CFD Analysis of Hydroxyl Technology to Reduce Risk of Indoor Pathogen Transmission

BY KISHOR KHANKARI, PH.D., FELLOW ASHRAE; CONNIE ARAPS, PH.D., MEMBER ASHRAE; DAVID CROSLEY, PH.D.

Traditionally, HVAC ventilation has been used to reduce the concentration of microorganisms through dilution. Increased airflow supply rates (air changes per hour [ach]) can help dilute airborne contaminants and reduce their concentration. The effectiveness of ventilation depends on airflow patterns in the space, how effectively the clean supply air reaches the breathing zone, the resulting age of air and extent of air mixing and how effectively contaminated air is removed. Computational fluid dynamics (CFD) analysis of HVAC design has demonstrated how improved airflow dynamics can reduce the risk of pathogen transmission.[1] The purpose of this study is to use CFD analysis to assess how the effectiveness of HVAC ventilation can be further enhanced with hydroxyl air purification in reducing the risk of infectious pathogen transmission.

The authors hypothesize that hydroxyl radical formation generates airborne sanitizing agents that can be distributed through HVAC ventilation systems and further reduce pathogen concentrations and transmission risk.

Atmospheric hydroxyl radicals are continuously produced in the lowest layer of the Earth's atmosphere by the action of the sun's radiated ultraviolet (UV) energy. Three to 10 million hydroxyls are in each cubic centimeter of ambient outdoor air during sunny daylight hours. Hydroxyl radicals are the primary atmospheric purifying agent in nature.[2-4] Hydroxyls decompose volatile organic pollutants by hydrogen atom abstraction. Volatile organic compounds (VOC) are progressively decomposed to ultimately yield carbon dioxide and water.[2]

Hydroxyls react with VOC in 20 to 50 milliseconds to form organic peroxy radicals (ROO), which are

Kishor Khankari, Ph.D., is president of AnSight LLC, Ann Arbor, Mich. Connie Araps, Ph.D., is president and CEO of Prometheus Strategies LLC, Delray Beach, Fla. David Crosley, Ph.D., is a consultant, Palo Alto, Calif.

themselves powerful sanitizing agents with much longer lifetimes than hydroxyls (minutes vs. milliseconds).[5] Each hydroxyl radical generates one ROO radical, which starts a chain reaction with another VOC to generate a new R′OO radical. This chain reaction persists until two radicals combine in a terminal reaction. The duration of the chain reaction is the radical lifetime.

Atmospheric hydroxyls and the natural organic oxidants they generate have been shown to reduce bacteria, virus and mold.[6] They react with the lipids, proteins, carbohydrates and other organic compounds that make up the cell membrane and disrupt the structure, leading to cell lysis (disintegration) and death.[6] Humans, animals and plants have evolved symbiotically with atmospheric hydroxyl radicals and developed outer surfaces and mucosa that are impervious to their oxidative effect at the concentrations found in nature.

Indoor environments do not contain atmospheric hydroxyl radicals as they react too rapidly to diffuse indoors. Hydroxyl technologies have been developed and commercialized that can produce hydroxyl radicals indoors, in the same concentrations found outdoors.[5–7] The equipment used in this study produces hydroxyl radicals with UV lamps that photolyze water vapor.[7] It can be inserted into ductwork, and the hydroxyl and organic peroxy radicals delivered through the supply air can reduce airborne and surface-bound virus, bacteria and mold, according to third-party testing.[8]

Other technologies that exist to generate hydroxyl radicals in indoor environments include photocatalytic oxidation devices, which project UV light onto a titanium dioxide catalyst to produce hydroxyl radicals on the catalyst surface, and terpene devices, which generate hydroxyl radicals in a mixing chamber by reacting ozone with limonene within the chamber.

Determination of Device Parameters for CFD Modeling

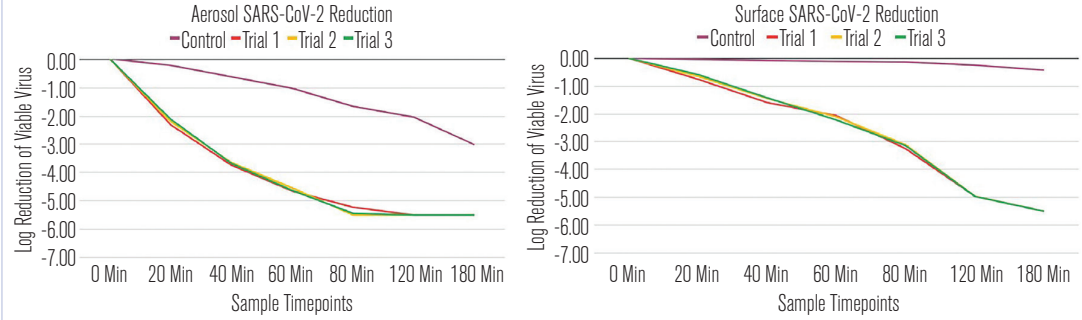
Chemical interactions begin when hydroxyl radicals react rapidly with ambient VOC to form the more stable organic peroxy radicals (ROO). The ROO radicals initiate chain reactions with VOC, which enable successive ROO moieties to circulate throughout the treatment area.

The network of radicals formed and the kinetics of reactions are too complex to use in CFD modeling. Instead, we determined one key parameter, the age of air, as a surrogate for the sum of the radical concentrations at any given point in the room. Owing to the configuration of the HVAC layout of the room and the resulting airflow patterns, the air at each location in the room has a unique age from the time it was injected into the room.

ROO radical chain reactions continue throughout the room and are terminated by radical-radical recombination. The "lifetime" of the radical is the length of time the chain reactions continue before termination. The value of the radical "lifetime" enables us to determine the concentrations of ROO radicals and hence their lethality as a function of the age of air at each point in the room.

We can determine this value using surface kill rate experimental data from an antimicrobial study, since the kill rates are attributed solely to the effect of ROO radicals in air. The effectiveness of a hydroxyl generating device in killing microorganisms was quantified by measuring the kill rate of airborne and surface-bound SARS-CoV-2 virus. A portable device was used to generate the hydroxyl radicals in the test chamber. The test nebulized and circulated virus uniformly through the chamber, and petri dishes inoculated with high concentrations of virus were also placed on a table in the chamber 18 ft (5.5 m) from the device. The study measured the concentration over time of aerosolized and surface-bound SARS-CoV-2, following the introduction of hydroxyl and ROO

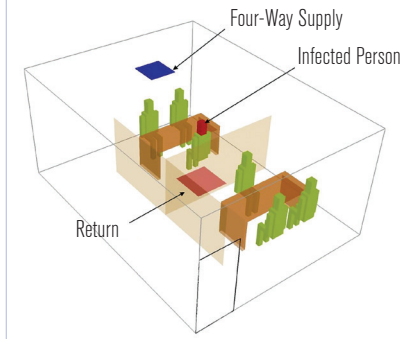
FIGURE 1 Biosafety Level 3 laboratory test results for the aerosol and surface inactivation of SARS-CoV-2 virus due to ROO radicals.



radicals into the chamber.

Live aerosolized virus was reduced 99% in 20 minutes and 99.99% in 60 minutes, relative to controls, while live surface-bound virus was reduced 99% in 60 minutes and 99.999% in 120 minutes, relative to controls. (As shown in *Figure 1*, a 1.00 log reduction is equivalent to a 90% reduction in microbial count, a 2.00 log reduction is equivalent to a 99% reduction and so forth.)

FIGURE 2 Schematic of the office CFD model analyzed in this study.



Using this data, an average ROO radical lifetime of 12.5 minutes was determined. This lifetime is consistent with a calculation using published values of chemical kinetic rate coefficients for organic peroxyl radicals typical of those presented here, the known energy output of the UV optics used in the experiment and an average value for relative humidity. The average lifetime value was then combined with CFD age of air plots to determine the radical concentration at each point in the CFD room. These patterns were mapped over the entire room to calculate the amount of virus remaining at any time after the hydroxyl and ROO radicals were introduced.

Virtual Office Space—CFD Model Description

A three-dimensional, steady-state, isothermal CFD model for a typical small office space was developed. The space has a floor area of about 300 ft^2 (27.9 m^2) with a 9 ft (2.7 m) ceiling height and occupancy of six persons. As shown in *Figure 2*, the cubicles are separated by 5 ft (1.5 m) tall dividing partitions. Each cubicle has about 100 ft^2 (9.3 m^2) area. A common corridor is adjacent to these cubicles leading to the room door. Each cubicle has three occupants seated at a desk. An infected individual is facing the two other individuals located in a cubicle away from the door. The office space is designed for a supply airflow flow rate of 135 cfm (63.7 L/s) or a total of 3 air changes per hour (ach), which corresponds to the total cooling load of 3,000 Btu/h (968 W) for a 20°F (11°C) difference between the supply and return air temperature. The model has a single four-way ceiling supply diffuser located away from the door with a single return placed near the door.

The hydroxyl-generating device was assumed to be installed in a duct above the ceiling, where the hydroxyl radicals and subsequent ROO radicals are formed. Thus, the supply air was assumed to be loaded with the organic oxidants, which eventually reacted with pathogens in the space. The age of air is computed by solving the passive scalar transport equation.[13]

The life of ROO radicals and the aerosolized microorganism kill rate, combined with the age of air, were used to determine the rate of inactivation of infectious aerosols and the resulting spatial variation of radical concentration in the space. CFD analyses were performed to compare the results of dilution ventilation with the reactive organic oxidants. The CFD analysis results were also compared for 2 ach and 3 ach with and without organic oxidants.

The k-omega turbulence model, which is suitable for low Reynolds number recirculating flows, was used to compute the turbulent viscosity of the air. A computational mesh of about 0.75 million hexahedral cells was created by placing fine mesh near the strategic locations. The infectious aerosol release from an infected person is simulated as continuous tracer gas emission. The ventilation performance of each configuration is evaluated using the Spread Index as described below. The probability of infection is evaluated using the Wells–Riley correlation as described below.

Spread Index $(SI)_{TC}$

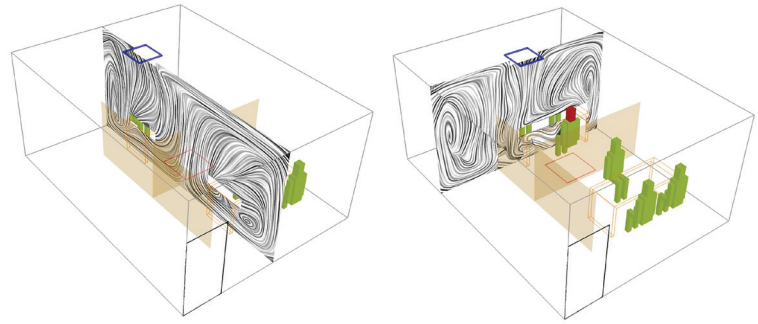
Ventilation performance for each case was analyzed using the Spread Index, which is the ratio of the volume of the space occupied by the infection risk level above a certain value to the total volume of the space.[9] Ideally, the ventilation systems should minimize the spread of contaminants and reduce the probability of infection everywhere in the space. Assuming the target concentration is a safe exposure limit, the ideal $(SI)_{TC}$ should always be close to zero.

The safe level of concentrations can depend on several risk factors including the type and quantities of contaminants or pathogens in the space and their safe exposure limits. Therefore, for each space $(SI)_{TC}$ can be evaluated for various levels of target concentrations and infection levels based on the exposure risk. The organic radical lifetime, kill rate, radical concentration, airflow patterns and the resulting flow paths of airborne

contaminants play an important role in determining the $(SI)_{TC}$ levels in a space.

Spread Index provides a normalized comparison ventilation effectiveness between the dilution ventilation and ventilation with hydroxyl and ROO radicals. In this study, the Spread Index of the probability of infection is set arbitrarily at 10%; hence, $(SI)_{10}$ is evaluated.

FIGURE 3 Airflow patterns in an office space showing large recirculation zones.



Probability of Infection

Infection risk assessment is performed by using the Wells–Riley model, which has been extensively used for quantitative infection risk assessment of respiratory infectious diseases in indoor spaces.[1,9,10] This model as stated in *Equation 1* considers the intake dose of airborne pathogens in terms of the number of infectious quanta (dose that will cause an infection in 63% of a susceptible population) to evaluate the probability of infection

$$P_I = \frac{C}{S} = 1 - exp\left(-\frac{Iqpt}{Q}\right) \quad (1)$$

where P_I is the probability of infection, which is a ratio of the number of infection cases to the number of susceptible persons, I is the number of infectors, p is the pulmonary ventilation rate of a person, q is the quanta generation rate per infector, t is the exposure time interval and Q is the room ventilation rate with clean air.

This model assumes well-mixed conditions and predicts a single number for the infection probability for an entire indoor space and thus ignores the spatial and temporal variations of pathogen concentration in a space. The present study demonstrates that the risk of infection depends on the location of occupants and HVAC configuration of the space.

In the present study the number of infectors (I) was assumed to be one and the exposure time (t) was assumed to be one hour. The quanta generation rate for influenza varies from 2 to 128 quanta per hour. The q value of 60 quanta per hour is assumed, which is most frequently used in the ventilation analysis.[10,11]

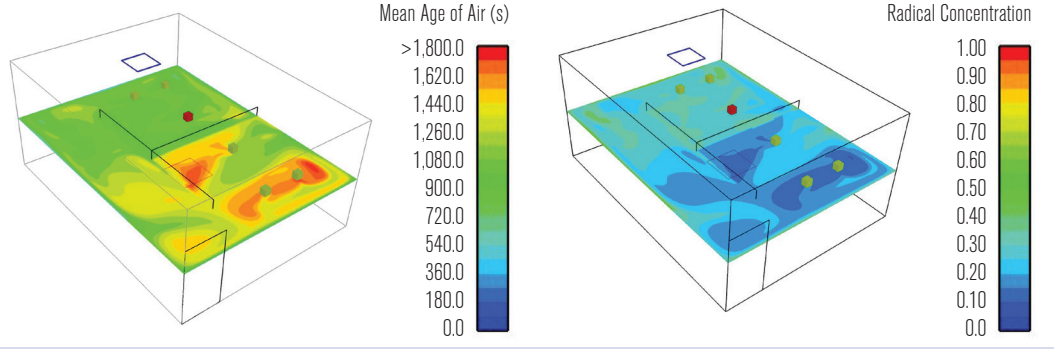
Results and Discussion

Airflow Patterns, Age of Air and Distribution of Organic Oxidants

Figure 3 shows the airflow patterns in the space in two orthogonal vertical planes passing through the center of a supply diffuser. This figure shows that the air exiting the diffuser travels along the ceiling, descends along the walls and moves inward along the floor away from the walls. Such airflow patterns create large recirculation loops along and across the room. These large recirculation zones form inside the cubicles between the room walls and the dividing partitions in the occupied zone. Three-dimensional airflow patterns (not shown here) are quite complex, which promote mixing in the entire space as expected from such diffusers.

Figure 4 shows the resulting distribution of the mean age of air (s) and resulting radical concentration at the center horizontal plane. Under ideal conditions for a single pass flow, for the 3 air changes per hour (h^{-1}) supply airflow rate, the average mean age of air should be 1,200 s (20 min). However, recirculation zones that also promote stagnant zones cause nonuniform distribution of the age of air. The large air recirculation

FIGURE 4 Age of air (s) and resulting radical concentration at a breathing plane at 4.5 ft (1.4 m) from the floor.



zones in the second cubicle, which is close to the door, form a stagnation zone in which the age of air is higher than the average value. Higher values of age of air reduce the concentration of radicals as explained above, which results in relatively lower concentration in the second cubicle.

FIGURE 5 Impact of organic oxidants on the distribution of infection probability at the breathing zone at 4.5 ft (1.4 m) from the floor—ach: 3 h^{-1}.

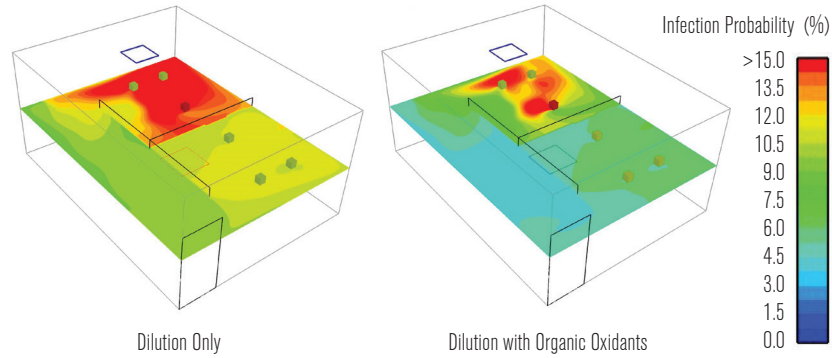
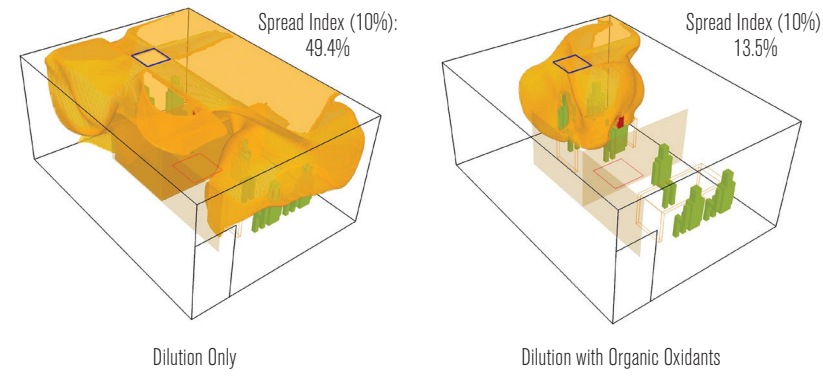


FIGURE 6 Impact of organic oxidants on the Spread Index of probability of infection $(SI)_{10}$ indicating the extent of the space volume at or above the 10% infection probability–ach: 3 h^{-1}.



Probability of Infection and Spread Index

Figures 5 and *6*, respectively, show the resulting risk of infection computed per *Equation 1* at a breathing level and the extent of infection spread in the space above 10% probability. For the case of no organic oxidant (dilution only), the airflow patterns described above create a nonuniform distribution of contaminant concentration with a zone of high infection probability in the vicinity of the infected person. The lowest concentration is in the adjacent corridor. The stagnation of the air in the recirculation zones promotes the accumulation of contaminants. The Spread Index $(SI)_{10}$ is 49.4%, indicating about half the room space is at or above 10% probability of infection. Zones of high and low risk of infection divide the space along the length of the room.

Figures 5 and *6* show that by adding the organic oxidants into the space (dilution with organic oxidants), the risk of infection and the resulting Spread Index $(SI)_{10}$ reduce significantly. The average probability of infection at the breathing plane reduces from 11.3% to 7% (about 38% reduction). Likewise, the Spread Index $(SI)_{10}$ reduces from 49.4% to 13.5% (about 73% reduction) with the zone of high infection shrinking to only the vicinity of an infected individual.

The impact of the organic oxidants ROO is equivalent to 6 ach for dilution ventilation. In spite of the relatively higher concentration of radicals in the vicinity of the infected individual, the highest probability occurs surrounding the infected individual. It indicates that the probability of infection cannot be nullified unless the source of pathogens (an infected individual) is removed from the room.

Effect of Air Change Rates

The effect of supply airflow rate, or ach, was analyzed by comparing infection probability for the case of dilution ventilation with 3 ach with the case of organic oxidants with 2 ach. *Figure 7* shows that by adding the organic oxidants into the supply stream and reducing the ach, the breathing level probability of infection remains almost equivalent or slightly better than the case with dilution ventilation with 3 ach with an equivalent ach of 3.3. Similarly, the resulting Spread Index SI_{10} reduces by almost 25%, limiting the zone of high infection to only the vicinity of the infected individual (*Figure 8*). These results indicate that addition of organic oxidants to the supply airstream can enhance the dilution ventilation by inactivating the infectious aerosols.

Summary and Conclusions

The evaluated hydroxyl technology generates reactive organic oxidant air cleaning agents (ROO radicals) that

can inactivate indoor infectious aerosols and complement traditional dilution ventilation to reduce the risk of pathogen transmission. When the organic oxidants are introduced, the indoor airflow patterns play a crucial role in their distribution. Additionally, the life of the radicals and their respective kill rate are the most important parameters that determine the efficacy of this reactive air cleaning technology. This study, with the help of CFD simulations, systematically evaluated the impact of the ROO organic oxidant radicals on the probability of infection at a breathing zone level and the spread of infection probability in a typical office space with two cubicles.

The analysis predicts that introduction of hydroxyl-generated OH and ROO and radicals into the supply airstream can reduce the average probability of infection at the breathing zone of occupants by about 38% and the zone of the probability of infection (Spread Index, SI_{10}) by 73% with an equivalent ach of 6. The analysis further predicts that the addition of hydroxyl-generated organic oxidants can reduce the required dilution ach by 33%. The efficacy of this hydroxyl technology primarily depends on the concentration and lifespan of the circulating reactive agents and their effective kill rates. Once these parameters are determined with controlled experiments, CFD can help not only in determining the efficacy of the air cleaning technology but also in optimizing HVAC layout and strategic locations for introduction of such reactants to maximize the reduced probability of infection in indoor spaces.

FIGURE 7 Impact of organic oxidants with reduced ach 2 h^{-1} on the distribution of infection probability at the breathing zone at 4.5 ft (1.4 m) from the floor.

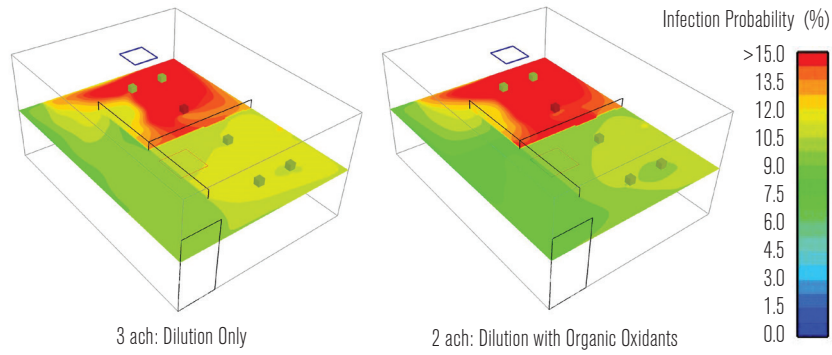
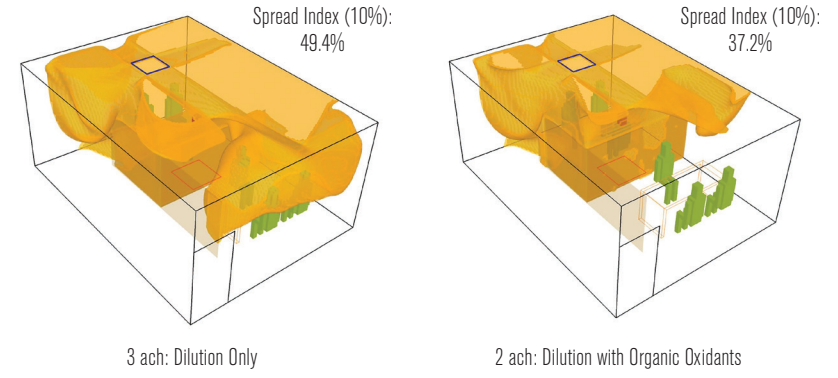


FIGURE 8 Impact of reducing the ach with organic oxidants on the Spread Index of probability of infection $(SI)_{10}$ indicating the extent of the space volume at or above the 10% infection probability.



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