Novel computational tool for indoor air quality.

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Abstract. This article introduces a novel computational tool for analysing concentrations of particles and gaseous impurities in mechanically ventilated indoor spaces. The computation routine exploits mass balance model assuming well-mixed conditions, and accounts for the most significant means of entry and loss of contaminants. The analysis inputs include time-dependent outdoor concentrations, indoor generation rates, filtration efficiencies and deposition rates. The model was validated using size resolved particle concentrations measured during an experimental campaign. The predicted indoor concentrations were in good correlation with experimental data over wide particle size range. To demonstrate the computational capabilities, indoor concentrations of particles and carbon dioxide were analysed with various combinations of supply air filtration efficiency, ventilation rate, recirculation ratio, air purifiers, and occupancy. Subsequently, a relative sick leave estimate based on time-averaged exposure to total particle mass concentrations was computed. The results emphasised the effectiveness of supply air filtration to limit the exposure to ambient air pollution. Replacing a coarse filter with a high efficiency filter resulted in reduction of an order of magnitude in the relative sick leave estimate. In comparison, increasing recirculation ratio or exploiting air purifiers demonstrated noticeable, but lesser impact.

Keywords. Indoor air quality, Modelling, Ventilation, Filtration, Air purifier, Morbidity, Sick leave.

1. Introduction

The World Health Organization (WHO) has recognised air pollution as the most significant environmental threat to human health and WHO Global Air Quality Guidelines (AQG) estimated ambient and indoor air pollution to annually cause 7 million premature deaths and loss of hundreds of millions of healthy years (WHO, 2021). Furthermore, the World Bank estimated that in 2013, air-pollution-related welfare losses corresponded to 2.2 to 7.5 percent of regional gross domestic product, which globally amounted to $5.11 trillion, and global labour income losses of $225 billion (The World Bank & Institute for Health Metrics and Evaluation, 2016). The World Bank reported that from 1990 to 2013, welfare and labour income losses have increased by almost 100 and 40 percent, respectively. Moreover, the report highlighted that by 2013, approximately 87 percent of the global population was living in areas where air pollution exceeded WHO Air Quality Guidelines of that time, which have tightened since.

Considering the notable health and economic burden of air pollution, reducing the exposure is of utmost importance. Exposure to air pollution can occur both outdoors and indoors. As people spend up to 90% of their time indoors (Klepeis et al., 2001), reducing exposure to contaminants in indoor environments can significantly impact total exposure.

The outdoor contaminants consist of particulate matter and gaseous compounds, which can reach indoor spaces along supply air or through building envelope. Substantial evidence exists to support the efficacy of ventilation as a means of airborne contamination control (Sundell et al., 2011). Therefore, efficient supply air filtration and tight building envelope constitute important aspects of providing good indoor air quality (IAQ).

However, keeping ambient air pollution out may not be sufficient to guarantee good indoor air quality as contaminants may also be generated indoors. For example, cooking and burning in a fireplace generate particles whereas carbon dioxide and volatile organic compounds (VOCs) are generated through exhalation and typically from building materials, respectively.

Considering the complexities related to assessing IAQ, the design process requires tools to compare various options and to quantify their benefits. However, few tools exist for modelling IAQ dynamics with respect to local conditions and custom requirements, and especially for quantifying costs and benefits of each option. Local ambient air quality, climate and weather conditions, as well as occupancy and indoor activities, significantly affect the requirements for heating, ventilation, and air conditioning (HVAC) systems. Furthermore, COVID-19 pandemic and current energy crisis have highlighted the need for resilient design solutions both in terms of health safety and energy efficiency.

This article introduces a novel computational tool for IAQ analysis. The approach enables computing time dependent concentrations of size resolved particles and gaseous impurities in mechanically ventilated indoor spaces. The computation routine exploits mass balance model assuming well-mixed conditions, and accounts for the most significant means of entry and loss of contaminants: Entry with supply air or by penetrating the building envelope, and removal by exhaust air, air purification, and for particles also deposition, are considered. The computational methodology utilises time-varying ambient air pollution levels and indoor generation rates of size resolved particle concentration and gaseous pollutant concentrations. As a result, time dependent indoor concentrations can be obtained and exploited in further analyses

The computational capabilities of the novel tool were demonstrated by computing concentrations for fine particles and carbon dioxide with various combinations of supply air filtration efficiency, ventilation rate, recirculation ratio, air purifiers, and occupancy. Additionally, the relative sick leave estimates based on time-averaged particle concentrations were computed.

2. Methods

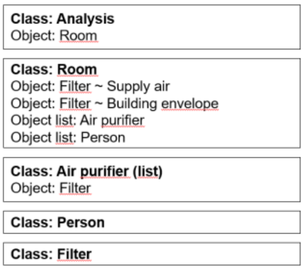
The methodology description for this study consists of two parts. In the first part, the implementation of the calculation tool is presented, whereas the second part discusses the validation methodology and analyses conducted to evaluate indoor air quality and its effects on the occupants, namely sick leave prevalence, in various settings.

2.1 Calculation tool

The calculation tool has been implemented using an object-oriented python code, which both facilitates modular modelling approach and enables capability extension in the future. The tool consists of several classes representing various aspects related to the IAQ analysis. Figure 1 shows the hierarchy within the analysis and the following sections introduce the contents of each class and the inputs they require.

Figure 1

Description of the classes and hierarchy of the objects in the computational tool.



Class: Analysis
Object: Room

Class: Room
Object: Filter ~ Supply air
Object: Filter ~ Building envelope
Object list: Air purifier
Object list: Person

Class: Air purifier (list)
Object: Filter

Class: Person

Class: Filter

2.1.1 Filter. The *Filter* class contains the information related to filtration efficiencies for various particle sizes. The name of each particle bin in the data, represents the average diameter of the particle within the respective bin. The data is stored in a dictionary the bin name being the key and the respective filtration efficiency is stored as a value. The current implementation does not support filtration of gaseous contaminants.

2.1.2 Air purifier. The *Air Purifier* class exploits the *Filter* object to quantify the filtration efficiency of the air purifier. Additionally, airflow rate needs to be specified for the air purifier to compute its clean air delivery rate (CADR)

$$CADR(d) = q_{AP}E_{AP}(d), \tag{1}$$

where q_{AP} and $E_{AP}(d)$ denote the airflow rate through the air purifier and the filtration efficiency of the filter in the air purifier, respectively.

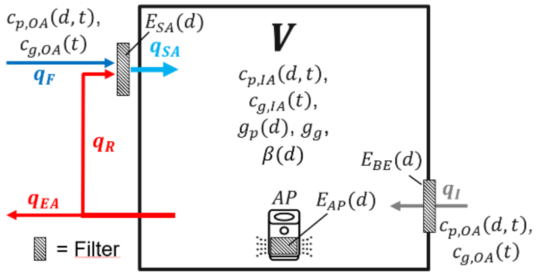
2.1.3 Person. The *Person* class characterises an occupant within the space of interest. It specifies the carbon dioxide and particle (bioaerosol) generation rates from an individual person and allows persons to have different generation rate from each other.

2.1.4 Room. The *Room* class combines all the information related to the space to be analysed. The basic information to describe the space consists of floor area and room height. Additionally, *Persons* and *Air Purifiers* can be assigned to the space, and *Filter* objects are exploited to describe both the supply air filtration and penetration through the building envelope. To characterise the ventilation system, airflow rates for fresh air, recirculation and infiltration need to be specified. The supply air filtration is applied to both fresh and recirculated air.

2.1.5 Analysis. The A*nalysis* class contains all the computation routines and its object-oriented implementation facilitates running several analyses with varied inputs. The inputs for the analysis consist of a *Room* object and contaminant data. For particles, both generation and deposition rates are specified along with initial indoor concentration and time-dependent outdoor concentration. All particle data is given in a particle size resolved format. For each gaseous contaminant, indoor generation rate, initial concentration and time-dependent outdoor concentrations are specified.

The analysis itself consists of computation routines for both particle and gaseous contaminant concentrations, and handlers for data inputs and outputs. Figure 2 provides a schematic representation of the analysis.

Figure 2
Schematic representation of the computational tool for a space with volume V.



The computation of particle concentration is based on mass balance model assuming well-mixed conditions within the space of interest. The mass balance equation for particles can be written as (Riley et al., 2002)

$$\begin{aligned}\frac{V\,dc_{p,IA}(d,t)}{dt} &= q_F c_{p,OA}(d,t)(1-E_{SA}(d)) \\ &+ q_R c_{p,IA}(d,t)(1-E_{SA}(d)) \\ &+ q_I c_{p,OA}(d,t)(1-E_{BE}(d)) \\ &- (q_F+q_R+q_I)\cdot c_{p,IA}(d,t) \\ &+ g_{gen}(d) - g_{loss}(d),\end{aligned} \tag{2}$$

where V, $c_{p,IA}(d,t)$, $c_{p,OA}(d,t)$, q_F, q_R, q_I, $E_{SA}(d)$, $E_{BE}(d)$, $g_{gen}(d)$ and $g_{loss}(d)$ denote the volume of the room, the indoor concentration, the outdoor concentration, the fresh air delivery rate, the recirculation airflow rate, the infiltration airflow rate, the supply air filtration efficiency, the building envelope filtration efficiency, the generation rate, and the loss rate, respectively.

Because of time-dependent outdoor concentration $c_{p,OA}(d,t)$, the indoor particle concentration cannot be solved from the equation (2) in a closed form. Therefore, the computation routine exploits numerical methods for time stepping to resolve the concentration. The concentration at time t_{i+1} can be solved as

$$c_{p,IA}(d,t_{i+1}) = c_{p,IA}(d,t_i) + \Delta c_{p,IA}(d,t_i), \tag{3}$$

and the term $\Delta c_{p,IA}(d,t_i)$ can be expressed as

$$\Delta c_{p,IA}(d,t_i) = \left(f_{p,SA} + f_{p,EA} + f_{p,LA} + f_{p,AP} + g_{p,gen} + g_{p,dep}\right)\cdot\frac{\Delta t}{V}, \tag{4}$$

where the supply air particle flux can be written as

$$f_{p,SA} = \left(q_F\cdot c_{p,OA}(d,t_i) + q_R\cdot c_{p,IA}(d,t_i)\right)\cdot(1-E_{SA}(d)), \tag{5}$$

the extract air particle flux as

$$f_{p,EA} = -(q_F+q_R+q_{LA})\cdot c_{p,IA}(d,t_i), \tag{6}$$

the particle flux through building envelope as

$$f_{p,LA} = q_{LA}\cdot c_{p,OA}(d,t_i)\cdot(1-E_{BE}(d)), \tag{7}$$

the particle flux removed by air purifiers as

$$f_{p,AP} = -c_{p,IA}(d,t_i)\cdot CADR(d), \tag{8}$$

and the particle deposition flux as

$$g_{p,dep} = \beta(d)\cdot c_{p,IA}(d,t_i)\cdot V, \tag{9}$$

where $\beta(d)$ denotes the size-dependent deposition rates. Finally, $g_{p,gen}(d)$, Δt, and V denote the particle generation rate, the time step, and the volume of the room, respectively.

Similarly, the gaseous contaminant concentrations can be solved numerically and the concentration at time t_{i+1} can be written as

$$c_{g,IA}(t_{i+1}) = c_{g,IA}(t_i) + \Delta c_{g,IA}(t_i), \tag{10}$$

and the term $\Delta c_{g,IA}(t_i)$ can be expressed as

$$\Delta c_{g,IA}(t_i) = \left(f_{g,SA} + f_{g,EA} + f_{g,LA} + g_{g,gen}\right)\cdot\frac{\Delta t}{V}, \tag{11}$$

where supply air gaseous contaminant flux can be written as

$$f_{g,SA} = \left(q_F\cdot c_{g,OA}(t_i) + q_R\cdot c_{g,IA}(t_i)\right), \tag{12}$$

the extract air gaseous contaminant flux as

$$f_{g,EA} = -(q_F+q_R+q_{LA})\cdot c_{g,IA}(t_i), \tag{13}$$

and the gaseous contaminant flux through building envelope as

$$f_{g,LA} = q_{LA}\cdot c_{g,OA}(t_i). \tag{14}$$

Finally, $g_{g,gen}$, Δt and V denote the gaseous contaminant generation rate, the time step, and the volume of the room.

After having solved particle and gaseous contaminant concentrations for all time steps, they are stored in an output file for further processing.

2.1.6 Processing the concentration data.

The analysis outputs raw concentration data which is processed using another python code to compute time-averaged concentrations and indoor-to-outdoor concentration ratios (I/O ratios), converting particle number concentration to mass concentrations, and calculating the relative sick leave estimates.

The particle number concentration is converted into particle mass concentration using the average particle diameter to compute the mass concentration for each particle bin as

$$c_{p,m} = c_{p,n}\rho_p\left(\frac{4\pi}{3}\left(\frac{d_p}{2}\right)^3\right), \tag{15}$$

where $c_{p,m}$, $c_{p,n}$, ρ_p, and d_p denote particle mass concentration, particle number concentration, particle density, and bin average particle diameter, respectively. For all analyses, the particle density was assumed to be 1000 kg/m^3. The total mass concentration is computed based on the mass concentrations computed for each bin. Additionally, mass concentrations for PM1, PM2.5, PM4 and PM10 are computed.

Finally, the relative sick leave estimate, in days per person per year, can be computed as (Salmela et al., 2017) based on earlier work by (Seppänen & Fisk, 2006)

$$SIC_p = 0.3108 \cdot c_{p,mtot}^{0.674}, \tag{16}$$

where $c_{p,mtot}$ denotes the time-averaged total particle mass concentration in the indoor environment. The model assumes that 60 percent of the ventilation related sick leaves are due to exposure to particles (Salmela et al., 2017). The relative sick leave estimate can be written as

$$SIC_{rp} = \frac{SIC_p}{d_{work}}, \tag{17}$$

where d_{work} refers to the number of working days in a year. In this study the number working days per year was assumed to be 220.

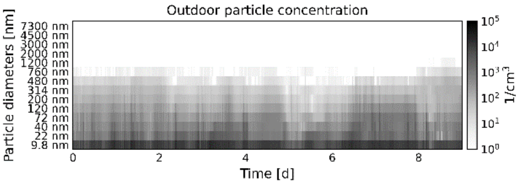
2.2 Validation and analyses

The calculation procedure was validated using experimental data obtained from a measurement campaign carried out in an office space located in Helsinki city centre. The volume of the office space was 66 m^3 with a floor area of 25 m^2. The supply airflow rate was constant and equivalent to five air exchanges per hour (5 ACH) with recirculation ratio of 0.6.

During a two-week period, both outdoor and indoor particle number concentrations were monitored. The experimental campaign and its results are detailed by Kulmala et al. (2022) and Silvonen et al. (2022). Figure 3 shows the time-dependent size resolved particle concentration for outdoor air. Outdoor carbon dioxide concentration was not monitored and was assumed to be constant 425 ppm. The supply air filtration efficiency was measured on-site with an optical particle counter (Palas Fidas Frog), and the filtration efficiency was determined to correspond to F7 class filter according to the standard EN 779 (European Standard EN, 2012). Furthermore, the infiltration airflow rate ($q_I = 19$ m^3/h) through the building envelope was determined processing the measurement data according to the methodology presented by Kulmala et al., (2020). The building envelope penetration was estimated using data from literature as reported by Kulmala et al., (2022).

Figure 3

Outdoor particle concentration during the monitoring period.



After having completed the validation of calculation procedure, the model was used to evaluate indoor air quality in various scenarios. The office space from the measurement campaign was used for these analyses with varying supply air filtration options, recirculation ratios and ventilation rates. Furthermore, the effect of air purifiers on the indoor particle concentration was analysed.

During the measurement campaign, the office space was unoccupied, however, in the analyses following the validation, it was assumed that there were four occupants in the space. The occupants were assumed not to generate particles, but to generate carbon dioxide at a constant rate of 5.0e-6 m3/s, which corresponds to breathing rate of 6 litres per minute typical for light office work.

2.2.1 Supply air filtration. The effect of supply air filtration on indoor particle concentration was studied with filters ranging from G4 to H13 class according to the standards EN 779 (European Standard EN, 2012) and EN 1822 (European Standard EN, 2019a) using typical filtration efficiencies for clean filters. Apart from supply air filtration, other parameters were kept constant compared to the validation case.

2.2.2 Recirculation ratio. The effect of recirculation ratio on indoor particle concentration was studied at four recirculation rates $R = \{0.6, 0.4, 0.2, 0.0\}$. The other parameters were kept equal to the validation case.

2.2.3 Air purifier. The effect of air purifiers on the indoor particle concentration was studied in a scenario in which the performance of a class G4 supply air filter was boosted by air purifiers with constant airflow rate equal to twice the fresh air delivery rate. The recirculation ratio was assumed zero ($R = 0.0$) for these analyses. Three variants of the air purifier with filtration units of classes F7, E10 and H13 were analysed. Additionally, the effect of increasing CADR was studied comparing air purification performance of multiple air purifying units equipped with a F7 class filter.

2.2.4 Ventilation rate. Contaminant concentrations were compared with various ventilation rates corresponding to different categories in the standard EN 16798 assuming low polluting building (European Standard EN, 2019b). Table 1 presents the resulting ventilation rates. Additionally, leakage flow rate was assumed negligible for this case to simplify the computation and no air recirculation was used. The indoor air quality was analysed both in terms of particle and carbon dioxide concentrations. The ventilation rates were calculated as

$$q_{EN16798} = N_{person} \cdot q_{person} + A_{room} \cdot q_{room}, \qquad (18)$$

where N_{person}, q_{person}, A_{room}, and q_{room} denote the number of persons in the room, the ventilation rate per person (m^3/h), the room floor area (m^2), and the ventilation rate per floor area (m^3/h/m^2), respectively (European Standard EN, 2019b).

Table 1

Ventilation rates corresponding to EN 16798 categories for the studied space with four occupants.

Category	Supply airflow rate [m3/h]
I	234.0
II	163.8
III	93.6
IV	63.0

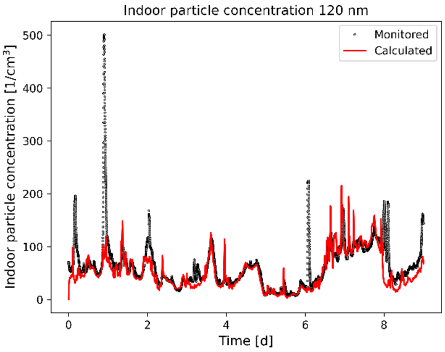
3. Results

3.1 Calculation tool validation

The modelled particle concentrations show good correlation to the monitored data for particle size range up to 760 nm. For larger particle sizes, the monitored concentrations for both outdoor and indoor air were low and intermittent, thus the data are not sufficient for an accurate analysis. Figure 4 presents an example of the validation results for 120 nm particle size.

Figure 4

Particle number concentrations for monitored and modelled data show good correlation.



3.2 Supply air filtration

The results of the comparison show that supply air filtration can efficiently reduce indoor particle concentrations. Figure 5 highlights the differences in the filter performance between coarse filter (class G4) and more efficient filter options.

Figure 5

Particle indoor-to-outdoor concentration ratios for various supply air filtrations options.

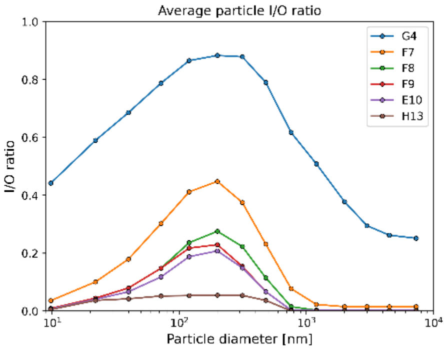
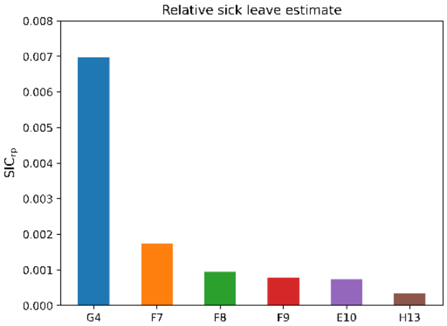


Figure 6 presents the relative sick leave estimates for different supply air filtration options and shows that efficient filtration can significantly reduce the exposure to ambient air pollution in indoor spaces, and subsequently the resulting sick leaves.

Figure 6

Relative sick leave estimate for various supply air filtration options.



3.3 Recirculation ratio

The comparison on the recirculation ratios reveals that increasing recirculation ratio results in reduced indoor particle concentration when combined with an efficient F7 class supply air filtration. Figure 7 and Figure ***8*** show the reductions in I/O ratio and sick leave estimate, respectively, as the recirculation ratio increases.

Figure 7

Particle indoor-to-outdoor concentration ratios for various recirculation ratios.

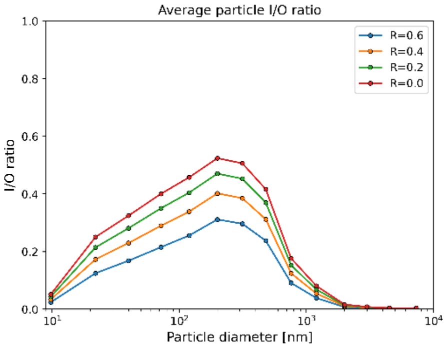
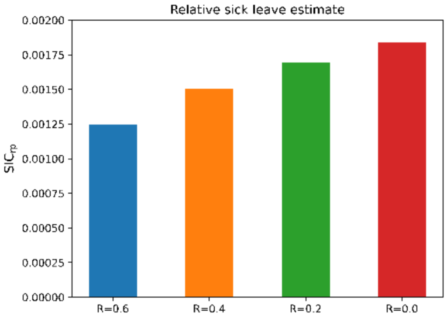


Figure 8

Relative sick leave estimate for various recirculation ratios.



3.4 Air purifier

Figure 9 shows that air purifiers can significantly reduce the indoor particle concentrations in the case where supply air filter is coarse class G4. Equipping an air purifier with higher efficiency filter reduces the indoor particle concentrations. Nevertheless, increasing the number of air purifier units equipped with F7 class filter decreases the I/O ratio more efficiently, apart from the most penetrating particle sizes. Additionally, the marginal benefit of an added air purifier reduces as the number of units increases.

Figure 9

Particle indoor-to-outdoor concentration ratios without and with air purifier with varying filtration efficiencies.

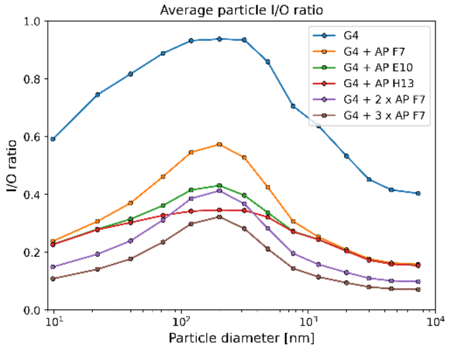
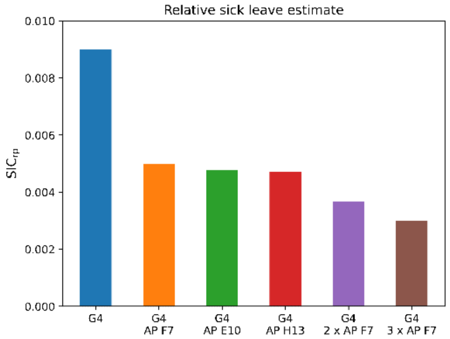


Figure 10 shows that air purifiers significantly decrease the sick leave estimate, however, adding more efficient filtration to the air purifying unit seems to have limited benefit, whereas increasing the amount of air purifier units, or CADR, is a more effective solution.

Figure 10

Relative sick leave estimate without and with air purifier with varying filtration efficiencies



3.5 Ventilation rate

In contrast to insignificant differences in indoor particle concentrations, Figure 13 shows substantial increases in the resulting carbon dioxide concentrations as the ventilation rate is gradually decreased from category I to category IV. This results from the fact that the carbon dioxide sources, the four occupants, are within the analysed space.

Figure *11* shows that the particle concentration I/O ratios for the ventilations rates corresponding to the EN 16798 categories I-IV are almost identical, which is an expected result as outdoor concentrations and supply air filtration efficiencies (F7 class) are identical in the analyses, and there are no indoor particle sources. Furthermore, the sick leave estimates in Figure 12 also show very similar values for all categories.

In contrast to insignificant differences in indoor particle concentrations, Figure 13 shows substantial increases in the resulting carbon dioxide concentrations as the ventilation rate is gradually decreased from category I to category IV. This results

from the fact that the carbon dioxide sources, the four occupants, are within the analysed space.

Figure 11

Particle indoor-to-outdoor concentration ratios for different EN 16798 ventilation categories.

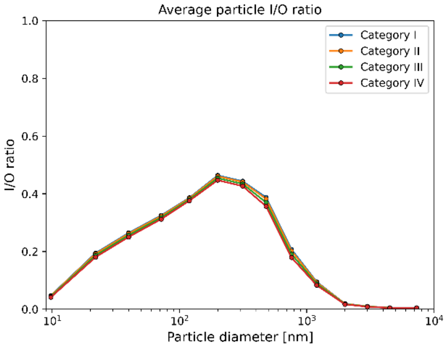


Figure 12

Relative sick leave estimate for different EN 16798 ventilation categories.

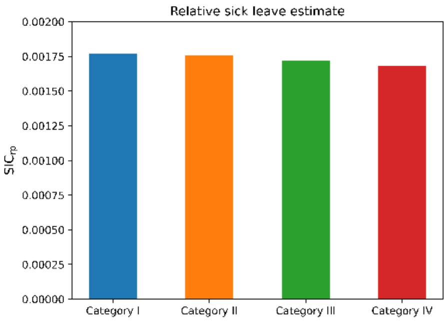
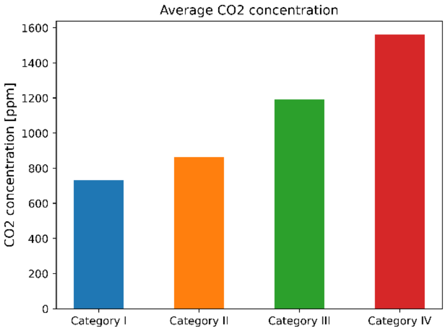


Figure 13

Carbon dioxide concentrations for different EN 16798 ventilation categories.



4. Discussion

The results confirm that supply air filtration is an efficient means to reduce the indoor particulate matter originating from ambient air pollution. The relative sick leave estimate decreased by an order of magnitude when a coarse filter was replaced by a high efficiency filter in the analysis. However, retrofitting an improved supply air filtration unit might not be a straightforward task. Typically, higher efficiency filters have higher pressure loss, which might result in HVAC system being unable to deliver the required amount fresh air, or at least, the system requires more energy to produce equal airflow rate.

If ventilation system cannot be retrofitted with high-efficiency filter, air purifiers may provide an effective solution to reduce indoor particle concentration. However, air purifiers should be considered as a temporary solution to occasional periods of poor ambient air quality, such as pollen season or dust storms, rather than a permanent solution. They are also useful in pandemic situations when the indoor concentration of pathogens, such as SARS-CoV-2 viruses, need to be reduced.

Additionally, the results show the effect of various recirculation ratios on the indoor air quality. Like air purifiers, air recirculation with high-efficiency supply air filtration can significantly reduce the indoor particle concentration.

Even though particulate impurities can be filtered from the air, the fresh air delivery rate needs to be sufficient to provide enough fresh air for the occupants in the space. As the results of this study show, the carbon dioxide concentrations within the space vary significantly depending on the fresh air delivery rate. It has been shown that elevated carbon dioxide concentrations impair the cognitive performance, therefore, providing fresh air is important to support better learning outcomes at schools and increased productivity at workplaces (Wargocki & Wyon, 2017).

The relative sick leave estimates provide an insight to the health effects of particulate air pollution. This is an important aspect from cost-benefit point of view. It will be easier to justify investments in IAQ improvements if quantitative evidence exists to support their benefits. In the current approach, total particle mass concentrations were used to compute the relative sick leave estimates. However, it has been well documented that finest particles sizes pose the greatest danger (EUROVENT, 2022; WHO, 2021). Therefore, it would be important to separately study the effects of PM1, PM2.5, PM4 and PM10 instead of just focusing on total PM concentration. In addition to particulate matter, future research should scrutinise the health effects of other contaminants typically found in indoor environments.

The results indicate that the developed tool can be highly useful for investigating various means to achieve desired IAQ. For example, the tool can be used to design a supply air filtration concept with specific IAQ requirements considering local ambient air quality. Alternatively, the tool can be used to study the concentrations of gaseous contaminants, such as carbon dioxide, formaldehyde, and ozone, originating from both outdoor and indoor sources, or to evaluate airborne infection probability indoors.

Even though the tool has proved its usefulness in various scenarios, the current implementation has some limitations. Firstly, the analysis is limited to single indoor space assuming a well-mixed state, which might not be an accurate representation of contaminant dispersion in a wide-open space. Secondly, the infiltration flow rate is considered constant and needs to be explicitly specified. Thirdly, the occupancy of the space is considered constant, which is not a realistic assumption for multiday analyses. Finally, the current implementation does not provide capabilities for cost-benefit analyses.

In future research, the current shortcomings in the modelling are to be resolved. Furthermore, the modelling capabilities are to be extended to enable evaluation of HVAC system energy performance, and analysis with demand-controlled ventilation systems.

Finally, it should be noted that the analyses presented in this study were conducted using data from Helsinki, where the ambient air pollution is relatively low compared to many other locations in the world. Therefore, the benefits from the mitigation measures could be significantly greater elsewhere.

5. Conclusion

This study aimed to develop a novel computational tool for characterising particulate and gaseous contaminant concentration in indoor spaces. The validation results show good correlation with experimental data on a wide range of particle sizes. Additionally, several analyses were conducted to demonstrate the capabilities of the tool. The results reflect the factors affecting indoor contaminant concentrations, efficiency of mitigation measures, exposure levels in indoor spaces and their potential effect on health.

In the future, both the costs and the benefits of indoor air quality need to be considered more broadly to provide insight to the most cost-efficient means to improve IAQ. Additionally, the energy efficiency, resilience and sustainability of such approaches must be evaluated. Furthermore, the results highlight the importance of cross-disciplinary research to better connect the exposure to airborne contaminants to its effects both in short and long term.

6. Acknowledgements

This study was funded by the Business Finland project Future Spaces (grant number: 33250).

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