The impact of natural ventilation on airborne biocontaminants: a study on COVID-19 dispersion in an open office

Günsu Merin Abbas
Department of Architecture, Middle East Technical University (METU), Ankara, Turkey and
Department of Architecture, TOBB University of Economics and Technology, Ankara, Turkey, and
Ipek Gursel Dino
Department of Architecture, Middle East Technical University (METU), Ankara, Turkey

Abstract
Purpose – Biocontaminants represent higher risks to occupants’ health in shared spaces. Natural ventilation is an effective strategy against indoor air biocontamination. However, the relationship between natural ventilation and indoor air contamination requires an in-depth investigation of the behavior of airborne infectious diseases, particularly concerning the contaminant’s viral and aerodynamic characteristics. This research investigates the effectiveness of natural ventilation in preventing infection risks for coronavirus disease (COVID-19) through indoor air contamination of a free-running, naturally-ventilated room (where no space conditioning is used) that contains a person having COVID-19 through building-related parameters.

Design/methodology/approach – This research adopts a case study strategy involving a simulation-based approach. A simulation pipeline is implemented through a number of design scenarios for an open office. The simulation pipeline performs integrated contamination analysis, coupling a parametric 3D design environment, computational fluid dynamics (CFD) and energy simulations. The results of the implemented pipeline for COVID-19 are evaluated for building and environment-related parameters. Study metrics are identified as indoor air contamination levels, discharge period and the time of infection.

Findings – According to the simulation results, higher indoor air temperatures help to reduce the infection risk. Free-running spring and fall seasons can pose higher infection risk as compared to summer. Higher opening-to-wall ratios have higher potential to reduce infection risk. Adjacent window configuration has an advantage over opposite window configuration. As a design strategy, increasing opening-to-wall ratio has a higher impact on reducing the infection risk as compared to changing the opening configuration from opposite to adjacent. However, each building setup is a unique case that requires a systematic investigation to reliably understand the complex airflow and contaminant dispersion behavior. Metrics, strategies and actions to minimize indoor contamination risks should be addressed in future building standards. The simulation pipeline developed in this study has the potential to support decision-making during the adaptation of existing buildings to pandemic conditions and the design of new buildings.

Originality/value – The addressed need of investigation is especially crucial for the COVID-19 that is contagious and hazardous in shared indoors due to its aerodynamic behavior, faster transmission rates and high viral replicability. This research contributes to the current literature by presenting the simulation-based results for COVID-19 as investigated through building-related and environment-related parameters against contaminant concentration levels, the discharge period and the time of infection. Accordingly, this research presents results to provide a basis for a broader understanding of the correlation between the built environment and the aerodynamic behavior of COVID-19.

Keywords Indoor air contamination, Natural ventilation, COVID-19, CFD simulation, Infectious airborne virus, Integrated contaminant simulation

Paper type Research paper

1. Introduction
Indoor air quality (IAQ), natural ventilation and occupants’ health in shared indoor spaces have received increasing attention since the beginning of the 2000s with infectious airborne
virus risks such as SARS, MERS and recently with coronavirus disease (COVID-19, SARS-CoV-2). These pandemic outbreaks highlighted the vulnerability of indoor spaces with inadequate ventilation and high occupancy rates to higher risks of contamination. As a result, building occupants run the risk of experiencing health problems such as allergy, asthma, lung inflammation, airborne diseases and breathing problems, lung cancer from radon exposure and carbon monoxide (CO) poisoning (ASHRAE, 2009). Centers for Disease Control and Prevention (CDC) confirmed that airborne transmission is the primary means of COVID-19 spread as a result of coughing, sneezing, singing, talking or even breathing (CDC, 2020b). Infectious diseases spread either by contact transmission or airborne transmission via virus-laden droplets and aerosols (Pica and Bouvier, 2012). The key determinant of aerosol behavior is the particle size. Unless proper ventilation is provided, particles smaller than 5 μm can remain airborne for indefinite periods (Fennelly, 2020). When inhaled, particles such as COVID-19 (average particle size = 0.1 μm) deposit in the lower respiratory tract and pose serious risks for occupant health.

Natural ventilation is identified in the literature as the most effective means of reducing indoor airborne contaminant exposure (Atkinson et al., 2009; Qian et al., 2010; Zhou et al., 2018). However, the studies focusing on natural ventilation effectiveness on airborne contamination dilution is rather limited for shared indoor spaces, which is discussed in the following section in detail.

1.1 Existing research

Previous studies mainly focused on the aerodynamic behavior of airborne biocontaminants through the relation between contaminant dispersion/transmission and ventilation/airflow patterns. Li et al. (2007) investigated the relationship between infection transmission and ventilation rates and underlined the strong correlation between contaminant dispersion and ventilation. Ben-David and Waring (2016) compared the performance of natural ventilation with mechanical ventilation in the dilution of indoor contaminants and its influence on energy consumption. Aliabadi et al. (2011) studied ventilation in healthcare buildings within the scope of infectious airborne transmission. Previous research also specifically focused on airborne infection transmission in healthcare buildings. Qian et al. (2010) studied cross-infection risks of airborne diseases via natural ventilation for a hospital and found that natural ventilation has a higher capacity in reducing transmission risks as compared to mechanical and hybrid ventilation. Zhou et al. (2014) studied the effectiveness in contaminant dilution for natural ventilation in hospital buildings and concluded that larger windows offer better ventilation and lower contamination.

Despite previous studies focusing on healthcare buildings, research on contaminant dispersion in public indoor spaces is rather limited. Public indoor spaces require in-depth investigation since they are relatively more vulnerable to infection risks than healthcare buildings due to their lower ventilation rates (Morawska et al., 2020). In healthcare buildings, since the focus is on the patients’ well-being, the monitoring of ventilation effectiveness and IAQ is a widespread practice (Morawska and Cao, 2020). Additionally, in such buildings, ventilation effectiveness and IAQ are regulated by infection control procedures and guidelines defined by organizations such as the World Health Organization (WHO) (Atkinson et al., 2009). Also, with the widespread use of mechanical ventilation and dense occupancy patterns in public indoors, particularly in offices, airborne contamination becomes a vital problem. In high-rise office buildings, sealed façades and mechanical ventilation are usually preferred over user-operated natural ventilation due to concerns of safety, operational difficulties of hybrid ventilation (in mixed-mode buildings) and possible conflicts regarding different comfort expectations of occupants (Wood and Salib, 2013). However, research shows that mechanical ventilation can accelerate contaminant dispersion by recirculating the
indoor air and possibly increasing air humidity through the stagnant water in mechanical devices (Fink and Gilman, 2000).

Recently, the COVID-19 outbreak placed a greater need to study contaminant-related risks in indoor spaces. Faster human-to-human transmission makes COVID-19 a more hazardous disease than SARS and MERS (Fani et al., 2020; Petrosillo et al., 2020). COVID-19 is particularly contagious in indoors due to its distinct aerodynamic behavior, faster transmission rates and resilient viral replicability. Moreover, COVID-19 can be transmitted by both aerosol and droplets (Bourouiba, 2020). Aerosol particles travel relatively far and can remain contagious for up to 16 h (Fears et al., 2020). COVID-19 virus particles also show retention of replication competence, which makes virus particles to be capable of infecting and reproducing new virus particles (Fears et al., 2020). Also, such particles are in respirable sizes (Fears et al., 2020), which also increases infectability. Infected individuals are capable of generating contaminated bioaerosols that could remain airborne for more extended periods, which increases viral shedding and airborne virus transmission.

While investigating the effectiveness of natural ventilation in preventing infection risks in indoor spaces, the most critical parameters of contaminant dispersion are those related to the building (i.e. window configuration and opening ratio) and the environment (i.e. indoor air temperature and wind) (CDC, 2015; Fung and Lee, 2015). The relationship between natural ventilation and the building and environment-related parameters are particularly important since they determine the indoor airflow patterns and natural ventilation effectiveness (Yang and Clements-Croome, 2012). CDC presents a pyramid of the “hierarchy of control” to control viral spread, where a number of protective and preventive parameters and strategies are indicated. From the most effective to the least effective, those are (1) elimination, which is the physical removal of the hazard, (2) substitution, which is the reduction of the hazard by the replacement, (3) engineering controls, which is the isolation of the people from the hazard, (4) administrative control, which is to change the occupancy and working patterns, and (5) using personal protective equipment to control potential exposure (CDC, 2015). Among the abovementioned protective and preventive strategies, the built environment, where the most viral transmission occurs, has a considerable impact on the removal of the hazard (Morawska et al., 2020; Nishiura et al., 2020). However, the impact of the built environment and natural ventilation on the spread of COVID-19 is rather limited in the literature. Bhagat et al. (2020) explored the impact of mixing ventilation, natural and mechanical displacement ventilation, and wind-driven ventilation on the distribution, transportation and fate of airborne contaminants. They concluded that displacement ventilation could reduce the exposure risk due to the stratification based on the indoor temperature differences (Bhagat et al., 2020). Lipinski et al. (2020) reviewed the common ventilation strategies for reducing infection transmission and confirm that the central ventilation and recirculation systems contribute to the rapid spread of airborne infections and recommended natural ventilation to provide safer indoors. Ren et al. (2021) compared three airflow behaviors based on the various configurations of the inlets and outlets ((1) inlet–outlet on the same wall, (2) inlet–outlet on the opposite walls, (3) one inlet on the ceiling and two outlets on the sidewalls) for a hospital ward and their impact on COVID-19 dispersion. Although their research focuses on a mechanically ventilated space, the inlets–outlets’ various positions contribute to the understanding of the relationship between ventilation and built environment. Among the three inlet–outlet configurations, Ren et al. (2021) concluded that the inlet–outlet on the same wall located on the upper and the lower diagonal corners of the wall is the best performing option for contaminant removal. Abuhegazy et al. (2020) investigated aerosol transport and surface deposition in a classroom and explored the impact of the particle size, aerosol source location, glass barriers and opening the windows while the air conditioning runs. Although they study a mechanically ventilated room, their recommendations and experimental setup could provide insights into the contaminant discharge by natural ventilation. They have
confirmed that the air-conditioning system increased the contaminant concentration, opening windows while the air conditioning runs contribute to the particle removal, and the transmission behavior changes notably with respect to the contaminant’s location (Abuhegazy et al., 2020). Melikov (2020) underscored the importance of ventilation on airborne virus transmission and recommended an urgent paradigm shift in ventilation strategies.

A large number of COVID-19 research focuses on the prevention strategies to reduce COVID-19 transmission. Awada et al. (2021) addressed indoor environmental quality concerning the occupants’ health and presents strategies, challenges and research opportunities for enhancing the built environment for healthy indoors. They recommended further research to focus on building and occupant-related parameters addressing heating, ventilation and air-conditioning (HVAC) design and operations, humidity, spatial configuration and human-building interactions (Awada et al., 2021).

Coccia (2020) investigated preventive infection risk measures on an urban scale to reduce the built environments’ vulnerability to the COVID-19 and future epidemics and pandemics. Megahed and Ghoneim (2020) highlighted the importance of the built environment in COVID-19 transmission and reviewed the potential strategies such as improving ventilation, filtration and UV-based systems to reduce indoor transmission risk. Similarly, Aghalari et al. (2021) reviewed the COVID-19 transmission and discussed preventive measures such as physical distancing, personal hygiene, ventilation and air filtration for healthcare buildings. Melikov et al. (2020) presented intermittent occupancy and ventilation as a combined strategy to reduce viral exposure for a typical classroom and recommended continuous clean-air supply and short breaks of the occupancy every hour. Similarly, Zhang et al. (2021) proposed an occupancy-aided ventilation strategy to reduce infection risk and increase work productivity for a classroom and recommended shorter and reduced occupancy.

The other foremost focus in the literature is the relationship between mechanical ventilation and COVID-19 dispersion. Borro et al. (2020) discussed the impact of air-conditioning on COVID-19 transmission and proposed computational fluid dynamics (CFD)-based simulations to optimize air-conditioning. Guo et al. (2021) reviewed the HVAC operation guidelines of different countries during COVID-19 and compared outdoor air, operation of HVAC systems, temperature and humidity setpoints, pressure differentials, filters for HVAC, air cleaning and heat recovery equipment as the COVID-19 countermeasures. Pease et al. (2021) investigated potential aerosol transmission via central ventilation systems by two scenarios with indoor and outdoor contaminant sources in order to evaluate filtration, air change and outdoor air fraction.

Existing research mainly focuses on the transmission prevention strategies and the relationship between mechanical ventilation and COVID-19 airborne dispersion. There is a gap in the literature on the impact of natural ventilation and built environment on COVID-19 airborne transmission. Accordingly, this research addresses this gap by focusing on the relationship between natural ventilation and various parameters of the building and environment and their impact on indoor COVID-19 dispersion and infection risk to guide the designers, occupants and building operators.

Currently, various methods are used to calculate and assess airborne infection risks. A standard infection risk assessment method is Wells–Riley’s method that assumes a constant, equally distributed and steady contaminant concentration (Pease et al., 2021; Sun and Zhai, 2020). Also, Monte Carlo simulations are broadly exploited in COVID-19 research to estimate overall infection risk (Buonanno et al., 2020a; Maltezos and Georgakopoulou, 2020; Riediker and Monn, 2021; Xie, 2020). However, the complex airflow patterns in naturally ventilated buildings call for detailed methods to calculate the uneven contaminant dispersion. CFD-based methods can perform such detailed airflow behavior and contaminant dispersion analysis.
1.2 Research motivation

This research investigates indoor air contamination of a free-running (no space conditioning is used), naturally-ventilated room with a COVID-19 infected occupant. The room contamination is evaluated using building-related parameters and an environment-related parameter. A simulation pipeline, which performs integrated contamination analysis, coupling a parametric 3D design environment, CFD and energy simulations, is implemented through a number of design scenarios, where indoor air contamination is evaluated for different contaminant concentration levels, discharge periods and the time of infection.

CFD, energy and multi-zone IAQ and contaminant transport simulations are performed for an open-office space, and four simulation setups were analyzed with evaluation metrics. This research contributes to the current literature by presenting simulation-based results, where the presented scenarios aim to provide a basis for a broader understanding of the correlation between the building and environment-related parameters and the aerodynamic behavior of COVID-19 in naturally-ventilated indoor spaces.

2. Methodology and experimental setup

This research adopts a simulation-based approach and implements an integrated pipeline. Computer-based simulations enhancing the designer’s capabilities facilitate the detailed investigation of the potential indoor transmission risks (Megahed and Ghoneim, 2020). The integration of various modeling and simulation tools has brought accuracy, well-informed and data-driven design decisions to the design process. Accordingly, this research develops and implements a pipeline that integrates CFD, energy and contaminant transportation simulation that aims to increase the accuracy of the simulation results. Particularly, CFD-based analyses need to be augmented with other tools since the accuracy of CFD-based methods relies on the correct definition of microclimatic conditions of the indoor spaces and the outdoor environmental conditions.

CFD analyzes fluid-flow behavior (Kundu et al., 2004) and is applied in various fields, from aeronautics engineering to architecture. In the built environment, CFD is commonly used for simulating potential wind loads of the buildings, assessing urban wind flow, pedestrian wind comfort and indoor/outdoor ventilation performance and façade systems (Blocken, 2015; Prohasky et al., 2016; Ramponi and Blocken, 2012; Van Moeseke et al., 2005). In COVID-19 research, CFD simulations are commonly used for the exploration of COVID-19 transmission and transport dynamics (i.e. humidity, airflow, temperature, particle size and spreading distance) (Abuhegazy et al., 2020; Bourouiba, 2020; Liu et al., 2021; Vuorinen et al., 2020) and the relationship between the COVID-19 transmission and HVAC (Bhattacharyya et al., 2020; Borro et al., 2020; Ren et al., 2021). However, in the current literature, no research has been conducted that addresses the indoor contaminant concentration levels at the different areas of the naturally-ventilated room, where both the indoor and outdoor environmental conditions are crucial parameters. It is critical to explore the relatively vulnerable areas to the infection risk due to complex airflow patterns and contaminant dispersion behavior.

In this research, CFD is used for simulating detailed airflow behavior, which provides indoor air pressure and velocity data for both indoors and the building surfaces for selected given building geometry and environmental conditions. The building geometry data are provided to the CFD engine by a parametric 3D modeling platform. The environmental data are provided by the weather files and the energy simulations since the outdoor and indoor temperatures and wind significantly impact the airflow and the contaminant dispersion behavior, as the latest literature addressed (Carleton and Meng, 2020; Islam et al., 2020; Qi et al., 2020; Rosario et al., 2020; Sanchez-Lorenzo et al., 2020; Wang et al., 2020). Additionally, the contaminant’s characteristics (i.e. molecular weight, particle diameter and effective density) are other significant determinants in airborne transmission, which are required by
contaminant transportation simulations. Leung et al. (2020) address the different transmission rates of COVID-19, influenza and rhinovirus. As a result, we particularly develop and use a pipeline that integrates CFD, energy and contaminant models and simulations to increase the accuracy and the validity of the simulation results. The analyses are context (i.e. wind speed, wind direction and temperature) and contaminant-dependent (i.e. influenza, SARS and MERS). Accordingly, the proposed pipeline can be generalized to calculate the dispersion behavior and the infection risks of other airborne viruses and contexts.

2.1 The implemented pipeline
The pipeline involves a number of tools for modeling and simulation-based analyses. CFD simulations are performed using OpenFOAM, which is a piece of open-source CFD software (The OpenFOAM Foundation, 2011). Energy modeling and simulations are performed in EnergyPlus (U.S. Department of Energy’s Building Technologies Office, 2001a). Contamination analyses are performed using NIST CONTAM, multi-zone IAQ and ventilation analysis software that supports the simulation of airflows, contaminant concentrations and occupants’ contaminant exposure (Dols and Polidoro, 2015). For 3D modeling of the building geometry, Rhinoceros 3D (Robert McNeel and Associates, 2020) is employed.

Contamination simulation is the central tool that calculates transient contaminant concentrations and exposure in an indoor space. For a given time and specific weather conditions, accurate data regarding the indoor space, dry-bulb air temperature ($T_i$) and wind pressure coefficients ($C_p$) are critical parameters that influence contaminant behavior. Therefore, rough assumptions in $T_i$ and $C_p$ lead to incorrect results and imprecise correlations between the actual indoor/outdoor conditions and contaminant exposure. To this end, the seamless integration of transient energy simulations to obtain $T_i$, and CFD simulations to obtain $C_p$ values for a specified location and transient environmental conditions are necessary. These values, after they are calculated by the corresponding simulation tools, need to be used in the contamination model.

The proposed pipeline also supports parametric modeling by employing Grasshopper 3D (Rutten, 2007), a visual programming environment that supports the algorithmic design and operates within Rhinoceros 3D. Grasshopper enables the seamless integration of CFD and energy simulations with parametric design capabilities through various simulation tools such as EnergyPlus and OpenFOAM via Ladybug Tools plug-in (Honeybee, Ladybug and Butterfly) (Roudsari and Mackey, 2012), which are used for energy and CFD simulations in this study. As such, rapid geometry manipulations and the easy exploration of a wide range of parametric variations are made possible. The pipeline has three phases: (1) CFD simulation, (2) building energy simulation and (3) contaminant simulation (see Figure 1).
2.1.1 CFD simulation. In this research, CFD simulations are performed using OpenFOAM and operationalized through the Butterfly plug-in (Roudsari and Mackey, 2012), which is a Python library that performs CFD simulations (Chronis et al., 2015). To generate the CFD model, first, the 3D design geometry of the case building is modeled in Rhinoceros 3D, and then the geometry is defined in Grasshopper and Butterfly. The walls, ceiling, floor slabs and openings are modeled as surfaces. The wind characteristics such as the prevailing wind direction and the average velocity are obtained from an EnergyPlus weather file (EPW) that contains 8,760-h annual weather data for the selected location and simulation period. CFD simulations are conducted to obtain $C_p$ for each opening defined in the geometry. First, $C_p$ is calculated and used to generate the wind pressure (WP) profiles at each opening as follows (Cóstola et al., 2009):

$$C_p = \frac{P_x - P_0}{P_d} ; P_d = \frac{\rho U_h^2}{2}$$

where $P_x$ is the pressure ($P_x$) derived from a test point on the building façade, $P_0$ is the freestream reference pressure, $P_d$ is the dynamic pressure, $\rho$ is the air density (kg/m$^3$) and $U_h$ is the wind speed (m/s) at the room altitude.

A CFD model is built for the entire building, and a test section in this building is defined for the room. There are two existing approaches to CFD simulations: coupled and decoupled approaches (Ramponi and Blocken, 2012). In the coupled approach, indoor and outdoor environments are a single computational domain (CD), where wind interacts with both indoor and outdoor at the same time via assuming openings as voids in the CFD model (Ramponi and Blocken, 2012). In the decoupled approach, indoor and outdoor environments are two different CDs isolated from each other, where wind only interacts with the envelope of the building that the $C_p$ is calculated for (Ramponi and Blocken, 2012). The openings are assumed to be solid surfaces in the CFD model, and the WP is calculated on these surfaces (Ramponi and Blocken, 2012). As a result, the boundary conditions of the contamination simulation are obtained. In this research, we selected the decoupled approach for CFD simulations, which are only performed to obtain $C_p$ on the opening surfaces, as wind is acting upon the building as a sealed body.

CD of the CFD model is defined following the best practice guidelines (Franke et al., 2011) as follows:

1. for the vertical extension (between the building’s roof and the vertical boundary of CD), the top of CD is regarded as 5H,
2. for the lateral extension (between the building’s sidewalls and the lateral boundary of CD), the sides of CD are regarded as 5H,
3. for the leeward extension (the longitudinal region between the building’s leeward wall and the boundary of CD), the distance is regarded as 15H and
4. for the windward extension (the longitudinal region between the building’s windward wall and the boundary of CD), the distance is regarded as 3H,

where H is the height of the building.

Reynolds-averaged simulation (RAS-kEpsilon), also known as Reynolds-averaged Navier Stokes (RANS) turbulence model, is used for steady incompressible flows. The simulations are performed for a densely built environment, where the terrain is covered by buildings with similar heights. This dense environment, when selected in the CFD tool, automatically changes the wind profile and adjusts the wind speeds that act upon the building. The CFD simulations are performed for 100 iterations and eight directions with 45° intervals. The final $C_p$ values are calculated using the WP values obtained in the $100^{th}$ iteration. To determine the number of iterations, the residual values are considered to assess the convergence of the CFD solutions. According to the CFD best practice guidelines, the acceptable residual value is 1E-4
All final residual values of velocity, pressure and turbulence parameters for the 100th iteration remained below this upper limit. Accordingly, 100 iterations were performed in this study. Finally, the obtained \( C_p \) values for eight directions are integrated into (1) the AirflowNetwork (AFN) in the energy simulations and (2) the contamination simulation as the openings’ WP profiles.

2.1.2 Energy simulations. Following the CFD simulations, energy modeling and simulations are performed to calculate \( T_i \). To generate the energy model, the design geometry that is previously generated in Grasshopper is used as a base. AFN is a crucial component of the energy model, as it simulates the performance of an air distribution system, supply/return leaks and calculates multi-zone airflow induced by wind and HVAC systems (U.S. Department of Energy, 2015). In EnergyPlus, there are two possible representations for natural ventilation: “wind and stack area” and AFN. AFN-integrated energy simulations are found to be more accurate, as they can incorporate actual \( C_p \) values in its calculations (Gu, 2007). Accordingly, in this research, the AFN model is used to calculate the transient thermal conditions that are affected by the airflow distribution through natural ventilation. The original modeling environment Honeybee is built upon the OpenStudio SDK (Mackey and Roudsari, 2018), in which AFN is not yet implemented (Marshall et al., 2020). Therefore, the energy model is built in two consecutive stages. In the first stage, an initial model without EnergyPlus AirflowNetwork is built-in Honeybee and saved as an EnergyPlus input data file (IDF). Following, this IDF file is edited using the IDF Editor to manually add the AirflowNetwork to the room with the \( C_p \) values calculated in the previous step (Figure 2).

From the energy simulations, hourly \( T_i \) values are obtained. Following, an average \( T_i \) value is calculated for the contaminant analysis period. This is because transient \( T_i \) values are not permitted in CONTAM. Finally, both the WP profiles that are calculated from \( C_p \) values and the average \( T_i \) are given as inputs to CONTAM.

2.1.3 Contamination simulations. CONTAM, multi-zone airflow and contaminant transport analysis software, performs CFD analyses using CFD0 as an external CFD zero-turbulence model link to calculate the indoor contaminant concentrations by predicting potential impacts of the WP distributions on the building exterior (Wang et al., 2010). Both CONTAM and the proposed pipeline follow CONTAM–CFD0–CONTAM path to obtain contaminant exposures. CONTAM–CFD0 link offers two models of coupling as (1) coupling for building exterior simulations and outdoor contaminant concentrations and (2) embedding a CFD zone within CONTAM AFN for the contaminant transport simulations (Wang et al., 2010). A CFD zone is a single space in a building that the CFD simulations are performed for (Dols and Polidoro, 2015). Since the \( C_p \) values are determined by the CFD simulations that are performed at the CFD phase in the pipeline, the second coupling model is used. The CONTAM model supports dynamic coupling between CONTAM and CFD0, based on the iterative exchange of the boundary conditions (Wang et al., 2010). Once the required data (i.e. weather data and \( C_p \) values) is provided, \( C_p \) values on the openings and flow rates are obtained for the CFD zone. CFD0 calculates airflow behavior and provides feedback to CONTAM (Wang et al., 2010).

To perform contamination simulations, CONTAM requires a building geometry drawn in the 2D CONTAM SketchPad environment. Also, a weather file is required in CONTAM weather file (WTH) format, which can be converted from EPW files using CONTAM Weather File Creator online tool (NIST, 2010). The transient outdoor air temperature values (\( T_o \)) are

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**Figure 2.**

AFN integration into the energy model.
extracted from the EPW-converted WTH weather file. CONTAM also requires a contaminant model that specifies the contaminant’s molecular weight (molar mass), particle diameter and the effective density. COVID-19 is selected as the bio-contaminant species in this study. The molecular weight of COVID-19 is 33797.0 Da (33.79 kg/kmol) (Jin et al., 2020). The diameter of COVID-19 is set to 100 nanometers (0.1 μm), which is the average value of the diameter range (between 60–140 nanometer) (Zhu et al., 2020). The particle’s effective density, which defines the mass and mobility relation of the particle, is set to 1.0 g/cm³ (Dols et al., 2020).

The CONTAM constant-coefficient contaminant model is used, which requires contaminant generation and removal rates. Contaminant generation rate is the measure of the virus particles that are introduced into space by a contaminant source to calculate the amount of contaminant amount in the environment (Dols and Polidoro, 2015). This value is needed for the determination of the number of virus particles emitted by the contaminant source. In this study, the generation rate for COVID-19 is used from the empirical study of Leung et al. (2020), which can be found below. The removal rate is the measure of the rate that the contaminant is deposed from the space (Dols and Polidoro, 2015). There are only a limited number of studies focusing on the removal rate of COVID-19. The recent studies highlight the unsteady character of the removal/deposition rate, which changes according to the thermal and physical conditions (i.e. airflow behavior, thermal properties and the placement of the openings) (Abuhegazy et al., 2020). Also, the size of the particle has a direct impact on the deposition rate; the larger particles are transported rapidly on the ground, whereas the smaller particles are transported to different areas of the space (Abuhegazy et al., 2020). Due to their size, COVID-19 aerosol particles revealed low and/or undetectable deposition rates in the recent empirical measurements in Wuhan hospitals and public spaces (Liu et al., 2020). Particularly, in their study, Liu et al. (2020) registered three virus particle copies per m³ as maximum for the particle size 0.1 μm. Accordingly, the removal rate for COVID-19 is assumed as zero in this study, also suggested by CONTAM for the constant-coefficient contaminant model since the removal is calculated by CFD (Dols and Polidoro, 2010).

In total, four scenarios that represent different indoor conditions are developed (Figure 3). In these scenarios, three independent parameters are investigated regarding the massive
impact of the built environment on the virus dispersion, highlighted by CDC, as abovementioned, are building-related parameters such as opening-to-wall ratio and the window configuration and environment-related parameter that is $T_i$. By using the pipeline, the indoor contamination levels, discharge periods and infection time are evaluated for each scenario.

2.2 Study metrics

In this section, we present the study metrics used in our analyses, which are the contaminant concentration level (CCL ($#/m^3$)), contaminant discharge period ($T_{discharge}$) and time of infection ($T_{infection}$). All metrics are calculated for all scenario categories and scenarios.

(1) CONTAM calculates airborne contaminant concentrations on the level of user-defined sensors in the room ($CCL_{Sensor1}$ to $CCL_{SensorN}$), which usually represent the location of occupants exposed to the contaminant. The total airborne contaminant concentration of a room ($CCL_{Total}$) is calculated as the average total sum of all sensors for the total occupancy period (6 h) as follows:

$$CCL_{Sensor} = \sum_{i=0}^{m} VP_i$$

(2)

$$CCL_{Total} = \frac{\sum_{k=0}^{k} \sum_{s=0}^{n} \sum_{i=1}^{VP_s} S}{S}$$

where $VP(#/m^3)$ is the number of the virus particles per $m^3$ of air, $i$ is the timestep, $m$ is the index of the final timestep, $s$ is the sensor index, $n$ is the index of the last sensor timestep, $c$ is the scenario category index, $k$ is the index of the selected scenario category, $VP_s$ is the total number of particles for $s$ during $i$ and $S$ is the total number of sensors.

(2) $T_{discharge}$ is the time required to get completely discharge the room from the contaminant particles. In this research, $T_{discharge}$ is calculated as the period between the time that the contaminant source leaves the room and the time that contaminant concentration is completely discharged. $T_{discharge}$ also determines the occupant’s exposure period to the viral particles, which is also necessary to calculate the time and risk of infection in the room. For scenario categories, $T_{discharge}$ is calculated as an average value of $T_{discharge}$ of each scenario.

(3) $T_{infection}$ is the time of an occupant becoming infected due to her/his exposure to pathogenic agents. In total, four parameters are considered in this research for $T_{infection}$: (1) $VP_s$ in the room that a healthy occupant is exposed to during the occupancy period, (2) the sensor index, (3) the volume of the occupant’s air exchange (inhalation/exhalation) and (4) the assumed infectious dose of COVID-19. To calculate $T_{infection}$, the following variables were considered:

- Inhalation rate of humans ($R_{inh}$) is the measure of the inhaled dose of air, and it can range relying on the metabolic rate (age, sex, weight and health conditions), activity level and activity duration (US Environmental Protection Agency, 2011). A typical person exchanges 0.5 m$^3$/h air for sedentary activities (Engineering Toolbox, 2003), which we selected for this research.

- The infectious dose, which is the number of particles to cause an infection, is set to 280 particles for COVID-19, following previous research on SARS-Cov-1 and influenza A virus (Buonanno et al., 2020b; Schröder, 2020). However, recent studies indicate that further clinical research is required to find the exact infective dose of
COVID-19 for successful infection (Buonanno et al., 2020a, b; Schröder, 2020). As a result, $T_{\text{infection}}$ calculations might be in need of modification in the future.

Based on these variables, the $T_{\text{infection}}$ is calculated as follows:

\[ VP_T = \sum_{i=0}^{n} VP_s^i \cdot R_{inh} \tag{4} \]

\[ T_{\text{infection}} = T_{CE} + t_i \tag{5} \]

where $R_{inh}(m^3/h)$ is the rate of inhalation of an occupant, $VP_T$ (#) is the number of virus particles inhaled by an occupant, $i$ is the timestep (hourly), $s$ is the sensor index, $VP_s^i (\#/m^3)$ is the total particle number for the selected sensor during the selected timestep, $T_{\text{infection}}$ is the time that the occupant is infected, $T_{CE}$ is the time the contaminant enters the room and $t_i$ is the amount of time after which $VP_T$ is higher than the infectious dose. For each scenario, $VP_T$ is calculated for each sensor as the average value of all the sensors.

2.3 Case study design

The pipeline is implemented for the analysis of a single-zone room with 16 × 16 m dimensions with a 4 m floor height. The room is assumed to be on the 13th floor (52 m altitude) of a 25-floor open-plan office building. The building is set to be located in a dense cityscape in (for CFD simulations), Istanbul, Turkey. In our study, the mid-building floor is selected, which represents a sample case through the atmospheric boundary layer. Istanbul belongs to the dry-summer subtropical (referred to as Mediterranean) climate according to the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) climate classification. For all scenarios, the simulation period was set to a typical summer day as the building is free-running, between 12:00 and 18:00. For only one scenario category, a typical spring day is also set as a simulation period, also regarding the date for the building to be free-running.

In our study, first, a baseline scenario category (SC-B) for the room and the environmental conditions are established, against which three different scenario categories will be benchmarked. In SC-B, the room is naturally ventilated through operable windows. During the simulation day, the building is considered free-running, where no space conditioning is used. The surfaces of the simulated room are two-floor slabs that are set to adiabatic surfaces and four walls that are exposed to outdoor conditions. The U-values of the walls and windows are set to 0.60 W/m²K and 2.4 W/m²K, respectively, according to the Turkish Thermal Insulation Requirements for Buildings Standard (TS 825) for Istanbul (Turkish Standards Institution, 2009). Solar heat gain coefficient (SHGC) of the windows is 0.78.

2.3.1 Weather. An EPW file that represents a typical meteorological year (TMY) of Istanbul is acquired from the EnergyPlus website (U.S. Department of Energy’s Building Technologies Office, 2001b). In this file, the average wind speed and average temperature for July 8 between 12:00–18:00 are calculated as 7.27 m/s and 30.24°C, respectively (Figure 4). For the same day, the prevailing wind direction ranges between 30–100°.

2.3.2 Contaminant. In all studies, the infected occupant is assumed to enter the room at 12:00 and exit the room at 13:00. The height of the contaminant is set to 1.20 m for a sitting occupant. In the literature, different accounts for COVID-19 generation rate exist, based on different experimental setups. COVID-19 generation rates vary greatly with respect to human activities (breathing, speaking, coughing, sneezing, even changes with the vocalization while speaking), the infection phase and particle characteristics (WHO, 2020). In this study, the generation rate is taken from the study of Leung et al. (2020), which measures the aerosol VS...
rates of patients with COVID-19, rhinovirus and influenza. In their study, COVID-19 infected breath samples are analyzed during 30 min of breath sampling (Leung et al., 2020). COVID-19 is detected in 40% of the aerosol samples (4 out of 10 participants with maximum 10^{4.7} and minimum 10^{2.8} particles per 30 min). The calculated average viral shedding is 35,366 aerosol virus particles per hour (maximum 100,237 and minimum 12,621 particles per hour). In our scenarios, average viral shedding value is used.

2.3.3 Occupant. The occupants that are exposed to contaminants are assumed to be engaged in office activities. Occupants’ activity levels are determinant of their respiratory activities, which are used in our studies to calculate (1) virus generation rate from a contaminated occupant and (2) virus inhalation rate of an exposed occupant. For different activity levels (resting, standing, light exercise, moderate exercise and heavy exercise), results can vary significantly, due to metabolic rates, expiratory activities and therefore the virus emission/generation rates. In our simulations, the consideration of office activities is also consistent with our use of viral shedding rates by Leung et al. (2020).

We analyze a baseline scenario and three different scenario categories (Table 1): The parameters considered in the scenarios are as follows (Figure 5):

(1) **Window configuration (WIN_CONFIG):** Two different window configurations are modeled: (1) the opposite configuration (OPP), where the openings are placed on the two opposite walls, and (2) the corner-adjacent configuration (ADJ), where the openings are placed on two adjacent walls that are perpendicular to each other. The openings are assumed to be fully opened. The openings are located on the east and west façades in OPP to receive the eastern winds, while on the north and east for ADJ to receive both northern and eastern winds.

(2) **Opening-wall ratio (OWR):** 5 and 10% OWRs are studied. OWR differs from the window-wall ratio (WWR), where WWR is the percentage of the exterior glazed surface area is divided by the exterior wall area, whereas OWR is the percentage of the exterior opening surface area that allows natural ventilation is divided by the exterior wall area.

(3) **Contaminant source location (CS):** Five contaminant sources are placed at the center, southeast, southwest, northeast and northwest in the room that are C, SE, SW, NE and NW, respectively.

(4) **Indoor air temperature (T_i):** EnergyPlus calculates indoor air temperature of the scenarios regarding scenario-specific window configurations and OWR. The scenario SC-T simulates the impact of T_i on contaminant concentration.
3. Implementation and results

In this section, we present the results of the simulation-based analyses that investigate the air contamination rates, time of infection and discharge period of the case study room. First, a baseline scenario category (SC-B) was developed and modeled. Following, three scenario categories were similarly developed to be benchmarked against SC-B. These scenarios are grouped into two: the first scenario category focuses on building-related parameters (window configuration and OWR), while the second scenario category focuses on an environment-related parameter ($T_i$). For each scenario category, new models (energy, CFD and contamination) are built by modifying the baseline models. The pipeline is implemented
using these new models, and the study metrics are calculated as a result of the simulations. For each contaminant model, a separate simulation is performed for the 16 sensors in the room. The total number of simulations is 320. The analyses are performed for the scenario categories and scenarios. Tables 2 and 3 show all the simulation results for scenario categories and scenarios, respectively.

3.1 Analysis of scenario categories
Analyses of scenario categories explore the overall impact of the studied parameter on the metrics, which are assessed by using calculated average values. Follow-up simulations are performed for SC-B and SC-T, as $T_{\text{discharge}}$ extends beyond the simulation period.

Among all the scenario categories, SC-O results in the lowest and SC-T in the highest CCL$_{\text{Total}}$ values. SC-O shows an 87% decrease, and SC-T shows a 50% increase in CCL$_{\text{Total}}$ as compared to SC-B (Table 2). SC-O requires 4H25M shorter $T_{\text{discharge}}$, whereas SC-T requires 0H10M longer $T_{\text{discharge}}$ as compared to SC-B. SC-W shows a 50% decrease in CCL$_{\text{Total}}$ and requires 2H25M shorter $T_{\text{discharge}}$ as compared to SC-B (Table 2).

### Table 2.
Simulation results and the risk assessment for all scenarios

<table>
<thead>
<tr>
<th>Scenario categories</th>
<th>Scenarios</th>
<th>CCL$_{\text{Total}}$ ($#/m^3$)</th>
<th>$T_{\text{discharge}}$ (hour/minute)</th>
<th>$T_{\text{infection}}$ (HH:MM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>SC-B</td>
<td>40523</td>
<td>6H30M</td>
<td>13:10</td>
</tr>
<tr>
<td>Window configuration</td>
<td>SC-W</td>
<td>10,616</td>
<td>7H40M</td>
<td>13:00</td>
</tr>
<tr>
<td>Opening-wall ratio</td>
<td>SC-O</td>
<td>2,747</td>
<td>2H50M</td>
<td>0H50M</td>
</tr>
<tr>
<td>Temperature</td>
<td>SC-T</td>
<td>31,598</td>
<td>5H25M</td>
<td>13:20</td>
</tr>
</tbody>
</table>

### Table 3.
Simulation results and benchmarking of all scenarios (The lowest and the highest CCL within the scenario category are highlighted with blue and orange, respectively)

<table>
<thead>
<tr>
<th>Scenario Categories</th>
<th>Scenarios</th>
<th>CCL$_{\text{Total}}$ ($#/m^3$)</th>
<th>$T_{\text{discharge}}$ (hour/minute)</th>
<th>$T_{\text{infection}}$ (HH:MM)</th>
<th>CCL$_{\text{Total}}$ (L or S)</th>
<th>$T_{\text{discharge}}$ (L or S)</th>
<th>Compared Scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Baseline</strong></td>
<td>SC-B1 (C)</td>
<td>40523</td>
<td>6H30M</td>
<td>13:10</td>
<td>-</td>
<td>-</td>
<td>SC-B3</td>
</tr>
<tr>
<td></td>
<td>SC-B2 (SE)</td>
<td>56588</td>
<td>7H40M</td>
<td>13:00</td>
<td>2722% increase</td>
<td>3H45M L</td>
<td>SC-B2</td>
</tr>
<tr>
<td></td>
<td>SC-B3 (SW)</td>
<td>2005</td>
<td>3H15M</td>
<td>14:35</td>
<td>77% decrease</td>
<td>4H30M S</td>
<td>SC-B4</td>
</tr>
<tr>
<td></td>
<td>SC-B4 (NE)</td>
<td>3485</td>
<td>4H20M</td>
<td>13:00</td>
<td>-</td>
<td>-</td>
<td>SC-B5</td>
</tr>
<tr>
<td></td>
<td>SC-B5 (NW)</td>
<td>2557</td>
<td>3H40M</td>
<td>13:00</td>
<td>-</td>
<td>-</td>
<td>SC-B5</td>
</tr>
<tr>
<td><strong>WIN-CONFIG</strong></td>
<td>SC-W1 (C)</td>
<td>2111</td>
<td>2H30M</td>
<td>14:20</td>
<td>96% decrease</td>
<td>4H30M S</td>
<td>SC-B1</td>
</tr>
<tr>
<td></td>
<td>SC-W2 (SE)</td>
<td>13091</td>
<td>3H10M</td>
<td>14:35</td>
<td>77% decrease</td>
<td>4H30M S</td>
<td>SC-B2</td>
</tr>
<tr>
<td></td>
<td>SC-W3 (SW)</td>
<td>6096</td>
<td>3H00M</td>
<td>13:00</td>
<td>264% increase</td>
<td>0H15M S</td>
<td>SC-B3</td>
</tr>
<tr>
<td></td>
<td>SC-W4 (NE)</td>
<td>123</td>
<td>3H30M</td>
<td>13:00</td>
<td>96% decrease</td>
<td>0H15M S</td>
<td>SC-B4</td>
</tr>
<tr>
<td></td>
<td>SC-W5 (NW)</td>
<td>31661</td>
<td>3H20M</td>
<td>13:10</td>
<td>1138% increase</td>
<td>0H20M S</td>
<td>SC-B5</td>
</tr>
<tr>
<td><strong>Opening-Wall Ratio</strong></td>
<td>SC-G1 (C)</td>
<td>1</td>
<td>0H20M</td>
<td>13:10</td>
<td>100% decrease</td>
<td>6H10M S</td>
<td>SC-B1</td>
</tr>
<tr>
<td></td>
<td>SC-G2 (SE)</td>
<td>13463</td>
<td>2H45M</td>
<td>14:20</td>
<td>76% decrease</td>
<td>4H35M S</td>
<td>SC-B2</td>
</tr>
<tr>
<td></td>
<td>SC-G3 (SW)</td>
<td>273</td>
<td>0H15M</td>
<td>13:00</td>
<td>86% decrease</td>
<td>3H30M S</td>
<td>SC-B3</td>
</tr>
<tr>
<td></td>
<td>SC-G4 (NE)</td>
<td>0.09</td>
<td>0H15M</td>
<td>13:10</td>
<td>100% decrease</td>
<td>4H05M S</td>
<td>SC-B4</td>
</tr>
<tr>
<td></td>
<td>SC-G5 (NW)</td>
<td>0.22</td>
<td>0H25M</td>
<td>13:25</td>
<td>853% increase</td>
<td>1H25M L</td>
<td>SC-B5</td>
</tr>
</tbody>
</table>

L: Longer than; S: Shorter than.
The simulation results are investigated to identify the exact time of infection, according to the occupant’s virus exposure load as calculated for sedentary inhalation rate (0.5 m³/h). There is an inverse correlation between CCL\textsubscript{Total} and T\textsubscript{infection} where higher CCL\textsubscript{Total} results in earlier T\textsubscript{infection}. Among the scenario categories, only SC-O is free of risk of infection (Table 2).

The overall analysis of the scenario categories shows an expected correlation between CCL\textsubscript{Total} and T\textsubscript{discharge}. This confirms the recent studies (Sun and Zhai, 2020); where lower CCL\textsubscript{Total} results in shorter T\textsubscript{discharge}. According to this correlation, the increase in OWR (to 10%) and adjacent window configuration are effective strategies to reduce the infection risk as compared to 5% OWR and opposite window configuration. However, lower T\textsubscript{i} results in higher CCL\textsubscript{Total} and longer T\textsubscript{discharge}. In this respect, higher T\textsubscript{i} results in shorter duration for the removal of the contaminant. However, it must be added that the occupants’ comfort should also be considered and assessed in higher T\textsubscript{i}, particularly for cooling periods.

### 3.2 Analysis of scenarios

Analysis of scenarios explores the impact of the altered parameter on the study metrics for each scenario that are grouped under the scenario categories. Scenarios are simulated for five contaminant placements (C, SE, SW, NE, NW). Follow-up simulations are performed for the scenarios that are grouped under SC-B and SC-T, as T\textsubscript{discharge} extends beyond the simulation period.

Among 20 simulation sets, SC-B2 results in the highest CCL\textsubscript{Total} (56,588 #/m³) and the longest T\textsubscript{discharge} (7H40M), whereas SC-O4 results in the lowest CCL\textsubscript{Total} (0.09#/m³) and the shortest T\textsubscript{discharge} (0H15M) (Table 3). Similarly, SC-B2 has the earliest T\textsubscript{infection} (13:00), while SC-O4 does not result in a risk of infection and therefore T\textsubscript{infection}. In total, ten of the scenarios result in no risk of infection, while the other ten of them result in a risk of infection, where T\textsubscript{infection} ranges between 13:00 and 15:40. Only, all the scenarios of SC-T scenario category result in a risk of infection, where T\textsubscript{infection} also ranges between 13:00 and 15:40. As typical in other scenario categories, SW and NE contaminant placement do not pose a risk of infection.

We also investigated the impact of contaminant placement on CCL. CCL\textsubscript{Total} is calculated as an average of each scenario for the specific contaminant placement (i.e. the average CCL\textsubscript{Total} is calculated for C as the average of SC-B1, SC-W1, SC-O1 and SC-T1) (Table 4). Among all scenario categories, the SW contaminant placement resulted in the lowest average CCL\textsubscript{Total} (12,489#/m³). In contrast, SE resulted in the highest average CCL\textsubscript{Total} (28,363#/m³). Although SW contaminant placement of has an advantage over SE in SC-B, SC-W and SC-O, SE contaminant placement resulted in 1.4-fold lower CCL\textsubscript{Total} as compared to SW in SC-T.

#### 3.2.1 Scenarios category-B: baseline

In this section, we first investigate the CCL\textsubscript{Total}, T\textsubscript{discharge} and T\textsubscript{infection} of the scenarios, and then we investigate the airflow behavior to calculate the contaminant dispersion and accumulation in the room.

Among the five baseline scenarios, a sharp difference is observed between (1) SC-B1, SC-B2 and (2) SC-B3, SC-B4, SC-B5. CCL\textsubscript{Total} of SC-B1 and SC-B2 were approximately six-fold higher as compared to SC-B3, SC-B4 and SC-B5 (Figure 6). Similarly, SC-B1 and SC-B2 have a

<table>
<thead>
<tr>
<th></th>
<th>(1) C</th>
<th>(2) SE</th>
<th>(3) SW</th>
<th>(4) NE</th>
<th>(5) NW</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC-B</td>
<td>40528</td>
<td>56588</td>
<td>2005</td>
<td>3485</td>
<td>2557</td>
</tr>
<tr>
<td>SC-W</td>
<td>2111</td>
<td>13091</td>
<td>6096</td>
<td>123</td>
<td>31661</td>
</tr>
<tr>
<td>SC-O</td>
<td>13463</td>
<td>3039</td>
<td>41584</td>
<td>9214</td>
<td>24371</td>
</tr>
<tr>
<td>AVG. CCL\textsubscript{TOTAL}</td>
<td>23788</td>
<td>28363</td>
<td>12489</td>
<td>3205</td>
<td>14647</td>
</tr>
</tbody>
</table>

Table 4. The contaminant placement and CCL\textsubscript{TOTAL}
Among five contaminant placements, SC-B2 resulted in the highest CCL\textsubscript{Total} (56,588 #/m\textsuperscript{3}), which is 28 times higher than SC-B3 lowest CCL\textsubscript{Total} (2,005 #/m\textsuperscript{3}) (Table 3). SC-B2 has the longest $T_{\text{discharge}}$ (7H40M) as expected. Similarly, SC-B3 was expected to show the shortest $T_{\text{discharge}}$ due to the lowest CCL\textsubscript{Total}. However, SC-B5 has shown the shortest $T_{\text{discharge}}$ (3H55M), whereas SC-B3 has the second shortest $T_{\text{discharge}}$ (3H55M). We qualitatively investigate the airflow behavior through CFD simulations and observe that the air follows a circular route, entering the room from the eastern façade and leaving the room from the western and eastern façade (Figure 7). On the eastern façade, a considerable amount of the air enters the room from W12. With the openings on the western façades, a limited amount of air also leaves the room from W7, W8, W9 and W10. As such, the airflow drags the contaminant toward the west and circulates in a clockwise direction. The simulations also show that the airflow accelerates at the periphery (0.90–7.86 m/s) and decelerates in the center of the room (0.10–0.90 m/s). Accordingly, the contaminant remains airborne relatively longer in the center (sensors S6, S7, S10 and S11) as compared to the areas that are in the close proximity of the outlets (S1, S5, S9 and S13). The dispersion is rather limited, which increases in the center (CCL\textsubscript{S6} and CCL\textsubscript{S7}). Accordingly, SC-B1 had higher CCL\textsubscript{Total} as expected. It is assumed that the contaminant’s proximity to the openings has the potential to decrease CCL\textsubscript{Total}, as observed in SC-B3, SC-B4 and SC-B5. This correlation was also expected for SC-B2, where the contaminant is placed at the southeastern periphery of the room. The contaminant is expected to discharge the contaminated air quickly due to the wind vectors acting upon the contaminant. However, CFD results showed that the airflow coming from W12 increases the dispersion of the contaminant in the room and delays the discharge, which explains the higher CCL\textsubscript{Total} in SC-B2 and SC-B1. Contrarily, in SC-B3, SC-B4 and SC-B5, the contaminant is largely discharged before it disperses in the room.

We also performed a detailed inspection for each scenario to determine the areas that are vulnerable to the risk of infection due to higher CCL\textsubscript{sensor} (Figure 8). There is a direct correlation between CCL\textsubscript{sensor} and the occupants’ risk of infection. The results suggest that SC-B4 has relatively better-mixed air due to the even contaminant distribution. The CCL\textsubscript{sensor} ranges between 103#/m\textsuperscript{3} and 85#/m\textsuperscript{3}, where the difference between the CCL\textsubscript{sensor} is
narrowest (18#/m³) among the scenarios. In contrast, SC-B2 has the most uneven distribution of the contaminant by having the widest difference in CCL_{sensor} (781#/m³) that ranges between 1,920#/m³ and 1,138#/m³.

3.2.2 Scenario category-W: window configuration. SC-W investigates the impact of two different window configurations (OPP5% and ADJ5%) on CCL_{Total}, T_{infection} and T_{discharge} for five contaminant placements. Accordingly, five simulation sets are performed for 16 sensors, and the results are presented in Table 3. Among the five scenarios, SC-W5 resulted in the highest CCL_{Total} (31,661#/m³) and the longest T_{discharge} (3H20M). SC-W4 resulted in the lowest CCL_{Total} (123#/m³) and the shortest T_{discharge} (1H55M) (Figure 9). There is no infection risk in SC-W1, SC-W3 and SC-W4, whereas the occupants potentially get infected during the occupancy in SC-W2 (14:35) and SC-W5 (13:10).

Simulations highlight a significant impact of the window configuration on CCL_{Total} and the risk of infection. Table 2 suggests the advantage of SC-W over SC-B, which led to a two-fold decrease in CCL_{Total} and T_{discharge}. Despite the overall decrease in the study metrics, SC-W3 and SC-W5 resulted in an increase in CCL_{Total}. Particularly, despite having the second and the first highest CCL_{Total} in SC-B, in SC-W, SC-W1 and SC-W2 show a significant decrease in CCL_{Total} and T_{discharge} (Table 3).
SC-W3 and SC-W5 showed a three-fold and a 12.3-fold increase in CCLTotal, respectively, compared to SC-B3 and SC-B5. However, such increase in CCLTotal was expected to result in longer $T_{\text{discharge}}$ due to the direct correlation between CCLTotal and $T_{\text{discharge}}$: Typically, higher CCLTotal is expected to discharge slower, which is also consistent with the results in recent studies (Sun and Zhai, 2020). In contrast to our initial assumptions, SC-W3 requires 0H55M,
and SC-W5 requires 0H20M shorter $T_{\text{discharge}}$ as compared to SC-B3 and SC-B5, respectively. Accordingly, airflow behavior is visually inspected through CFD outputs.

Visual analyses based on CONTAM CFD0 results show that the northern openings in ADJ allow wind to enter the room, increasing the internal WP difference for a relatively longer time as compared to OPP (Figure 10). In ADJ, the pressure gradient force increases as a result of a shorter distance between the northern and eastern openings. Consequently, the wind speed increases and accelerates the discharge rate and shortens $T_{\text{discharge}}$. OPP demonstrates a lower pressure gradient force as compared to ADJ, which retains the contaminant in the room for a longer period. The circular route of the airflow in ADJ also contributes to rapid discharge. Accordingly, the airflow could reach the contaminant and accelerate the discharge as in SC-W3 and SC-W5. At this stage, due to the indoor air pressure and airflow behavior, ADJ has an advantage over OPP due to its shorter $T_{\text{discharge}}$.

A detailed inspection is performed for each scenario to determine the vulnerable areas to the risk of infection, correspondingly the occupants who might have a higher risk of infection due to higher CCL$_{\text{sensor}}$ (Figure 11). The simulation results, which are similar to those of SC-B, suggest that SC-W4 has relatively better-mixed air due to the even contaminant distribution, whereas SC-W2 shows the most uneven contaminant distribution. In SC-W4, CCL$_{\text{sensor}}$ ranges between 3.70#/m$^3$ and 3.16#/m$^3$, with the difference narrowest (0.54#/m$^3$) between the CCL$_{\text{sensor}}$. Contrarily, SC-W2 shows the widest difference between the CCL$_{\text{sensor}}$ (923#/m$^3$) that ranges between 1.129#/m$^3$ and 206#/m$^3$.

3.2.3 Scenario category-O: opening-wall ratio. SC-O investigates the impact of OWR on CCL$_{\text{Total}}$, $T_{\text{discharge}}$ and $T_{\text{infection}}$. We investigate two ratio values: 5 and 10% in scenarios SC-B and SC-O, respectively (Table 1). The simulation results show that there is an inverse correlation between OWR and CCL$_{\text{Total}}$ (Table 2). The higher OWR results in lower CCL$_{\text{Total}}$, shorter $T_{\text{discharge}}$ and longer $T_{\text{infection}}$ (Figure 12). All SC-O scenarios show a decrease in CCL$_{\text{Total}}$ and $T_{\text{discharge}}$. This similarly delays $T_{\text{infection}}$ in SC-O. Only SC-O2 poses a risk of infection at 14:20, whereas there is no IR in SC-01, SC-03, SC-04 and SC-O5 (Table 3).

The airflow behavior studies indicate a two-fold increase in the airflow speed observed in CFD outputs of SC-O (average wind speed: 9.03m/s) as compared to SC-B (average wind speed: 4.36m/s) (Figure 13). Similar to SC-B, airflow accelerates at the periphery (1.80–12.63 m/s) and decelerates in the center (0.10–1.80 m/s) of the room. This increase also shortens $T_{\text{discharge}}$ and reduced IR. However, it must be noted that accelerated airflow can cause occupant discomfort due to potential draft at the periphery of the room. Further investigation should be considered for occupant comfort in future studies.

The simulation results are visualized for each scenario to determine the areas that are vulnerable to the risk of infection (Figure 14). Similar to SC-B and SC-W, the results suggest that SC-O4 has relatively better-mixed air due to the even contaminant distribution. In SC-O4, CCL$_{\text{sensor}}$ ranges between 3.27E-03#/m$^3$ and 2.29E-03#/m$^3$ that the difference is the narrowest (9.8E-04#/m$^3$). In contrast, SC-O2 has the most uneven distribution of the contaminant, where CCL$_{\text{sensor}}$ ranges between 987#/m$^3$ and 302#/m$^3$, having the widest difference (684#/m$^3$).

3.2.4 Scenario category-T: indoor air temperature. SC-T explores the correlation between $T_i$ and the study metrics CCL$_{\text{Total}}$, $T_{\text{discharge}}$ and $T_{\text{infection}}$. In general, indoor air temperature is the determinant in buoyancy-induced airflow through windows. The degree to which $T_i$ is influential in contaminant discharge is the subject of this scenario category. Different $T_i$ values resulting from the transient thermal balance in the room can be calculated hourly by energy simulations. In total, two days are selected for SC-B and SC-T that are a typical summer day and a typical spring day that does not require heating, respectively. The average $T_i$ values calculated by EnergyPlus (between 12:00 and 18:00) are 29.30 and 23.30°C, respectively, for the two scenarios. Although the $C_p$ values on typical spring day in SC-T are
Figure 10.
Airflow behavior in OPP and ADJ (wind and pressure) between 12:00–18:00 (15 min timestep)
different than those of SC-B, we used the $C_p$ values of SC-B for both scenarios to be able to observe the impact of $T_i$ in isolation (Table 1).

In all SC-T scenarios, the occupants get infected, where $T_{infection}$ ranges from 13:00 to 15:40 (Table 3). The calculated average of all SC-T scenarios suggests an inverse correlation between CCL$_{Total}$ and $T_i$, where a 6°C decrease in $T_i$ resulted in a 1.5-fold increase in CCL$_{Total}$ (Table 3). This correlation is observed in SC-T3, SC-T4 and SC-T5 (Figure 15). However,
SC-T2 showed a linear correlation, where 6°C decrease in \(T_i\) resulted in a 1.9-fold decrease in \(CCL_{\text{Total}}\) and required 1H25M shorter \(T_{\text{discharge}}\) as compared to SC-B2.

Within five scenarios, SC-T4 resulted in the lowest \(CCL_{\text{Total}}\) (9,214#/m³), which is 2.7-fold of SC-B4. This increase also led to 0H05M increase in \(T_{\text{discharge}}\) as compared to SC-B4. SC-T1 resulted in the highest \(CCL_{\text{Total}}\) (52,514#/m³), which shows a 1.3-fold increase as compared to SC-B1. However, in contrast to our initial assumptions, simulation results suggest an inverse correlation between \(CCL_{\text{Total}}\) and \(T_{\text{discharge}}\), where SC-T1 requires 0H15M shorter \(T_{\text{discharge}}\) as compared to SC-B1. SC-B1 was expected to require longer \(T_{\text{discharge}}\) due to the increase in \(CCL_{\text{Total}}\) and its contaminant location at the center, where airflow is decelerated. Accordingly, indoor airflow behavior is visually investigated through CFD outputs. Slower airflow is observed in CFD simulations of SC-T as compared to SC-B. Although SC-B has a relatively higher airflow velocity in the room (SC-B: 0–8.73m/s and SC-T: 0–8.69m/s), SC-T has higher airflow velocity in the center of the room between 15:00–16:00 as compared to SC-B (Figure 16). This can possibly shorten \(T_{\text{discharge}}\) despite the increase in \(CCL_{\text{Total}}\).

To determine the vulnerable areas in the room, \(CCL_{\text{sensor}}\) is calculated for each scenario (Figure 17). The simulation results suggest that SC-T4 has relatively better-mixed air due to

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**Figure 13.**
Airflow behavior in OPP10% (\(h = 1.20\) m)
(60 min timestep)
the even contaminant distribution. Similarly, to SC-B, SC-W and SC-O, this is due to the narrowest difference of CCL_{sensor} (48.92/#/m³) ranges between 270.77/#/m³ and 221.95/#/m³. In contrast, the contaminant is distributed more unevenly in SC-T1, where CCL_{sensor} ranges between 1589.58/#/m³ and 1201.90/#/m³, where the difference between CCL_{sensor} (387.68/#/m³) is the widest.
4. Discussion and conclusion

Public indoor spaces have a significant impact on the acceleration of airborne infections, as it is confirmed by the current COVID-19 pandemic. Natural ventilation is a critical aspect of the risk of infection and is identified as the most effective means of reducing indoor airborne contaminant exposure in the literature. However, the impact of natural ventilation on building-related and environment-related parameters relating to COVID-19 transmission remains unclear. Accordingly, there is a need for further exploration of natural ventilation, built environment and its impact on the risk of infection. Identification of their impacts through specific scenarios presents a broader understanding of the correlation between natural ventilation, building, occupant and environment-related parameters, and the aerodynamic behavior of COVID-19. Additionally, in the literature, studies specifically focus on healthcare and education buildings. However, the shared working spaces also pose a significant infection transmission risk for respiratory infections. Accordingly, this paper problematizes indoor air contamination of a free-running, naturally-ventilated room contaminated by COVID-19.

In this study, we implement a simulation pipeline that couples CFD, energy and the multi-zone IAQ-contaminant transport simulations to increase the accuracy in calculating transient
contaminant concentrations for actual weather conditions. We develop four scenario categories and five possible contaminant locations. As a result, 20 scenarios are modeled and simulated by implementing the developed pipeline. We calculated CCL_{Total}, T_{discharge} and T_{infection}. We explore the correlations between the parameters that are outlined in Table 1. Accordingly, this research draws a number of conclusions:

(1) SC-T resulted in 50% increase in CCL_{Total}, whereas a decrease of 50 and 87% are observed for SC-W and SC-O as compared to SC-B. As a result, SC-O has a higher potential for reducing the risk of infection as compared to SC-W. The comparison between the baseline case and the three scenarios are as follows:

- **SC-O**: Confirming the study of Fung and Lee (2015) and Zhou et al. (2014), larger windows (higher OWR) offer better ventilation and lower contamination. As expected, higher OWR in SC-O results in faster contaminant discharge due to lower CCL_{Total} and T_{discharge}. CDC advises resuming occupancy at least 24 h after the previous occupancy period for public spaces under infection risk (CDC, 2020a). The required period could differ in different cases. In this study, it is observed that the required time is reduced 84% (4H25M) by SC-O as compared to SC-B. However, it must be noted that higher OWR runs the risk of occupant discomfort due to potential draft problems. The combined evaluation of thermal comfort and indoor contamination is currently an understudied area that requires further investigation in the future.

- **SC-W**: Confirming the study of Fung and Lee (2015), the window configuration has a considerable impact on the ventilation performance and the indoor contaminant concentration. ADJ has a 98% advantage over OPP based on their CCL_{Total} Values. Window configurations result in unique indoor air pressure and...
velocity, therefore pressure gradient force. The higher level of change in the air pressure accelerates the indoor air velocity and shortens $T_{\text{discharge}}$. However, the results cannot be generalized. Calculating not only the wind direction and speed but also the gradient force is essential to the determination of the openings. The combined evaluation of energy, CFD and contaminant transportation simulations is necessary to reliably understand the complex airflow and contaminant dispersion behavior.

- **SC-T**: In the available literature, due to the complexity in the weather conditions, the impact of temperature on the transmission of COVID-19 is yet to be confirmed. However, the majority of the research studies report the impact of the ambient air temperature on COVID-19 transmission that the higher infection risk occurs in colder ambient air temperatures, whereas lower infection risk occurs in warmer ambient air temperatures (Carleton and Meng, 2020; Islam et al., 2020; Qi et al., 2020; Rosario et al., 2020; Sanchez-Lorenzo et al., 2020; Wang et al., 2020). Carleton and Meng (2020) reported that with 1°C increase in local temperature resulted in 13% fewer cases. In our study, 6°C increase in indoor air temperature resulted in 50% decrease in infection risk. The results of SC-T contribute to the existing literature by confirming the studies that report the higher $T_i$ can help to reduce the risk of infections compared to lower $T_i$. Therefore, the free-running periods (typically in spring and fall) can pose higher infection risk as compared to summer. However, higher $T_i$ could lead to the occupants’ discomfort and must be evaluated accordingly. Comfort studies need further investigation.

(2) The existing literature indicates a linear correlation between contaminant concentration levels and the discharge period. Contrarily, our studies point to the correlation between CCL$_{\text{Total}}$ and $T_{\text{discharge}}$ is not linear in all conditions. This linear correlation is observed in all scenario categories. However, contrasting the recent studies, an inverse correlation is observed in SC-T1, SC-W3 and SC-W5. The contaminant location and $T_i$ have an impact on the correlation between CCL$_{\text{Total}}$ and $T_{\text{discharge}}$ due to the gradient pressure forces and airflow velocity that act upon the contaminant, where the case-specific and microclimatic conditions require further investigation during the design decisions.

(3) The simulation results suggest that there is a strong relationship between contaminant placement and CCL$_{\text{Total}}$ in all scenarios. Among all scenario categories, the SW contaminant placement resulted in the lowest average CCL$_{\text{Total}}$. In contrast, SE resulted in the highest average CCL$_{\text{Total}}$. Also, the vulnerable areas of the room change according to the contaminant placement. In all scenarios, NE has better-mixed air due to the relatively even distribution of the contaminant. In contrast, SE (in SC-B, SC-W and SC-O) and C (in SC-T) pose a higher risk of infection to the occupants at certain locations in the room due to the relatively uneven contaminant distribution.

Based on the simulated scenarios, this research recommends a number of practical implications to reduce indoor COVID-19 transmission risks:

(1) For the existing buildings:

- The determination of the reoccupancy: With COVID-19, the occupancy and the ventilation control of the shared spaces becomes essential to reduce the potential transmission risk. Particularly, the calculation of the required period for reoccupancy is crucial. Accordingly, the existing buildings must first be
evaluated for their infection risk potential and following, the required period for the re-occupancy must be determined. The pipeline presented in this research can guide such evaluation and regulation process for different buildings and climates and can be beneficial for designers, occupants, and building operators.

- The refurbishment process: With COVID-19, there is an increasing need for the refurbishment of existing buildings to provide adequate ventilation. With ventilation adequacy, the potential contaminant concentration levels and the airflow behavior in existing buildings, which are important parameters in preventing the viral transmission indoors, must be evaluated. The modification of window configuration and OWR are potential refurbishment actions to improve effective ventilation.

- Contaminant location: Although the primary aim of this research was not to evaluate the room layout, the relationship between the contaminant location and the spatial depth appeared as an issue that requires further inquiry. The analysis of different plan layouts and window configurations is a crucial area that requires further investigation. This research shows that, the contaminant is dispersed unevenly in the room due to the airflow behavior. The dispersion behavior is also related with the placement of the contaminant in the room. It is important to determine the infection-vulnerable locations that have relatively higher contaminant exposure. The presented case study setup shows that a contaminant located in close proximity to the inlets increases the dispersion of the contaminant and results in higher contamination levels. A contaminant located in distant proximity to the inlets results in significantly lower contaminant levels. The determination of the infection-vulnerable locations could reduce the transmission risk by guiding the indoor circulation and occupancy.

(2) For new buildings:

- The design of the openings: This research highlights the impact of the window configuration and OWR as design parameters which determine the indoor airflow and ventilation adequacy. Accordingly, the window configuration and OWR can be determined for the new designs by employing a simulation-based procedure to analyze the ventilation, contaminant discharge and infection risk potential.

Our study also confirms that each building setup is a unique case that requires a systematic and detailed investigation using simulations. Our results were calculated for typical summer and spring conditions. For other physical contexts and weather conditions (i.e. different wind profiles and $T_e$), the results can significantly vary from ours. Other parameters that need to be studied further include building program, occupancy, internal loads, HVAC systems (especially mechanical ventilation systems, if any).

Within the scope of this study, two limitations were identified. First, occupants can act as contaminant sinks as they inhale contaminated air and retain a portion of the contaminant source. In our simulations, this condition is not considered. In a room occupied by a high number of people, our results can overestimate the actual contaminant concentrations. Therefore, a high number of occupancies can reduce the contamination concentration in the room, and if this the case, a contaminant sink should be inserted inside the model. We leave this issue as future work. Second, we used the actual weather data in this research, which has brought both not only the site-specific and context-dependent results but also a number of challenges to the analyses. The impact of wind and the air temperature was not analyzed in
isolation in the scenarios. Accordingly, further work should focus on the effect of air temperature isolated from wind to clarify the direct relationship between the thermal conditions and COVID-19 contaminant dispersion. Also, contaminant concentration analyses cannot be regarded in isolation from other performance measures such as energy use, daylighting and occupant comfort.

The simulation pipeline presented in this study can serve as a supporting tool for the integrated analysis of building performance. The existing building stock must be reevaluated, and the new designs should be assessed for the existing and future microclimatic conditions. Metrics, strategies and actions to minimize indoor contamination risks should be addressed in future building standards to minimize the building and environment-related airborne virus transmissions. This study specifically focuses on COVID-19. However, the pipeline can be utilized for other airborne contaminants and design scenarios. Further studies can address and simulate different occupant densities and occupant profiles, particularly with masks. The benefits of this pipeline can also be realized by integrating it to decision-making for the adaptation of existing buildings to pandemic conditions, as well as the design of new buildings.

References


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Supplementary data
The supplementary material is available online for this article.

Corresponding author
Günsu Merin Abbas can be contacted at: merin.abbas@metu.edu.tr

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