

Assessment of the air purifier manufactured by the company UniqAir in a reference room using CFD simulations for analysis of air flow and respiratory air distribution

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TÜV SÜD Advimo GmbH Technical Advisory Services Sherwin Falsafi Yannick Renaud



Projektbeteiligte

Auftraggeber	UniqAir	
	Maximilianstrasse 16 67346 Speyer	
	Tel. +49 6232 67727 0	
Herr Mika Wilska	Email: mika.wilska@uniqair.de	
Nummerische Simulationen	TÜV SÜD Advimo GmbH	
	Brandsende 2-4 20095 Hamburg T +49 221 500857-19 M +49 170 8319456	
Herr Falsafi	Email: Sherwin Falsafi@tuvsud.com	
Herr Renaud	Email: Yannick.Renaud@tuvsud.com	
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1. Initial situation and task formulation

The company UniqAir has developed an air purifier that can extract and clean polluted aerosols from the air with integrated HEPA H13 and activated carbon filters. Due to the high room air exchange rate and the built-in filter, air purification is supposed to take place so that the risk of contracting coronaviruses is reduced. TÜV SÜD Advimo is to examine this concept by means of 3D flow simulations. For this purpose, as an sample a waiting line in front of a reception desk is simulated and evaluated in terms of breathing air and velocity distributions to examine the extent to which one or two purifiers could cover the room, how the exhaled air is distributed in the room and how much of the exhaled air is captured by the UniqAir purifiers.

1.1 Work procedure

The evaluation of the air conditions that arise within the reference room is carried out with the aid of a 3D flow simulation.

The dimensions and arrangement of the reference room and its occupants and objects are agreed upon in communication with UniqAir. A waiting line in front of a cashier counter is chosen as the reference room and on this basis a 3D CAD model is constructed by TÜV SÜD Advimo. A computational grid was generated and tested for on the CAD model for numerical stability and sufficient numerical accuracy.

Two types of simulations are carried out for the reference room, namely steady-state and transient, each using three arrangements: 1) without any air purifier, 2) with a single air purifier, 3) with two air purifiers. The steady-state simulations serve to obtain the equilibrium conditions in the room after a long period of time, while the transient ones are done to observe the temporal evolution of the air condition in the room. Different breathing models are prescribed for the manikins depending on the simulation. One of the manikins is marked in each simulation as "infected", such that the hazardous exhalation is discerned from normal exhalation. Since the bigger droplets (> 50 µm) produced during breathing/speaking are relatively heavy, they fall down and settle on the floor before complete evaporation. These droplets are neglected in the simulations, as they are more difficult to be vented. The internal function of the purifier devices is not a topic of our assessment and is not simulated. Instead, it is assumed that the 100% of the aerosols inside the air sucked into the device are removed by the implemented filters and other internal mechanisms. Therefore, our simulations are useful to examine the extent to which the provided suction power of the device can capture the aerosol-containing air in this reference room. The results of the simulations are analysed and compared to assess the performance and efficiency of the purifiers.



2. Pre-processing

In this section an overview of the simulation setup and the defined boundary conditions are presented.

2.1 Geometric specifications

Pictures of the simulation domain of the reference room and the arrangement of manikins and objects are presented in Figures 1 and 2. The room has dimensions of 7.05 m×5 m×3 m and include four manikins positioned 1.8 m apart in a line, numbered starting from the rear of the room, a cashier counter (including a separating plexi-glass), a radiator, and air purifier(s). The purifiers are placed at 0.933 m away from the side walls. The manikins and the plexi-glass barrier are 1.698 m and 2.1 m high, respectively.

The manikin geometries are highly simplified to save on cell number during the mesh generation process and reduce the computational effort. The first and second purifiers are coloured by green and pink, respectively. A radiator is placed next to the rear wall to enhance buoyancy-driven advective mixing. The air purifier unit has four separate openings at the top for suction and four at the bottom for supply. The simulation domain is fully closed, that is no door or window is considered in the simulation setup. Therefore air input and output occurs only by respiration process of manikins and filtration process of the purifiers. Breathing of the manikins are modified by replacing the mouth geometry by a mask like extension. Manikin 3 is considered as infected. Therefore the aerosols originating from the infected and healthy manikins are differentiated.



Figure 1: The created CAD model of the reference room





Figure 2: Arrangement of the manikins and objects in the reference room. The infected manikin is marked with red.



Figure 3: Simplified CAD model adopted for manikins. The mouth geometry is replaced by a mask like extension.

2.2 Boundary conditions

Two types of simulations are carried, namely steady-state and transient, each using three arrangements: 1) without any air purifier, 2) with a single air purifier, 3) with two air purifiers. The steady-state simulations serve to obtain the equilibrium conditions in the room after a long period of time and cannot demonstrate the instantaneous behaviour of the system. The transient ones are done to observe the temporal evolution of the air condition in the room. However, due to more computationally demanding nature of transient simulations, they can only be conducted for a rather short duration. In this project, all transient simulations are performed for a duration of five minutes.

2.2.1 Velocity

The prescription of boundary conditions is different for steady-state and transient simulations. The stead-state simulations are initialised from a stationary (motionless) condition. A no slip boundary condition is applied to the surface of all walls and objects in the room, including the manikin bodies. The velocity boundary condition prescribed for the inlet and outlet patches of the air purifier(s) is set at constant flow rate of 330 m³/hr.



For transient simulations, a time-dependent sinusoidal function is adopted for the flow rate a the mouth (with mask extension) patches. This function produces an average air supply of 5.7296 L/min per person. The surface area of the mask extension is roughly 127 cm². Breathing occurs at a frequency of 0.2833 Hz. Considering the surface area of the mask extension, a velocity magnitude of approximately 0.0075 m/s is expected right at the mask. In Figure 4 the prescribed boundary condition for flow rate is shown. For the steady-state simulations, a constant volumetric flow rate equal to 5.7296 L/min is prescribed, as no time-changing behaviour can be considered.



Figure 4: Prescribed flow rate boundary condition for breathing

2.2.2 Temperature

The initial value of temperature of the room air as well as the temperature of the objects during the simulation is set to 20 °C. The surface of manikin bodies are kept at the constant temperature of 30 °C throughout the simulation, while the exhaled air is kept at 34.64 °C. The rear wall of the room is considered a cold wall (in contact with outside environment) with a constant temperature of 18.5 °C. The rest of the walls have a constant temperature of 20 °C. The radiator is set to have a constant temperature of 65 °C.

2.2.3 Concentration

Exhaled and infected air are the two variables considered in our simulation as concentration variables, which are introduced to the solver passive scalars, i.e. they are passively carried with the bulk flow and their concentration is so low that cannot affect the momentum of air flow actively, e.g. via buoyancy. The only source of input of these variable into the domain are from the exhalation of the manikins. The value of concentration is set to 1 [-] on the mask extension patches. The prescribed flow rate discussed in Section 2.2.1 is responsible for transport of the mentioned variables into the domain. Since we do have any knowledge of the volume fraction or concentration of aerosols in the respiratory air based on our literature research, using the analogy introduced in the Section 3.2 it is attempted to scale the concentration values in a rational manner and get a sense of the concentration values.

2.3 Steady-state and transient variants

As mentioned in Section 1.1, three setups are investigated for steady-state and transient simulations, namely with zero, one, and two purifiers. While the setups with one and two purifiers are identical for both steady-state and transient simulations, the zero-purifier setup is slightly different. It is possible for the transient zero-purifier setup to exclude the purifier entirely and only simulate the motion of air caused by breathing of the manikins and thermal buoyancy. However, a steady-state simulation would encounter numerical issues in absence of the purifier, as breathing is constant inflow to the domain and no other numerical outlet is defined, which violates the steady-state assumption. Therefore, for the steady-state zero-purifier simulation, one purifier is placed at the place of the first purifier (see Figure 2), but is only let to operate at 1% part load. Using this approximation, the simulations will yield converged results and the efficiency of the three setups can be compared. Therefore, hereafter the one-purifier setup with 1% part load simulated as steady-state is referred to as zero-purifier, although there is a working (although barely) device is present. The above mentioned setups are shown in Figure 5.



Both simulations are carried out taking the non-isothermal behaviour of the gas into account, i.e. the energy transport equation is solved coupled with the momentum equation. Gas compressibility due to thermal expansion/compression is allowed for using the equation of state of the ideal gas, which means the Boussinesq approximation is avoided. Therefore, the calculations can capture thermal lift as a result of air expansion due to heating. Turbulence was modelled using a linear two-equation eddy viscosity model.



Figure 5: The three setups simulated as transient



3. Results and discussion

3.1 Concentration distribution

The steady-state simulations are conducted to obtain the distributions of concentration of exhaled and infected air after a long period of time, and subsequently calculate the efficiency of the purifiers arrangements. In Figures 6 and 7 the concentration distributions of exhaled and infected air are shown, respectively, and compared for the three setups. In these figures regions containing at least 200 ppm and 80 ppm exhaled and infected air are shown, respectively. These values are uniform among all three setups in each figure to allow compare the spread of the aerosol-containing air. The ppm equivalent values are estimated using the assumptions explained in Section 3.2. In the zero-purifier setup the domain is, as expected, saturated by aerosol-containing air (exhaled or infected) after a long time, since the input into the domain does not exit the domain in any way. It must be noted that we still see saturation of the domain at the zero-purifier setup using a purifier device operating at 1% part load, because the input of aerosol-containing air is significantly higher than the output at the suction patches of the device. Both figures show that the spread of the region with relatively high concentration is reduced by adding more purifiers to the room. They also show that the high concentration region tends to be seen away from the breathing level and close to the ceiling.

In Figures 8 and 9 different concentration thresholds are used for the visualisation of each of the three setups, to be able to have a comparative sense of the resulting concentration levels in the room. It can be seen that for the exhaled air the zero-purifier case yields about roughly 70 times, and the one-purifier case 1.71 times more compared to the two purifier case. For the infected air these values are roughly 50 and 1.2, respectively. Again here for the purifier-containing rooms the high concentration region of the room is located in the middle of the room relatively away from the manikins and close to ceilings, while this is not the case for zero-purifier case.





Figure 6: Region with the concentration of at least ~200 ppm obtained by steady-state simulations; (top) zero-purifier (middle) one purifier (bottom) two-purifiers





Figure 7: Region with the concentration of at least ~80 ppm infected air obtained by steady-state simulations; (top) zero-purifier (middle) one purifier (bottom) two-purifiers





Figure 8: Region with the relatively higher concentration obtained by steady-state simulations; (top) zero-purifier at ~7400 ppm (middle) one purifier at ~180 ppm (bottom) two-purifiers at ~105 ppm





Figure 9: Region with the relatively higher concentration obtained by steady-state simulations; (top) zero-purifier at ~2000 ppm (middle) one purifier at ~48 ppm (bottom) two-purifiers at ~40 ppm

The distributions concentration of exhaled air of the three setups on the breathing level cutplane (~1.55 m), obtained from steady-state simulations are shown in Figure 10. The scaling of contour colours is unified. Here the values of concentration are not converted to ppm, and instead only the original value of the passive scalar is reported. Nevertheless, the influence of adding purifiers to the room is quite clear. Comparing the resulting fields, the following conclusions can be drawn: First, adding even a single purifier significantly reduces the concentration of exhaled air. Second, the positioning of the purifiers in close proximity to manikin No. 3 causes a slightly more spread in front of it. Third, the plexi-glass barrier serves to block the propagation of the exhaled air of manikin 3 towards manikin 4 and proves effective at containment of the spread of the unfiltered air. Since a unified scaling is applied here, the range of the concentrations of the setups cannot be directly compared. The range of concentration values on the breathing level is as follows:

• Zero purifier: 18.2% - 18.8%



- One-purifier: 0.327% 0.587%
- Two-purifiers: 0.148% 0.518%

Based on the given values, the significant drop of the concentrations on the crucial breathing level is evident.





Exhaled Air Concentration [-] 0.0025 0.003 0.0035 0.004 0.0045 0.005 0.0055 0.006



Exhaled Air Concentration [-] 0.0025 0.003 0.0035 0.004 0.0045 0.005 0.0055 0.006



Exhaled Air Concentration [-] 0.0025 0.003 0.0035 0.004 0.0045 0.005 0.005 0.006

Figure 10: The distributions concentration of exhaled air on the breathing level cut-plane (~1.55 m), obtained from steady-state simulations; (top) zero-purifier (middle) one purifier (bottom) two-purifiers



3.2 Scaling of the concentration variables

It is not possible to directly evaluate the amount of aerosol in the air, since evaporation, condensation and speech/breathing patterns, etc. affect the values. Furthermore, to our knowledge no body of literature is available, in which the concentration levels of virus particles or the volume fraction of aerosols in respiratory air are reported. Therefore, we adopt a simple method to scale the values of passive scalars to obtain rational concentration levels. Exhaled air contains roughly 4% CO₂ while exiting the mouth. Since there are well-established air quality regulations in place for the CO₂ content of the air, we assume that the aerosols occupy the same fraction of the exhaled air which can be used as a reference value to obtain an estimate for aerosol concentration.

3.3 Filtration efficiency and resulting equilibrium concentrations for the purified cases

On the basis of the assumption presented in Section 3.2, the filtration efficiency of the one- and two-purifier cases can be estimated as presented in Table 1 by calculating the accumulation of the passive scalars in the domain based on the input and output through corresponding boundaries.

Table 1: Estimation of the filtration efficiency of the purified cases

	Filtration Efficiency Exhaled air [%]	Filtration Efficiency Infected air [%]	
one UniqAir purifier	93.51	93.27	
two UniqAir purifiers	94.38	93.84	

This table shows that using a single purifier roughly 93.5% of the exhaled air passive scalar is filtered, that is gets sucked into the purifier. The filtration of the infected air happens with a similar efficiency (93.27%). This is a noteworthy observation, because the proximity of the purifier device(s) to the infected person does not affect the filtration efficiency significantly. This observation could be explained by the fact that the air flow is mostly upwards due to the buoyancy of the warmed air by the radiator, breathing of the manikins and their thermal plumes, which induces air circulation from the ceiling towards the floor adjacent to the walls.

Considering the mass balancing of the passive scalars and the filtration efficiency, the total fractions and concentrations of the unfiltered exhaled and infected air are calculated and reported in Table 2. Here the ppm values fall below the recommended value of 1000 ppm (IRK 2008, UBA 2017). However, comparing the values reported in Tables 1 and 2 for one- and two-purifier cases shows only slight improvement of filtration efficiency by adding an extra purifier. Therefore, we could expect that a single purifier should be enough for this specific reference room considering the dimensions and number of occupants.

Table 2: Estimation of the filtration efficiency of the purified cases

	Unfiltered fraction		Equilibrium concentrations	
	Exhaled air [%]	Infected air [%]	Exhaled air [ppm]	Infected air [ppm]
one UniqAir purifier	0.065	0.067	649	673
two UniqAir purifiers	0.056	0.062	562	616



3.4 Estimation of the required time for adequate filtration of the aerosols

Two transient simulations, are used two estimate the time it takes a single purifier to extract the aerosols from the air. The instantaneous concentration contours of these simulations are used to create videos that show the variation of the exhaled air in the domain over time. These videos have been previously delivered to UniqAir to accompany the presentation slides. The first case is a zero-purifier case initialised from a fully clean state, which is performed for 300 seconds and leads to spread of the aerosol containing exhaled air in the entire room. The final results of the first simulations is considered as a contaminated room, which are then used as the initial conditions of the second case with one air purifier. This scenario is similar to a room, where the occupants are breathing with the purifier is turned off, and after 5 minutes the purifier is turned on and the concentration is measure for 5 minutes after the purifier is started. The video of the purified case show gradual reduction of the exhaled air in the room.

The values of total amount of exhaled air in the domain is measure at each 30 seconds until the end of the simulation. These measurements shows a linear drop in the amount of the exhaled air. Since running the simulation until the room is adequately clean is not feasible, the measurements in the first minutes are extrapolated to get an estimate for the time it takes a purifier to sufficiently clean the room. The result of this extrapolation is presented in Figure 11. The extrapolation shows that after 22 minutes the purifier sufficiently cleans the room. It must be noted that the assumption of the linear drop of the amount of exhaled air in the domain after 5 minutes has not been proven by our simulations. Therefore, the real required time filtration time could be higher, in case the behaviour becomes asymptotic after 5 minutes.



Figure 11: Extrapolation of the measured amounts of exhaled air in the domain in the five minutes of a transient simulation.

3.5 Velocity distribution

The distributions of velocity magnitude of the three setups on the breathing level cut-plane (~1.55 m), obtained from steady-state simulations are shown in Figure 12. Introducing UniqAir purifiers to the room increases overall mixing. At the breathing level compared to the room without purifiers the increase in velocity magnitude is for the one-purifier and two-purifier cases roughly 60% and 85%, respectively. This mixing is however not found to cause a chaotic spread of the aerosols in the room, since the high velocity flow occurs mostly close to walls an away from the middle of the room, where the manikins breath.









Velocity Magnitude [m/s] 0 0.05 0.1 0.15 0.2 0.25





Figure 12: Distributions of velocity magnitude of the three setups on the breathing level cut-plane (~1.55 m), obtained from steady-state simulations; (top) zero-purifier (middle) one purifier (bottom) two-purifiers



3.6 Quality of air

In order to assess the local freshness of the air in the reference room, the so called "Age of Air" variable is calculated. The age of air is the time duration that a parcel of air entering from a fresh air inlet patch, here only the purifier supply air openings, has resided in the domain. It can be used to calculate the air-change effectiveness of the room ventilation and identifying the dead zones. Using this variable, the age of air of the purified cases are visualised for the freshest 65% region of the room in Figure 13. These results are obtained using transient simulations after a duration of 300 s. Therefore, the blue region contains the air that is at most 200 s old.

Adding the purifiers introduces fresh air at the supply level close to floor, which is then deflected upwards after colliding with the walls. Although the increase in the portion of the fresh air two purifiers is significantly larger, it must be noted that excluded region containing the "old air" is not necessarily contaminated. These visualisations show the manner of supplying of clean air to the room. Comparing the distribution of fresh air in the lateral and longitudinal directions show that placing the UniqAir purifiers away from the walls make them more effective at providing fresh air.





Figure 13: The freshest 35% part of the room evaluated by age of air variable; (top) one-purifier case (bottom) two-purifier case



4. Summary and conclusions

The performance of the UniqAir purifier is assessed using CFD Simulations in a reference room, which includes three manikins in a waiting line in front of a cashier counter. Two sets of simulations of the reference room are carried out, namely steady-state and transient, on three cases, a room without any purifier, and rooms with one and one with two purifiers.

In this investigation the full-load operating mode is considered for the purifiers, which provides the room with about 3.1 h^{-1} and 6.4 h^{-1} air exchange rates for the one-purifier and two-purifier rooms, respectively. Since the simulation of the inner mechanisms of the device has not been the subject of this investigation, assuming a 100% internal filtration efficiency, the devices are found to improve the overall air quality by removing the aerosol-containing exhaled air.

Comparing the equilibrium concentration levels of the purifier-equipped room, with an unequipped room, it was found that adding a purifier can extract about 94% of the aerosol-containing air. Adding an extra purifier was found to slightly improve the air quality.

In absence of well-established evaluation methods, the concentration of CO_2 in the exhaled air is used as a reference value to scale the passive scalars and obtain values for concentrations of exhaled and infected air. The calculated concentrations of both scenarios are below the recommended value of 1000 ppm (according to IRK 2008, UBA 2017).

The positioning of the UniqAir purifiers is important, as placement too closed to walls or other large obstacles is expected to hinder the optimal performance of the device.

Considering the assumed room size and assuming the CO₂ analogy, one device can potentially provide sufficient purification. Further simulations could confirm and further optimise the effectiveness of the ventilation concept for other rooms with different sizes or arrangements.