Investigation of aerosol dispersion and air purifier performance in a hospital patient room using CFD and measurements

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Abstract. Transmission of airborne disease is a concern in many indoor spaces. Recent studies have identified correlations between poor indoor air quality (IAQ) and COVID-19 vulnerability and mortality. Studying the role building design and ventilation play in both the spread and mitigation of airborne viruses in high-density spaces is thus imperative. However, guidance for IAQ improvement and COVID-19 risk mitigation is general and insufficient for specific application in at-risk spaces like British Columbia’s (BC) patient settings and long-term care homes. What remains underdefined is a workflow for translating site specific data on indoor aerosol spread into actionable tools health officials can use towards building retrofit and intervention planning. The objective of this project was thus to develop a library of ‘digital twin’ models of at-risk indoor spaces that can provide accurate and rapid investigations of indoor air quality improvement measures using computation fluid dynamics (CFD) software. To calibrate these models, 41 repeated controlled experiments of aerosol dispersion and removal were conducted to assess the ventilation patterns of a 4-bed hospital room. From these experiments, a 3D CFD model of the room was created using the RhinoCFD modelling package, calibrated with measured IAQ sensor data, and validated against the results of the live study. This paper presents the methodology and in-progress results of this CFD modelling process.

1 Introduction

Debate surrounding the primary mode of transmission of the SARS-CoV-2 virus loomed large at the start of the COVID-19 pandemic [1]. Transmission through contact with an infected person or surfaces carrying virus-laden droplets prompted early recommendations for frequent hand-washing and social distancing [2]. However, increasing evidence has identified airborne transmission as the primary pathway for the spread of COVID-19 [2-5]. Inhaling aerosols shed by an infected person while talking, sneezing, or coughing has been largely considered the dominant pathway of transmission [6, 7]. The ability for micron-scale aerosols to remain suspended in the air for extended periods of time and travel distances of 10 m within enclosed indoor spaces brings established literature on indoor air quality (IAQ) and healthy ventilation systems to the forefront of the COVID-19 response [1, 6, 8].

The relationship between IAQ conditions in enclosed spaces and the susceptibility of building occupants to sickness and disease transmission is supported by a long history of evidence [9-13]. For decades, indoor CO2 concentration has been accepted as a proxy for indoor fresh air rate and found to negatively impact cognition at high indoor concentrations [14, 15]. Recent studies have begun to identify correlations between poor IAQ and COVID-19 vulnerability and mortality as well [16-19]. Studying this relationship in Northern Italy, Coker et al. found that a 1 μg/m3 increase in PM2.5 concentration was positively associated with a 9% increase in COVID-19 related mortality [16]. Cole et al., found a similar correlation in 255 municipalities in the Netherlands, where a 1 μg/m3 increase in PM2.5 concentration was associated with 9.4 times more COVID-19 cases, 3.0 times more hospital admissions, and 2.3 times more deaths [17].

In March 2020, the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) created the ASHRAE Epidemic Task Force to provide guidance on how to improve IAQ towards mitigating COVID-19 transmission risks. Providing adequate ventilation and air cleaning were amongst key recommendations to control aerosol and droplet spread indoors [20]. However, guidance provided by ASHRAE and related bodies has remained general and insufficient for specific application in at-risk spaces like British Columbia’s (BC) patient care settings. High-density, high-traffic spaces like hospitals and long-term care homes carry the highest risk aerosol transmission and cross-contamination. But public health officials in BC have not received clear indication on what IAQ measures should be provided in these settings or how they should be implemented.

Additionally, recent analysis of aerosol transmission studies by Jones et al. [21] notes that research of indoor airflow patterns and viral transmission are limited. Research focused predominantly on average indoor ventilation rate and failed to capture the complexity of
localized air flows and its affect on aerosol trajectory. Without a clear understanding of the localized airflow patterns ventilation systems create and the effects they have on the behaviour of aerosols, effective mitigation measures become difficult to implement and evaluate.

Computational fluid dynamic (CFD) simulation presents a proven and effective tool to understand aerosol transport within ambient flows. Creating virtual replicas or ‘digital twins’, of real physical spaces and conducting CFD simulations within these environments has become increasingly common, especially during the pandemic. The ability for virtual models to parametrically study the effect different boundary conditions, occupancy schedules, and system configurations have on aerosol transmission makes this tool a powerful one. Throughout the pandemic, CFD has been used to simulate the human sneeze, mask mechanics, and aerosol movement within aircrafts, vehicles, washrooms, and public spaces. In studies by, Abuhegazy et al. [22], Burgmann & Janoske [23], and He et al. [24], CFD software was used to model aerosol transmission in classrooms and the efficacy of different purifiers and their arrangement in the room.

Cheong & Phua [25], Qian & Li [26], and Cho [27] similarly used CFD to study the effect different exhaust locations and furniture arrangements had on airflow and pollutant distribution patterns in negative pressure patient isolation rooms. Each study validated their simulated results against in-field measurements and similarly found that ventilation strategies and furniture layouts had great influence on the airflow within the room. However, the literature base regarding CFD-based digital twins of multibed hospital wards remains scarce. Amongst few examples exists the work of Li et al. [28] who conducted a physical experiment to study bioaerosol cross infection in a two-bed hospital ward and compared their findings to a developed CFD model. They found that bioaerosol removal efficiency and breathing zone concentrations were lower using unilateral downward ventilation compared to bilateral downward ventilation.

Furthermore, what remains undefined in BC is a workflow for translating site specific data on indoor aerosol spread into actionable tools health officials can use towards building retrofit and intervention planning. To fill this gap, the objective of this study is to develop a library of ‘digital twin’ models that can accurately describe aerosol transmission in different patient care settings and provide rapid investigations of different IAQ improvement measures and their efficacy. To validate the accuracy of the models, repeated controlled experiments of aerosol spread was undertaken in a multi-bed hospital room. Various configurations of air purifiers and patient curtains was tested. The following presents the set up of the experimental phase of the project and the in-progress results of the CFD modelling process.

2 Methods

The experimental conditions and test sequence in the hospital room are described in Section 2.1, followed by a description of how the CFD model was generated and the process of calibrating the boundary conditions of the simulation in Section 2.2.

2.1 Experimental Setup

To assess the ventilation patterns in a 4-bed hospital room, sodium chloride aerosols were injected into the space using a nebulizer and tested under different configurations of air purifiers and curtains around the beds.

Fig. 1. Isometric representation of test room. The supply (inlet) grill is mounted on alcove drop ceiling edge, directing air to the SW wall. The return (outlet) grill is mounted above the entry door on the underside of the dropped ceiling.

To simulate realistic conditions, all experiments took place in a 4-bed patient room in Delta Hospital, British Columbia (Fig. 1). The room has an area of 37 m² (398 sf) and a 4.5 m² (48 sf) entry alcove. Within the dropped alcove ceiling is the room air supply pointed at the SW exterior wall and a return air grill directly above the entry door on the alcove’s underside. The room’s existing ventilation scheme creates a tumbling pattern of air that moves along the centerline of the room’s ceiling towards the SW window and returning at floor level to the entry door. Measurements prior to the experiment suggest flow rates of 3.5 ACH with 206 cfm (350 m³/h).

As active COVID-19 protocols were in effect at the hospital during the test period, the researchers conducting the study were required to stay within the empty room during all tests. Fully masked, the researchers either remained along the SE or NW walls. Each bed was surrounded by a sliding curtain that had gaps of approximately 50 cm at the top and bottom. In the "Long" curtain experiments, curtains were retrofitted with additions that extended to the floor.
Fig. 2. Plan of test room. Four cylindrical upflow air purifiers were placed in the corners of the room and horizontal towers on the floor placed between the beds. Particle sensors (RAMPS) were positioned at the head of the bed where a patient's head would lie. The Nebulizer is on the East bed.

Several different purifiers were used in the study. Four Blue Air 411 purifiers were positioned in each corner of the room near the head of the bed and 1.2 m off the floor. The purifiers use radial inflow through a cylindrical filter and exhaust vertically out the top of the unit. The nominal efficiency of these filters is 99% for PM_{2.5}. Each Blue Air purifier is rated for 5 ACH in a 15 sqm (161 sf) room, equivalent to 103 cfm (175 m³/h).

Two additional purifiers were located in between the beds along the NW and SE walls (Fig. 2). For the NW wall, the Honeywell HFD 310C (Air Genius 4) was used. This purifier uses a HEPA filter and produces 161 cfm (274 m³/h) within a 250 sqft room, equivalent to 2.7 ACH. Along the SE wall, the Honeywell HFD 122q was used, which has a nominal efficiency of 99% at 0.3 μm. The unit produces 109 cfm (185 m³/h) rated for 170 sf (16 m²). Both purifiers were positioned on the floor and exhaust horizontally either to its adjacent wall or towards the center of the room.

A full description of experiments conducted and results are provided in Rogak et al. [32].

2.2 CFD Simulation

CFD simulations were carried out in RhinoCFD FLAIR (version 2.1.5, powered by PHOENICS, CHAM), a plug-in to Rhinoceros3D an established CAD environment. This software was chosen for its ability to facilitate rapid design explorations and run CFD simulations natively within the same CAD environment. RhinoCFD has been used previously in the study of building surface wind pressure [33], natural ventilation of atrium spaces [34], and the efficacy of Ultraviolet Germicidal Irradiation devices for controlling SARS-CoV-2 virus spread in a hospital patient room [35].

2.2.1 Geometry & Mesh Generation

Geometry

A 3D model of the test room was created in Rhino3D (Fig. 1). However, due to lack of access to the test room and floorplans for privacy reasons during this phase of the study, the models were reconstructed from images and sketches of the room. Thus, the exact dimensions of the room and positioning of the purifiers in the corners were approximated. The oversimplification of interior geometry and the HVAC system are a limitation of the study. Further calibration of the models is currently underway.

The complex geometry of the beds and purifiers were simplified to minimize the computational resources and time needed to run each simulation (Table 1). For the same reason, the two researchers in the room were omitted from the simulation model.

<table>
<thead>
<tr>
<th>Geometry Name</th>
<th>X length (m)</th>
<th>Y length (m)</th>
<th>Z length (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Room</td>
<td>6.50</td>
<td>5.70</td>
<td>2.90</td>
</tr>
<tr>
<td>Alcove</td>
<td>3.50</td>
<td>1.30</td>
<td>2.40</td>
</tr>
<tr>
<td>Bed (4)</td>
<td>2.30</td>
<td>1.00</td>
<td>0.85</td>
</tr>
<tr>
<td>Table (4)</td>
<td>0.69</td>
<td>0.32</td>
<td>0.50</td>
</tr>
<tr>
<td>HVAC Return</td>
<td>0.42</td>
<td>0.42</td>
<td>0.19</td>
</tr>
<tr>
<td>HVAC Supply</td>
<td>0.39</td>
<td>0.39</td>
<td>0.19</td>
</tr>
<tr>
<td>Blue Air 411</td>
<td>0.20</td>
<td>0.20</td>
<td>0.44</td>
</tr>
<tr>
<td>HW HFD 310C</td>
<td>0.25</td>
<td>0.25</td>
<td>0.66</td>
</tr>
<tr>
<td>HW HFD 122q</td>
<td>0.25</td>
<td>0.25</td>
<td>0.66</td>
</tr>
</tbody>
</table>

For each simulation, a mesh was automatically generated using the cut-cell meshing tool PARSOL native to RhinoCFD. The PARSOL method distinguishes solid from fluids in each cell and automatically applies the correct boundary conditions. The cells in the mesh were rectilinear and totals ranged from 808,962 to 1,266,265 (Table 2). The minimum grid size ranged from 0.029670 m to 0.031737 m.

| Exp # Name     | Cell Count | Min. grid size (m) | Cells in | | | |
|----------------|------------|--------------------|----------| | | |
| 1 Baseline     | 1,266,265  | 0.031737           | 121 115 91 |
| 29 Four Corners| 808,962    | 0.02967            | 102 103 77 |

Fig. 3. Experiment 1 Baseline - RhinoCFD automatically generated mesh in XY-plane
2.2.2 Boundary Conditions

All walls in the live experiment were well-insulated and thus modelled as adiabatic and non-slip in the CFD simulations. The window in the SW exterior wall was modelled with a surface temperature of 16°C. The curtains and hospital beds were similarly modelled as adiabatic and with non-slip boundary conditions. The volumetric flow rate of the supply diffuser was modelled as 0.0972 m$^3$/s.

To simulate the saline solution aerosolized by the nebulizer in the experiment, an aerosol model was created in Rhinoceros with a diameter of 3 μm and a density of 2160 kg/m$^3$. The concentration of the aerosol was set at 100% at the nebulizer’s mouth in the 3D model. A mass flow rate of 3.283E-8 kg/s was applied to this geometry, calculated from measurements taken with the Sonair MedPro Ultrasonic nebulizer used on test day. Aerosols were subject to gravity and allowed to settle on surfaces.

The flow inside the room is assumed to be incompressible and turbulent. Pressure, momentum, and temperature variables are solved through the Navier-Stokes equations. To describe turbulence, the Realisable k-ε model proposed by Shih et al. (1995), was adopted for this study [36]. This model is a variant of the standard k-ε model that has shown improved performance with flows involving strong adverse pressure gradients.

The Blue Air 411 purifiers were modelled with a radial inflow rate of 0.0495 m$^3$/s and a filtration rate of 99%. The settings were calibrated by test day measurements.

Five probes were used as sampling points in the models to replicate the Remote Affordable Multi-Pollutant (RAMP) sensors used during the experiment. However, the exact location of these probes had to be approximated in the simulation model as well. This is another limitation of this study that we are continuing to calibrate and improve.

Table 3 summarizes all inputs and settings of the CFD model.

### Table 3. Summary table of CFD inputs and settings

<table>
<thead>
<tr>
<th>CFD model selection</th>
<th>Numerical Scheme</th>
<th>Navier-Stokes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Turbulence model</td>
<td>Realisable KE</td>
</tr>
<tr>
<td></td>
<td>Buoyancy model</td>
<td>Boussinesq</td>
</tr>
<tr>
<td>Aerosol characteristics</td>
<td>Diameter (m)</td>
<td>3.00E-06</td>
</tr>
<tr>
<td></td>
<td>Density (kg/m$^3$)</td>
<td>2160</td>
</tr>
<tr>
<td></td>
<td>Deposition model</td>
<td>Gravity</td>
</tr>
<tr>
<td></td>
<td>Boundary Conditions</td>
<td></td>
</tr>
<tr>
<td>Air inlets (m$^3$/s)</td>
<td>0.0972</td>
<td></td>
</tr>
<tr>
<td>BlueAir Purifier Outlet (m$^3$/s)</td>
<td>0.0495</td>
<td></td>
</tr>
<tr>
<td>Nebulizer (m/s)</td>
<td>8.57</td>
<td></td>
</tr>
<tr>
<td>Window (°C)</td>
<td>16</td>
<td></td>
</tr>
<tr>
<td>Walls/Ceiling</td>
<td>Adiabatic, non-slip</td>
<td></td>
</tr>
<tr>
<td>Initial Conditions</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2.2.3 Test Cases

Two experiments of the 41 were simulated as part of this study (Table 4). Experiment 1 was the Baseline with all purifiers turned off and the curtains removed from the simulation. In this experiment, the nebulizer was allowed to run for 10 mins before being shut off. After this point, the decay rate of the aerosols was observed for 15 minutes. Experiment 29 also has the curtains removed, but all four corner purifiers were turned on during the simulation and the nebulizer ran for 25 minutes to simulate steady state conditions. The decay rate was again observed for 15 minutes after the nebulizer was shut off.

### Table 4. Simulation Cases

<table>
<thead>
<tr>
<th>Exp. #</th>
<th>Description</th>
<th>Purifier State</th>
<th>Curtain Config.</th>
<th>Aerosol Generation</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Baseline</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>10 mins</td>
</tr>
<tr>
<td>29</td>
<td>NC 4 corners</td>
<td>4 corners</td>
<td>No</td>
<td>No</td>
<td>25 mins</td>
</tr>
</tbody>
</table>

Both experiments were simulated under transient conditions. A transient model was necessary to accurately account for temporary and complex airflows. Attempts were made to first simulate each experiment under steady state conditions. However, the complexity of the flow regime when the nebulizer or purifiers were first initialized necessitated a transient solution simulating each experiment with small enough time steps to achieve convergence. The total number of time steps varied between cases due to changes in length of simulated time, but the time step frequency averaged around 0.2 seconds. To initialize both simulations, the HVAC system and purifiers were turned on and simulated for 10 mins to establish the pre-existing air currents within the space before the aerosols were injected into the room. These conditions would then act as the initial values of a transient flow field simulating the aerosol dispersion and decay or purifier stages of the experiments.

The solution was assumed to be converged when all the scaled residuals stabilized and approached a minimum of 1.00E-2 for k, c, x, y, and z momentum equations.

3 Results and Discussion

3.1.1 Comparison of predicted results against experimental results: Experiment 1

Figure 4 shows the results recorded of the baseline experiment. The East sensor, nearest the nebulizer, reports the highest aerosol concentration of all sensors in the room. Despite being located behind the nebulizer, the circulation in the room transports the aerosols
backwards towards the sensor with a 2-minute delay. The four other sensors away from the nebulizer observe much lower aerosol concentrations, as well as a 2–4-minute response delay indicating the time it took for the aerosols to travel across the room. After the first 10-minutes when the nebulizer shuts off, the aerosol decay rate was observed. Aerosol concentrations at the five sensors all similarly reported a slight decay rate over this 15-minute period.

Figure 5 shows the results of the baseline simulation, which are in reasonable correlation with the measured results. The simulation similarly predicts the highest aerosol concentration to be measured by the East sensor for at least the first 10 mins of the experiment, indicating that the predominant air current in the test room directing the aerosols behind the nebulizer and back towards the East sensor was likely captured within the CFD simulation. The four other sensors similarly showed lower concentrations than the east bed and the same 2–4-minute delay accounting for the time for the aerosols to be transported across the room. Additionally, the simulated model also predicted that aerosol concentrations at each sensor would decay at a slight rate after the nebulizer shuts off at the 10-minute mark.

Figure 6 shows the aerosol distribution at the level of the probes taken at the 9-minute mark of the simulation. From this plan view, the aerosols had difficulty moving across the room to the North corner. This is likely due to the supply air directed along the centerline of the room towards the SW wall from the alcove diffuser that directed the aerosols away. This is similarly observed in the experimental data with the North sensor reporting the lowest aerosol concentrations throughout the experiment. Past the center sensor, aerosols were evenly distributed to the south and west beds. This observation likely describes the circulating air flow pattern in the south and west directions created by the supply air hitting the SW wall. The time for the aerosols to travel this distance of the room thus describes the observed delays.

The magnitude of the predicted concentration differs slightly from the measured values however, indicating that further refinement of the model’s boundary conditions and investigation of other possible factors affecting aerosol distribution not accounted for in the model is needed.

3.1.2 Validation of predicted results against experimental results: Experiment 2

Figure 7 shows the results of Experiment 29 (four purifiers and no curtains). Similar to the recorded results in Experiment 1, the East sensor recorded the highest aerosol concentration of the five in the room, while displaying a 1-minute delayed response. The results at this sensor did report greater fluctuation than in Experiment 1. The nebulizer was allowed to run for 25 minutes before being shut off. The four corner purifiers active throughout the experiment consequently dropped the aerosol concentration at each sensor at a similar rate after the nebulizer was shut off.

Figure 8 shows the simulated results for Experiment 29. The results however are significantly different and not as expected. The aerosol concentrations at each sensor are not reflective of the experimental results with the results from the East sensor being the most egregious. The simulation reports concentrations that are orders of magnitude lower than the aerosol concentrations observed in the test room.
Diagnosing these abnormal results, several factors that stem from limitations of the study come into play. Firstly, without the ability to revisit the test room for this study, measure its dimensions, measure the size of the diffuser grille, and to know the exact position the purifiers were placed in the room during the experiments, these key inputs were all estimated. These factors all likely play a large role in determining the actual airflow within the space and any inaccuracy in their specification results in a mischaracterization of the room’s flow patterns. Looking at Figure 8, there seems to be insufficient mixing of air within the space, resulting in lowered simulated aerosol concentration at all sensors. An approximation of the HVAC system and the purifiers likely play a hand in this characteristic. The sensitivity of results to grid mesh size was also not studied. Additionally, the removal of the researchers in the test room from the model and the thermal plumes they create could have eliminated another possible influence on the overall airflow in the room.

Another potential source for error is the possible inaccurate placement of the virtual sensors in the model. As mentioned previously, the sensor locations were approximated and not confirmed by test day measurements. Slight shifts in the sensors location could drastically change the reported aerosol concentrations.

Fig. 7. Experimental Results of Experiment 29 (four corner purifiers and no curtains). Dashed lines indicate the fitted curves used to estimate steady-state concentrations. Aerosol injection started at t=0.

Fig. 8. Simulated Results of Experiment 29 (four corner purifiers and no curtains). Aerosol injection started at t=0.

Further calibration of the simulation models is currently underway, however the work it took to achieve these results calls into questions whether very applied CFD software like RhinoCFD can be easily configured to realistically emulate real spaces without significant fine tuning and calibration. Although the model of Experiment 1 was able to come to some closeness to the test results, the flow regime of that simulation without any purifiers turned on was less complex. Both the computational time and effort to fine-tune different inputs through trial-and-error increased significantly as the purifiers were introduced and the complexity of the problem grew. To counterbalance this increased demand on computational resources with Experiment 29, we chose to simplify the model geometry. As demonstrated by our results in Section 3.1.2, over simplifying HVAC and indoor flow problems must be approached with caution. Finding the right balance between inputting enough information to accurately describe the flow patterns within a space and minimizing the immense computation cost CFD models demand is necessary to achieve CFD models fit for design exploration and evaluation.

In all, this study finds that general CFD modelling of indoor spaces remains – as always – highly sensitive to several parameters that are not immediately identifiable: geometry, mesh size, and physics. Near out-of-the-box simulation with a tool like RhinoCFD, while presenting a user interface that may be easy to use for building engineers and architects, must be used with care. The present work will continue to evolve in order to evaluate the simulations undertaken, determine sources of error, and calibrate existing models.

4 Conclusion

In this paper, the transmission of aerosols under different conditions in a multi-bed hospital room was studied numerically through CFD simulation and validated against experimental data. The experiments were performed in an unoccupied 4-bed hospital room using saline aerosols produced by an ultrasonic nebulizer, concentrations of which were measured in several positions in the room using IAQ sensors. The aerosol concentration decay rates were determined with different configurations of air purifiers in the room.

Two numerical models were produced using the RhinoCFD package seeking to replicate the in-field results of Experiment 1 (baseline; no purifiers, no curtains) and Experiment 29 (four corner purifiers, no curtains). The first numerical model was able to reproduce the baseline results with reasonable similarity, while the model of Experiment 29 (four corner purifiers, no curtains) produced unexpected results. Due to several limitations to modelling the physical test room with a high level of accuracy at this point in the study, the model and the simulation inputs can still be improved, which is currently underway.

Understanding the specific role building design and ventilation systems play in both the containment and spread of the SARS-CoV-2 virus is crucial to implementing effective mitigation strategies. However,
the flow patterns within indoor spaces are often highly complex and thus challenging to completely account for. A multitude of factors can drastically affect the distribution of aerosols, including uncertain boundary conditions and unknown sources of thermal flows. In simulating these complex conditions within CFD software, a balance must be struck with simplifying the problem enough to reduce immense computational cost, while still prescribing enough information to accurately capture the characteristics of the dominant flow pattern in the room. Validating computational models against experimental data thus becomes vital to this process and the workflow for translating site specific data into actionable tools for intervention planning and building retrofit.

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