroom with CFD-driven Machine Learning

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Abstract

Air residence time denotes the total time the air particles have spent inside a control volume. Analysis of a room's ventilation in terms of air residence times is vital to understanding critical zones and reducing the spread of infectious diseases that can spread via air. This case study performs flow and air residence time analysis for a classroom in the Department of Chemical Engineering, IIT Bombay, for various placements of exhaust fans. Based on the analysis, the optimal placement of exhaust fans and an additional intervention to improve the ventilation in the room are suggested. An ML model is also trained on the CFD data to predict air residence times without running the flow simulations, saving computational time and power.

1 Introduction

In modern times, humans are spending more time indoors than ever. Most of the office and educational activities are carried out in closed rooms for long periods of time. These places can become hotspots for spreading of airborne diseases. Therefore, it is essential to design buildings, meeting rooms and classrooms with proper ventilation. Ventilation designers need to optimize some design parameter to ensure air replenishment in such spaces at a pace fast enough to reduce chances of infection when different people cross the same area. One of the parameters used to track this is called the Air Residence Time (ART). [Sinha et al., 2021]

Commonly used ventilation systems in classrooms are air conditioners, exhaust fans, and table fans. The goal of this project is to analyse the changes in air flow and air residence time due to the varying location of exhaust fans in a classroom. To achieve this, the computational fluid dynamics (CFD) solvers in OpenFOAM v9 have been used. Running CFD simulations for all possible ventilation configurations of a large room is a very tedious and computationally heavy task. With the rise in machine learning algorithms, complicated systems can be modelled in a very simple manner for fast and accurate results. The application of 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 configurations, saving computational resources.

2 Problem Statement

A classroom in the Chemical Engineering Department, IIT Bombay, is used as a test case. The room is modelled as a cuboidal fluid domain containing air. 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 three walls. Air enters the room through the air conditioners, circulates inside the room, and leaves through the exhaust fans. The door is maintained at ambient conditions.

Fig 1 shows the different positions for which the simulation would be run, leading to a total of 24 simulations for the flow field and air residence time. At the end, based on the results, some interventions are introduced in order to minimize the air residence time in specified regions of interest.

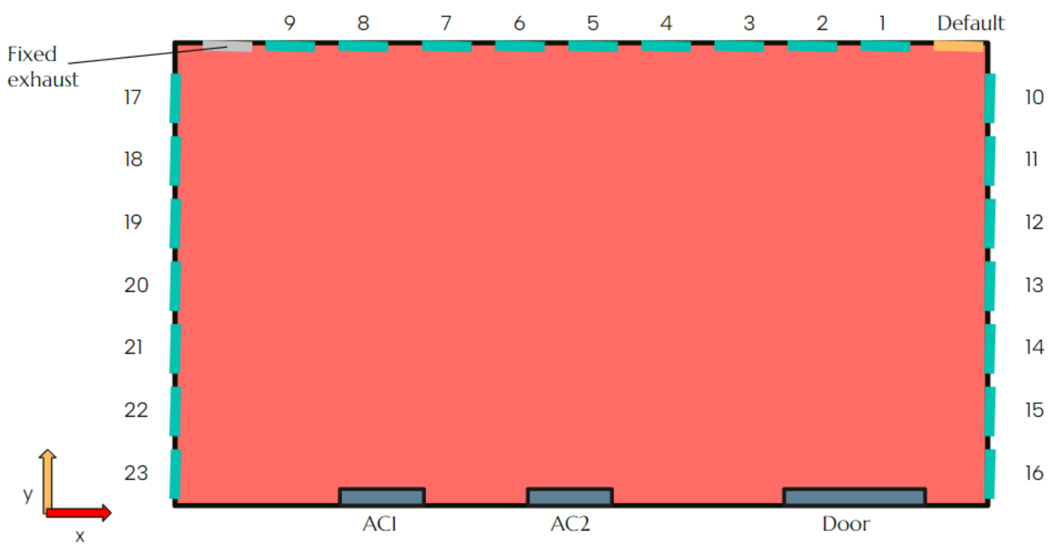

Figure 1: Positions of variable exhaust fan (1-23)

3 Governing Equations and Models

The incompressible Navier-Stokes equations are the governing equations for the flow of air inside the room. The continuity and momentum equations are of relevance to this case.

$$\nabla \cdot \vec{V} = 0 \tag{1}$$

$$\rho \frac{\partial \vec{V}}{\partial t} + \rho(\vec{V} \cdot \nabla)\vec{V} = -\nabla p + \mu \nabla^2 \vec{V} \tag{2}$$

To incorporate effects of turbulence, the Reynolds Averaged Navier Stokes equations were used, with the $k - \epsilon$ turbulence model for calculating turbulent viscosity.

$$\rho \frac{D}{Dt}(k) = \rho \nabla \cdot (D_k \nabla k) + P - \rho \epsilon \tag{3}$$

Here, k represents the turbulent kinetic energy (TKE), D_k is the effective diffusivity for k and P is the TKE production rate.

$$\rho \frac{D}{Dt}(\epsilon) = \rho \nabla \cdot (D_\epsilon \nabla \epsilon) + \frac{C_1 \epsilon}{k}\left(P + C_3 \frac{2}{3} k \nabla \cdot \vec{V}\right) - C_2 \rho \frac{\epsilon^2}{k} \tag{4}$$

In this equation, ϵ represents the turbulent kinetic energy dissipation rate, D_ϵ is the effective diffusivity for ϵ and C_1, C_2 and C_3 are the model constants.

$$\nu_t = C_\mu \frac{k^2}{\epsilon} \tag{5}$$

The turbulent viscosity is represented by ν_t, and C_μ is a model constant, generally having a value of 0.09.

To solve for the air residence time in the flow field, we first take the general passive scalar transport equation

$$\rho \frac{\partial \phi}{\partial t} + \rho \frac{\partial u_j \phi}{\partial x_j} = S \tag{6}$$

We then replace S with ρ, so that ϕ represents the air residence time, the quantity we want to solve for.

$$\frac{\partial \phi}{\partial t} + \frac{\partial u_j \phi}{\partial x_j} = 1 \tag{7}$$

4 Simulation Procedure

4.1 Geometry and Mesh

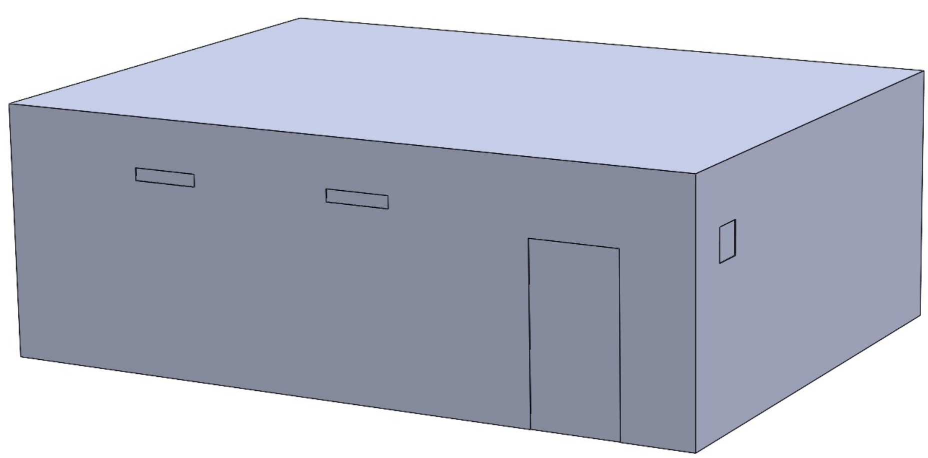

Figure 2: Chemical engineering classroom

The geometry as shown above has the following dimensions. All units are in centimeters. A single door is located near the room's corner and 2 ACs are fixed on the wall which has the door. One of the exhaust fans' position is fixed on the wall opposite to the door, and the other exhaust fan is moved along the three walls (other than the one containing the ACs) of the room.

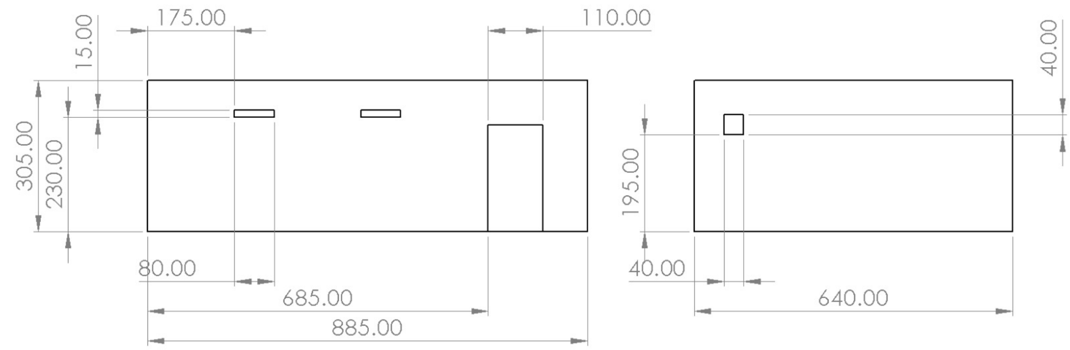

Figure 3: Dimensions of the classroom

The geometry and mesh were created using the blockMesh feature in OpenFOAM 9. The patches for air conditioners, door and exhaust fans were made using the topoSet and createPatch features, by specifying the coordinates and the area of each component. For all 3 directions, 20cm of domain from each wall was refined with a gradient of 10, as the mesh became finer near the external faces. This was done primarily for small y+ values. The rest of the domain had uniform hexahedral 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.

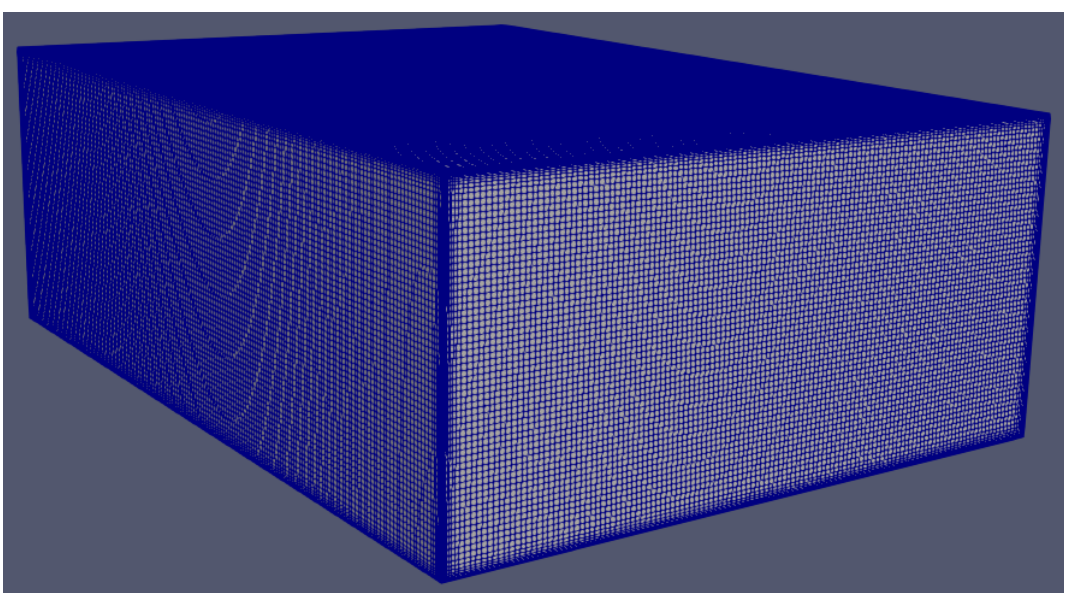

Figure 4: Mesh

Table 1: Overview of meshing parameters

Mesh Metric	Value
Max aspect ratio	10.21738153
Max skewness	1.451977157e-12
Max non-orthogonality	0

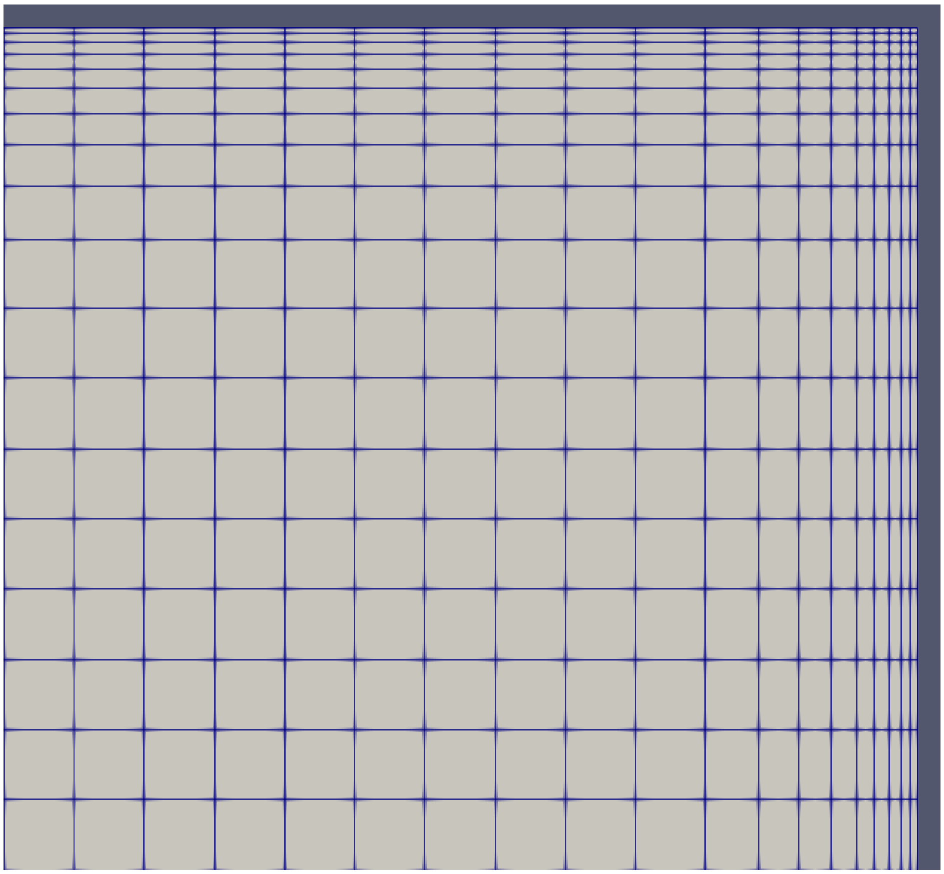

Figure 5: Grading in the mesh

The domain was divided into four blocks using topoSet. A shell 30cm thick from all 6 faces was formed, hereafter referred to 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 to 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 (approximately 1 foot) 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. The outer zone was isolated as it would generally have high air residence times and affect the volume averaged values of the other zones. The upper and lower zones would also have high air residence times in the presence of interventions like fans and desks, so further analysis into this classroom may require the air residence time values in those zones. Furthermore, data from these zones help in training the machine learning model, as shown later.

4.2 Initial and Boundary Conditions

The classroom is assumed to be having ambient air conditions, with the AC throwing in air and the exhaust fans acting as outlets. Air in deficit or excess is compensated by the presence of the door. All numerical value inputs were uniformly distributed over the inlet/outlet patches. The internal field of the domain was initialized with initial values of U, p, k and ϵ.

Table 2: All initial and boundary conditions of the simulation

	U	p	k	ϵ	ν_t	S (ART)
ACs	2m/s inlet @ 60º with vertical	Fixed flux pressure	Inlet value 0.015	Inlet value 2.95e-3	Calculated value 6.83e-3	Fixed value zero
Door	Pressure Inlet Outlet Velocity	Total pressure 101325 Pa	Inlet outlet	Inlet outlet	Calculated value	Fixed value zero
Exhaust fans	2m/s outlet	Fixed flux pressure	Inlet value 0.015	Inlet value 5.91e-3	Calculated value 3.43e-3	Zero gradient
Walls	No slip	Fixed flux pressure	Wall function	Wall function	Wall function	Zero gradient
Internal field	Uniform 0	Uniform 101325 Pa	Uniform 3.37e-5	Uniform 1.17e-5	Uniform 8.74e-4	Uniform 0

The values used in boundary and initial conditions of Turbulent kinetic energy (k), Turbulent dissipation rate (ϵ), and Turbulent viscosity (ν_t) were obtained through calculations shown below. Calculations were verified using online calculator [Fluid-Mechanics-101, 2021]

$$k = \frac{3}{2}(u_\infty I)^2 \tag{8}$$

where u_∞ is the free stream velocity, taken to be exhaust outlet velocity (2 m/s) and AC air velocity (2 m/s) for exhaust and AC, respectively. I is the turbulence intensity, taken to be 5% (standard value).

$$\epsilon = \frac{c_\mu k^{1.5}}{0.07L} \tag{9}$$

where c_μ is a k-ϵ model parameter, typically given as 0.09, k is the turbulent kinetic energy calculated above, and L is the characteristic length. L is taken as the larger length of the corresponding entity, for example, height for the door.

$$\nu_t = \frac{c_\mu k^2}{\epsilon} \tag{10}$$

where ϵ is as calculated from equation (9).

4.3 Solver

The simpleFoam solver was initially used to obtain the steady state flow field in the room. The fluid flow equations are solved using the existing SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm, with the temporal term set with a steady state condition. The $k - \epsilon$ turbulence model was used for modelling turbulence in the flow. The simulation ran for a total of 15,000 time steps till suitable convergence of the residuals was reached.

The inbuilt OpenFOAM solver was modified to develop a custom solver (artFoam) for air residence time. The equation 7 was discretized using finite volume method functions and used as the governing equation. The in-house artFoam solver was then used, with the velocity field solution as the input, to calculate the air residence time values throughout the domain.

The age function, an inbuilt OpenFOAM function, was used to calculate the ART immediately after each simulation to verify the values of the artFoam solver. Based on the results, the limitedLinear scheme was used as the divergence scheme for the artFoam solver, particularly to eliminate the presence of negative values of ART in some parts of the domain.

5 Results and Discussions

5.1 Flow and ART results

The 24 simulations as mentioned were run, and flow fields and air residence times were obtained. The extensive tabulated results for all zones (outer, inner upper, inner middle and inner bottom) can be found in the following linked spreadsheet: Tabulated Results
The y+ values obtained for case 23 are shown below:

	Min y+	Max y+	Average y+
Ceiling	0.00127	6.19	2.17
Floor	0.00036	12.22	3.14
Side Walls	0.00036	41.54	2.11

Table 3: y+ values for Case 23

The crucial areas prone to spread of infection are near human sitting and standing heights. In this regard, our 'inner middle' zone is of most interest, since it covers the region from 0.9m to 2.15m from the floor. The 'inner' zones exclude a 0.3m (1 Feet) distance from all walls (and floor), which generally have a high ART value but are not of much significance being outside regions of human occupancy.
Two quantities are used for analysis: maximum ART and volume average ART. The plots for ART vs coordinate of exhaust fan on each of the 3 walls is shown below.

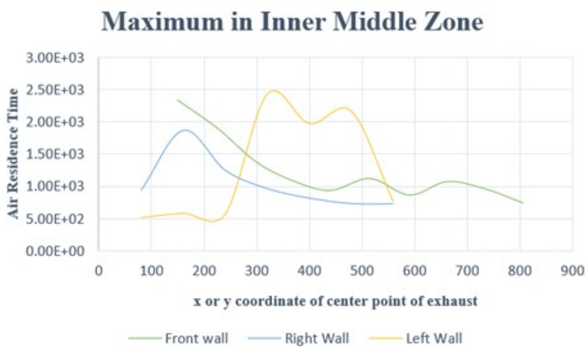

Figure 6: Max ART variation for the three walls

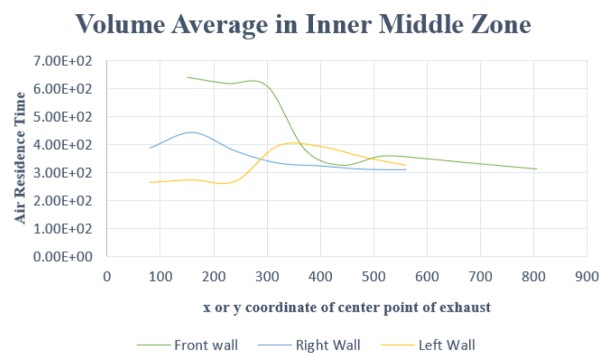

Figure 7: Volume average ART variation for the three walls

Based on these two quantities, the best cases for each wall are: Default case, case 10 and case 23. Results for these cases are summarized in the table below. Case 20 and Case 9 turned out to be the worst case scenarios, and their results are tabulated as well, showing the impact and relevance of exhaust fan placement on the ART. The flow streamlines for the best case (case 23) and worst case (case 9) and the ART contours at 1.7m height (around human standing height) follow. The scale in all the contours is 0 (Blue) to 750s (Red).

Case	Max ART	Volume average ART
Default case	744s	313s
Case 10	731s	308s
Case 23	510s	264s
Case 20	2431s	396s
Case 9	2334s	640s

Table 4: Comparison of ART for inner middle zone for various zones of interest

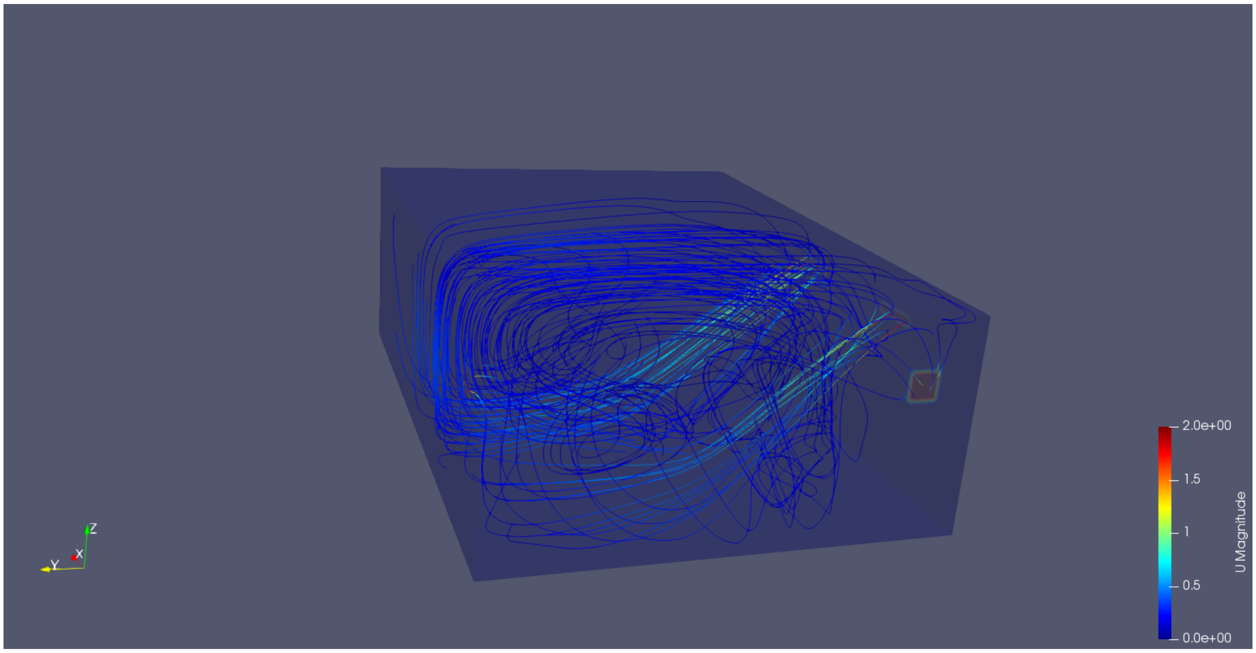

Figure 8: Velocity streamlines for case 23

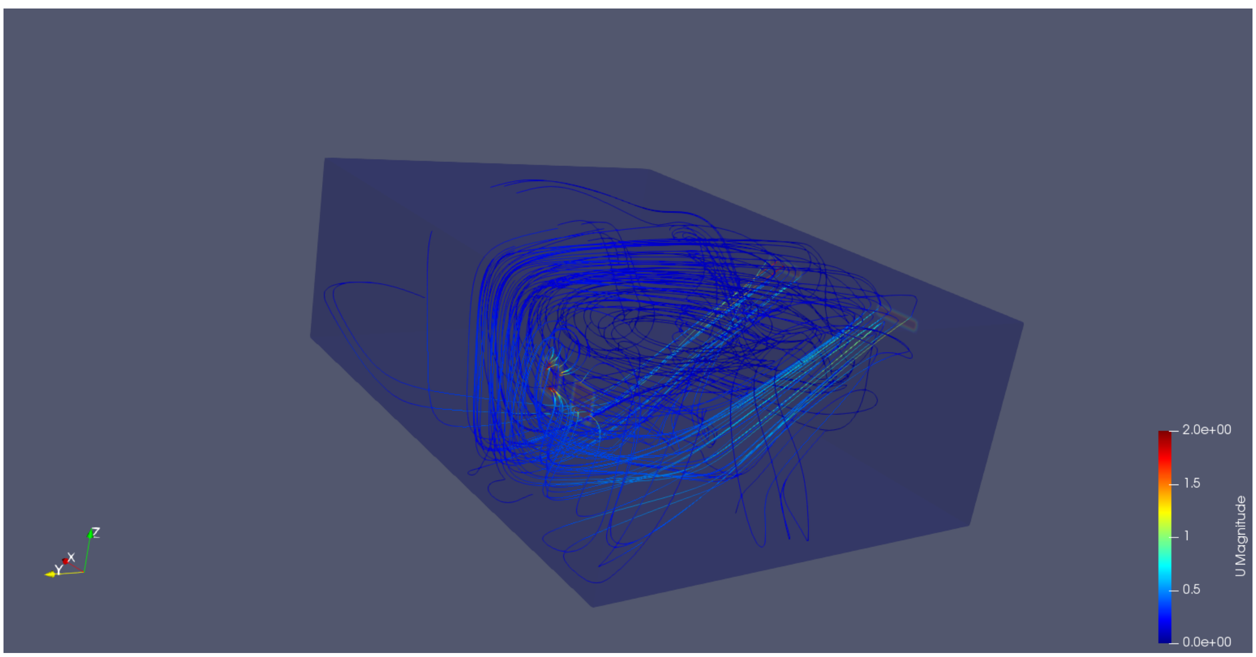

Figure 9: Velocity streamlines for case 9

As seen in the contours, there is a recirculation zone (red) on the left hand side of the room. In case 23, moving the exhaust fan near that recirculation zone helps break down the zone and reduces the ART. In case 20, which has the highest maximum ART, we see that even though the exhaust

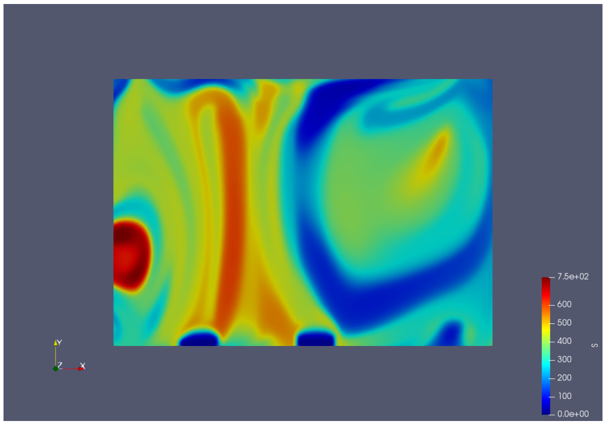

Figure 10: ART contour for Default case

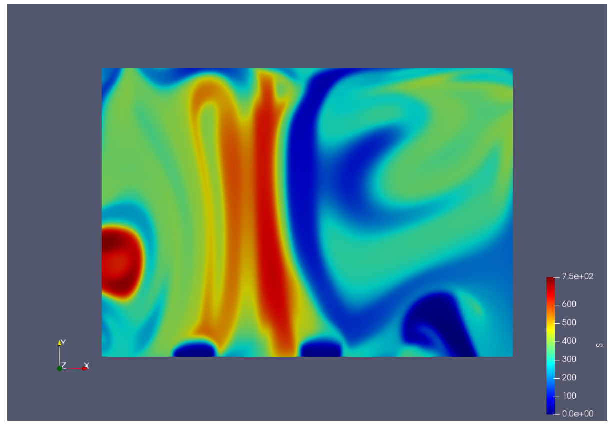

Figure 11: ART contour for Case 10

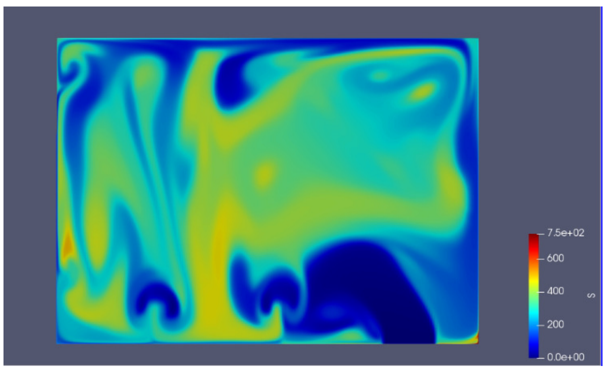

Figure 12: ART contour for Case 23

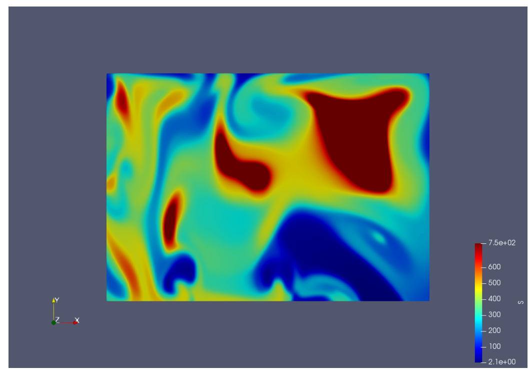

Figure 13: ART contour for Case 20

fan is placed on same wall as that in case 20, which has lowest max ART, the placement of exhaust fan affects the ventilation. In case 23, the exhaust fan 'pulls' the stream from AC towards itself, causing dead zones (very low flow) in the opposite corner of the room. In case 20, the exhaust fan manages to dissipate the recirculation in that corner of the room without affecting the AC flow much.

5.2 ML model

After performing over 24 CFD simulations, machine learning algorithms were used to track patterns in the maximum and volume averaged air residence time values of the room for the different positions of the variable exhaust fan.

Initially, the x and y coordinate of the center of the variable exhaust fan was used as input to the model, and the air residence time in various zones were set as target variables. The machine learning algorithm was run in four zones, i.e. the outer zone, inner upper zone, inner middle zone and the inner bottom zone for both the maximum value of air residence time and the volume averaged value of the air residence time in that zone. Thus, the model had to be run eight times to find out the prediction accuracies. Additional features were generated using polynomial features transformation from the Python library scikit-learn, to improve performance of the training algorithm. The data was then scaled appropriately and the linear regressor model from scikit-learn was used to train and test the data. Around 75% of the data was used for training and the remaining 25% for testing. However, the lack of sufficient amount of data caused large mean absolute percentage errors of around 60% during testing for almost all the zones.

To tackle this issue, data of each of the three walls where the exhaust fan was present was first isolated, after which 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). Simple linear regression was effective, as this improved the accuracy, and the mean absolute percentage errors in all the eight columns (one column corresponds to either maximum or volume averaged residence time for a particular zone) decreased to around 20%, except for some columns, but this also can be explained by lack of data as no particular trend could be seen.

In conclusion, the machine learning algorithm performed well when a simple linear regressor model was used on a single variable and single output case. This is because simple models often require fewer data to train and identify trends, even if they are not the most accurate. More complex models like artificial neural networks and convolutional neural networks could have been used to predict the air residence time if there was sufficient data for training. The model can be reverse trained too, such that an input ART gives x and y coordinates of the exhaust fan. This can be useful when trying to find fan positions for a room.

6 Ventilation Improvement

In order to improve the ventilation in the room, the best case among the 24 cases was picked up (case 23) and interventions were tested out to improve the ART in the room. A ceiling AC was placed at the center of the ceiling with velocity boundary condition as 5m/s. Turbulence parameters were calculated for the ceiling AC and input as inlet conditions. Rest boundary conditions were kept the same. A significant improvement in ART was observed because of the ceiling AC. The jet of stream from the ceiling AC hits the floor and gets diffused throughout the room, breaking up recirculation zones and improving the ventilation.

Case	Max ART	Volume average ART
Case 23	510s	264s
Case 23 with ceiling AC	238s	87s

Table 5: Improvement in ART for inner middle zone using ceiling AC

Note that the scale in Figures 15 and 16 is 0 (blue) to 500 (red), as compared to 0 to 750 in the Figures 10 to 13 in previous section.

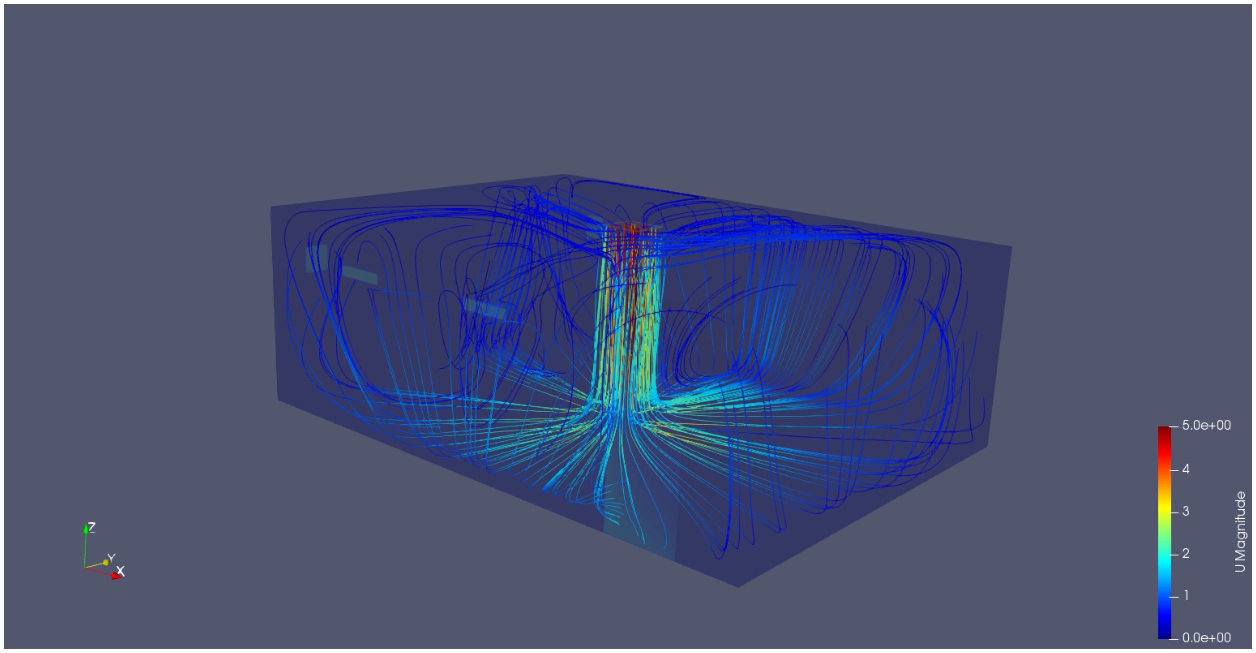

Figure 14: Velocity streamlines from the ceiling AC

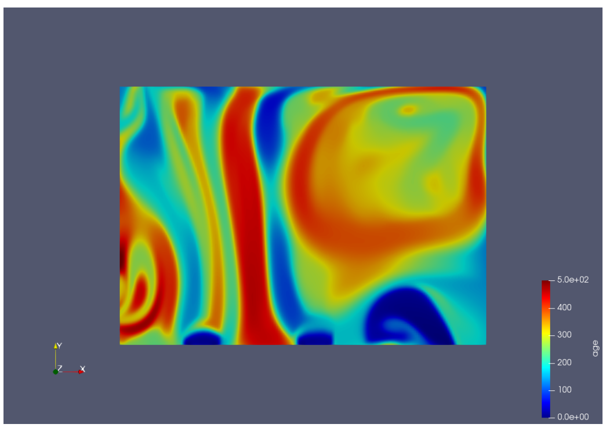

Figure 15: ART contour for Case 23

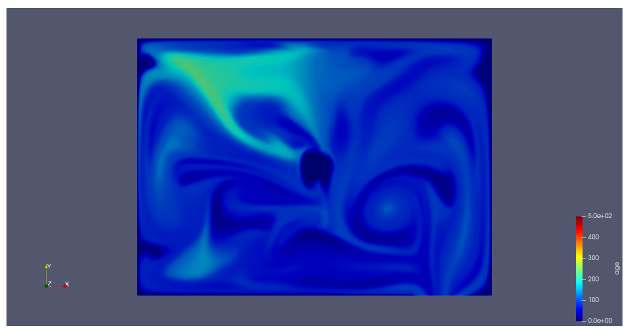

Figure 16: ART contour for Case 23 with ceiling AC

7 Conclusions

The flow and ventilation analysis of a classroom in Chemical Engineering Department at IIT Bombay was carried out. The air residence time for various placement of exhaust fans was obtained via OpenFOAM simulations, and the optimum position of the exhaust fan was determined. An ML model was trained on the data set to be able to directly predict the air residence time for the input of exhaust fan position to eliminate the high computational time and power required for the flow simulation. A ceiling AC was proposed as an intervention in the room to reduce the ART further, and flow simulation results show that the ceiling AC is very effective in achieving this.

References

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Sinha, K., Yadav, M. S., Verma, U., Murallidharan, J. S., & Kumar, V. (2021). Effect of recirculation zones on the ventilation of a public washroom. *Physics of Fluids*, *33*(11), 117101. https://doi.org/10.1063/5.0064337