An analytical approach for evaluating the concentrations of multiple generic air contaminants in EnergyPlus simulations.

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Abstract

The study of the concentration of indoor air pollution has become central to devising ventilation strategies that can improve the indoor air quality. Since the strategies used for ventilation and air filtration have an impact on thermal comfort and the energy used, the simulation of air pollutants has been integrated into energy modelling tools such as EnergyPlus. However, EnergyPlus runs simulations that can output only one air contaminant beside carbon dioxide. This paper presents a novel approach to enable EnergyPlus to output the concentrations of multiple air contaminants using equations scripted into EnergyPlus via the Energy Management System.

Highlights

- When compared to EnergyPlus results, the analytical approach proposed in the study could generate estimates for indoor air contaminants levels that are within an acceptable margin of error.
- The precision of the results generated using the method proposed seem to be impacted by the outdoor air inflow rate.
- The precision of the air contaminantion estimates can be slightly affected by the zone geometry.

Introduction

There is a growing interest in assessing indoor air quality (IAQ) in the built environment due to its significant impact on people's health and wellbeing, which has been of particular relevance in light of the recent COVID-19 pandemic (Lewis, Alastair C et al., 2022; World Bank, 2020; World Health Organization, 2010). This study aims to present an analytical approach that helps to evaluate the concentrations of multiple indoor air contaminants and can be deployed to implement ventilation operation controls accordingly in EnergyPlus simulations.

Since it performs complex air flow calculations in each timestep to calculate the energy balance, EnergyPlus has also been used and validated for the assessment of air contaminants concentrations and flow rates (Taylor et al., 2014). However, beside calculating carbon dioxide (CO_2) concentrations, EnergyPlus is limited to performing the calculations for only one generic air contaminant (GC) of outdoor origin that should be selected by the program user per simulation. Since indoor air quality can require a thorough and simultaneous consideration for multiple contaminants such as $PM_{2.5}$, PM_{10}, NO_x, Ozone, etc., performing multiple air contaminant evaluations can be implemented by methods such as co-simulation (performing another simulation in parallel to EnergyPlus to assess IAQ using another specialized tool like CONTAM) or iterative EnergyPlus simulations (running the simulation many times and evaluating an alternative contaminant in each iteration).

Regarding co-simulation, since CONTAM is a steady state air transfer modelling tool, coupling EnergyPlus with CONTAM is impeded by several interoperability issues of the two programs especially at feeding in the EnergyPlus model data into CONTAM in every simulation timestep (Dols et al., 2016; Justo Alonso et al., 2022). It is also challenging to override the EnergyPlus ventilation control to respond to the air quality results generated by CONTAM.

On the other hand, many issues would arise as a result to iterative EnergyPlus simulations to simulated multiple air contaminants, one contaminant per iteration. One main issue is the amplification of the computation power required. The other issue is the difficulty to make responsive ventilation controls that can consider all the contaminants simultaneously as the controls applied in the last iteration will override the previous ones.

Other studies have suggested post-processing EnergyPlus models to evaluate the levels for multiple generic contaminants simultaneously (Taylor et al., 2014). Such approach is effective at evaluating multiple air contaminants but might not support implementing IAQ-based HVAC controls.

In contrast to the methods available, the approach proposed in this study is based on implementing air balance equations in every simulation timestep to calculate the concentrations of indoor air contaminants of outdoor origin. The method should enable the simultaneous simulation of multiple air contaminants, enable application of responsive IAQ-based HVAC controls through Energy Management System (EMS) actuators, and hence facilitate building performance optimisation where the consideration of the trade-offs in energy consumption versus indoor air quality is required.

The focus on pollution from outdoor origin in this study stems from the existing availability of multiple indoor origin contaminants' simulation in EnergyPlus, the significant contribution of outdoor contaminants to indoor air quality levels (Leung, 2015), their impacts on health and mortality rates (Sang et al., 2022; World Bank, 2020), and the ready access to monitored outdoor pollution levels that could be used in this study. While the scope of this study focuses on $PM_{2.5}$, as an example of generic outdoor pollutants, the methodology however is applicable to other outdoor pollutants following the approach proposed.

Another reason to focus on contaminants from outdoor sources is that they require ventilation controls that contradict the default controls for providing a certain amount of outdoor air to reduce CO_2 levels (Clausen, 2003). For instance, introducing outdoor fresh air can reduce CO_2 levels and the pollution from indoor sources, but it will also increase the pollution from outdoor sources. Consequently, the study of pollutants of outdoor origin helps with optimising the default HVAC controls to balance the levels of the competing indoor/ outdoor contaminants.

Methods

In this study, the Energy Management System (EMS, a scripting tool within EnergyPlus) was used to calculate the concentration of indoor contaminants from outdoor sources. The calculation methodology was based on the principles of mass balance (Wallace & Hobbs, 2006) and adapted from contaminant concentration presented in the EnergyPlus Engineering Reference (U.S. Department of Energy, 2022). The EnergyPlus version used for simulation and EMS scripting in this study was 9.6.

With the calculations for the generic contaminants (and CO_2 for subsidiary understanding and validation for the analytical approach) in place, accomplishing acceptable margins of error against other validated methods would indicate that the script can be generalised to calculate the concentrations of any other contaminant given the outdoor concentration schedule and the deposition rate.

Generic contaminant (GC) calculation

As shown in Equation 5, the concentration of an indoor air contaminant (GC_{in}^{t}) at a certain timestep t in a certain building zone would be equal to the concentration of the contaminant in the previous timestep (GC_{in}^{t-1}) minus the change in contaminant concentration due to deposition (GC_{d}^{t}) plus the change in the contaminant concentration due to the air flow from outdoors ($GC_{o/i}^{t}$). If looking at contaminants of indoor origin, a term that evaluates the change in indoor pollution due to indoor sources at every timestep ($GC_{i/i}^{t}$) can be added to this equation, but this was assumed to be equal to zero in this study.

Equations 1-4 are sub-calculations that provide the input for Equation 5. Equation 1 shows the calculation of the air change rate for the contaminant deposition (ach_d) which is the contaminant deposition velocity (v_d), multiplied by 3600 for unit conversion from seconds to hours, multiplied by the total surface area of the zone (A_{tot}) and divided by the volume of the zone (Vol). Equation 2 is used to derive the change in pollutant concentration due to deposition (GC_{d}^{t}) which is based on the contaminant concentration in the previous timestep (GC_{in}^{t-1}) and the contaminant deposition air change rate (ach_d).

Equation 3 shows that the total air change rate at a certain timestep (ach_{tot}^{t}) is the summation of the air changes due to natural ventilation (ach_{nat}^{t}), mechanical ventilation (ach_{mech}^{t}), and infiltration/ exfiltration (ach_{inf}^{t}). Inter-zonal air exchange is assumed to be equal to zero and would be neglected in this case. Equation 4 shows that the change of contaminant concentration due to outdoor air flow ($GC_{o/i}^{t}$) is based on the concentration of outdoor pollution at a certain timestep (GC_{out}^{t}) and the total air change rate (ach_{tot}^{t}). Since the study focuses on indoor air contamination from outdoor sources, the contaminant concentration for the very first timestep GC_{in}^{0} was assumed to be equal to zero.

$$ach_d = v_d * 3600 * A_{tot}/Vol \quad (1)$$

$$GC_d^t = GC_{in}^{t-1} * \frac{ach_d}{1+ach_d} \quad (2)$$

$$ach_{tot}^t = ach_{nat}^t + ach_{mech}^t + ach_{inf}^t \quad (3)$$

$$GC_{o/i}^t = GC_{out}^t * \frac{ach_{tot}^t}{1+ach_{tot}^t} \quad (4)$$

$$GC_{in}^t = GC_{in}^{t-1} - GC_d^t + GC_{o/i}^t \quad (5)$$

These equations have been written using an EMS program to output the generic contaminant concentration at every timestep and the outputs were compared to the concentrations simulated in EnergyPlus using the same inputs of outdoor air conditions and contaminant deposition velocity.

Model inputs and workflow

Python was used to do all the back-end calculations and to conduct the EMS script. To do so, EMS sensors were defined to capture the air change rates for natural ventilation, mechanical ventilation, and infiltration in every timestep. The calculations for the zone volume and sum of the internal surface areas required to derive contaminant deposition air change rate were implemented using Eppy, a Python package that is used to read, edit, and run EnergyPlus files.

The main model inputs to implement the calculations are the outdoor air contaminant concentrations and the contaminant deposition rate. A deposition velocity of 0.000075 m/s for the GC ($PM_{2.5}$ is chosen in this study) has been assumed based on the literature (Liu et al., 2018). Real data for outdoor $PM_{2.5}$ concentrations monitored in Cairo received directly from the Ministry of Environmental Affairs in Egypt was used in the study. Two ways to input the outdoor contaminant concentration schedule were assessed:

1. A constant schedule with an annual mean outdoor contaminant concentration value.
2. A fluctuating hourly schedule with real data for outdoor contaminant concentration over a year.

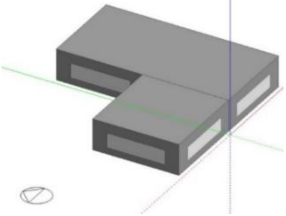

Figure 1: The two-zone shoebox model tested- modelled in DesignBuilder.

Data for ambient (outdoor) $PM_{2.5}$ concentrations have been collected from three weather stations in Cairo, Egypt, from January to December 2021. To eliminate the outliers and smoothen the hourly fluctuations, a Python script was used to derive and use the geometric mean of the hourly reading at the three stations combined.

A shoebox model that consisted of two adjacent zones with different sizes (10 x 20 m and 10 x 10 m, height = 3 m) was used to test the calculation method, shown in Figure 1. Trying to investigate the method caveats, the model consisted of two zones to see if the accuracy of the analytical approach will remain consistent across the zones or the zone geometry would rather have an impact on the accuracy of the script. The generated hourly outputs for annual simulations using the EMS script equations were compared against the EnergyPlus native outputs that resulted from the same inputs. A summary for the workflow is illustrated in Figure 2.

The following inputs for the HVAC/ air flow controls in the model were assumed:

- HVAC template: packaged terminal air conditioner (PTAC) with heating and cooling coils.
- Mechanical ventilation was available during occupancy hours. Outdoor air flow rate was equal to 10 liter/second/person.
- Natural ventilation was available through operable windows (95% of the window area can be opened). Wind pressure and occupancy schedules were taken into consideration as natural ventilation was modelled using DesignBuilder's default settings for the "By Zone" scheduled ventilation method while the maximum natural ventilation rate was assumed to be 5 ACH (DesignBuilder, 2022).
- Ventilation operation mode was mixed-mode (natural ventilation is turned off when cooling or heating is on).
- Cooling and heating setpoints were 24 and 18°C.
- The weather file chosen was the Cairo International Airport EnergyPlus weather file (epw).
- Occupancy density and schedules were set to follow the "Generic Office Area", a default standard EnergyPlus schedule for offices used to input an occupancy density of $0.111\, people/m2$.
- Variable infiltration rates that range from 0.5 ACH to 20 ACH have been tested with a step increment of 0.5 ACH from 0.5 ACH up to 5 ACH, and an increment of 5 ACH from 5 up to 20 ACH.

The choice of the HVAC equipment installed here (the PTAC template) is redundant to the study as the contaminantion levels should only be attributed to the ventilation strategy (intended outdoor airflow), infiltration/exfiltration rates (unintanded outdoor airflow). The HVAC equipment might only have an impact on the results in case relevant air filters are modelled to reduce the contamination levels but this is not the case in this study. The assumptions for natural and mechanical ventilation were settled for the different scenarios, but multiple values for infiltration were tested. This is because air infiltration here can be the most significant constituent and a convenient proxy for a variable total outdoor airflow as there is no need to change the three parameters that constitute the total outdoor air flow at the same time. Moreover, infiltration rates are likely to be the best way to test the caveats EMS script on a wide range for outdoor airflow scenarios as infiltration has a high variability range, assumed from 0.5 ACH to 20 ACH, and it is active on 24/7, unlike natural and mechanical ventilation that don't work simultaneously in a mixed-mode scenario, and will not be reaching significant air change values under typical conditions. This is illustrated in more detail in the results section.

Regarding the details of the EMS script, the calling point for the script was set to be "AfterPredictorAfter-HVACManagers", a calling point that executes the script during every simulation timestep and comes after the HVAC components have been sized and the air flow components have been modelled but before reporting the results, which makes this calling point convenient for implementing HVAC control actions that would override the default HVAC operation modelled in EnergyPlus. The number of timesteps used in the model was 6 timesteps per hour.

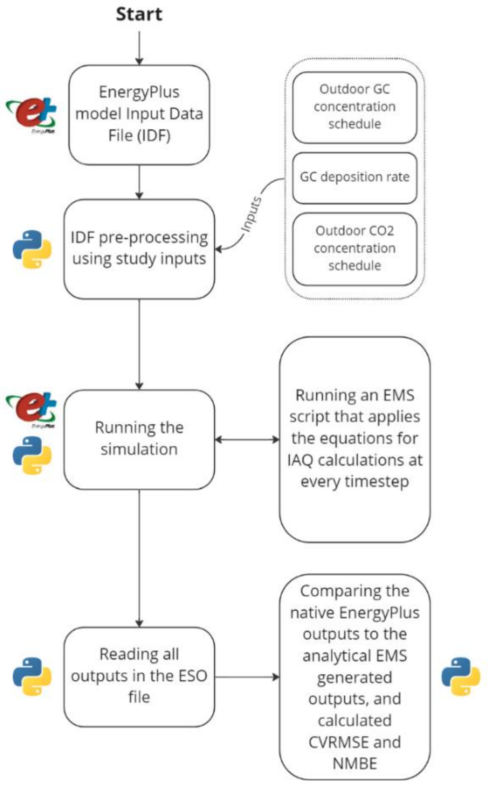

Figure 2: Summary of the study workflow

Validation method

Inspired by the concept of energy model calibration, a process where a simulated energy model is modified until it becomes representative of the actual metered performance, the calibration thresholds for errors were used in this study to check whether the method proposed can produce results within an acceptable margin of error in comparison to another validated simulation method. The acceptable threshold for calibration error set by ASHRAE Guide 14, shown in Table 1, was used in this study.

Both indices shown in the table quantify the difference between the reference data (EnergyPlus results in this case) and the estimated data (the analytical EMS script results).

The calculations for the error indicators: coefficient of variance of the root mean sqaure error (CVRMSE) and the normalised mean bias error (NMBE), are illustrated in by equations 6 and 7 where y_i and y_i' are the tested and the reference values at datapoint i, y'_{mean} is the annual mean for the reference values, and n is the number of datapoints ($n = 12$ for monthly calibration, and $n = 8760$ for hourly calibration). For a calibration exercise, meeting the requirements for either monthly calibration or hourly calibration should be sufficient. In contrast to NMBE, CVRMSE has a higher threshold because over estimated and underestimated results by the method proposed will not be cancelling each other as shown in Equation 6.

Table 1: Acceptable error for model calibration according to ASHRAE Guide 14

	Monthly data	Hourly data
CVRMSE	≤ 15%	≤ 30%
NMBE	≤ ±5%	≤ ±10%

$$CVRMSE = \frac{\sqrt{\frac{\sum_i (y_i - y_i')^2}{n}}}{y'_{mean}} * 100 \tag{6}$$

$$NMBE = \frac{\sum_i (y_i - y_i')}{n * y'_{mean}} * 100 \tag{7}$$

CO$_2$ calculation

For subsidiary validation for the approach, the same workflow but with different equations was applied to evaluate the level on indoor CO$_2$ and the results were compared to the results generated from EnergyPlus. The Equations 8-11 were used to calculate the concentration of CO$_2$ in a zone at every timestep ($CO2^t_{in}$).

$$CO2^t_{o/i} = CO2^t_{out} * \frac{ach^t_{tot}}{1 + ach^t_{tot}} \tag{8}$$

$$G_{ach-p} = GR_{people} * \frac{3600}{Vol} \tag{9}$$

$$CO2^t_{people} = G_{ach-p} * ER_{people} * n^t_{people} \tag{10}$$

$$CO2^t_{in} = CO2^{t-1}_{in} + CO2^t_{o/i} + CO2^t_{people} \tag{11}$$

As shown in Equation 11, the concentration of CO$_2$ ($CO2^t_{in}$) is equal to the sum of the CO$_2$ concentration in the previous timestep, the change of CO$_2$ due to the air entering the building from outside through ventilation and infiltration ($CO2^t_{o/i}$), and the additional CO$_2$ emitted from the occupants ($CO2^t_{people}$). Equation 8 shows that the CO$_2$ generated from outdoor sources ($CO2^t_{o/i}$) is based on the outdoor CO$_2$ concentration ($CO2^t_{out}$) assumed to be a fixed value during the simulation at $400 ppm$, and the total air changes in the building (ach^t_{tot}) already calculated in Equation 3.

Equation 10 shows that the CO$_2$ generated from the people ($CO2^t_{people}$) is the product of three terms:

1. The CO$_2$ generation air change rate from a person (G_{ach-p}). This is calculated in Equation 9 by multiplying the CO$_2$ generation rate of people (GR_{people}) by 3600 (for unit conversion from seconds to hours) and divided by the zone volume (Vol). The CO$_2$ generation rate for people was assumed to be the EnergyPlus default value of $0.0000000382\ m3/(W.s)$.
2. The CO$_2$ emission rate of people (ER_{people}) which was assumed to be $35{,}000\ ppm$. The normal range is between $35{,}000\ ppm$ and $50{,}000\ ppm$ (WSU, 2013).
3. The number of people inside the zone at a certain time (n^t_{people}), a number the script can derive from any EnergyPlus model by scanning the "People" EnergyPlus objects related to every zones.

Results

First, the combination of the intended outdoor air flow (mixed mode ventilation during occupancy hours according to the assumptions discussed in the methods section) created a monthly average of intended air flow rate of less than 0.6 ACH, shown in Figure 3. Given that infiltration rates in this study would range from 0.5 ACH to 20 ACH, the resulting outdoor air flow combination confirms that the infiltration rates will be more decisive in defining the total outdoor air flow, and testing the robustness of the script on various infiltration scenarios can be a sufficient proxy for a varying outdoor flow.

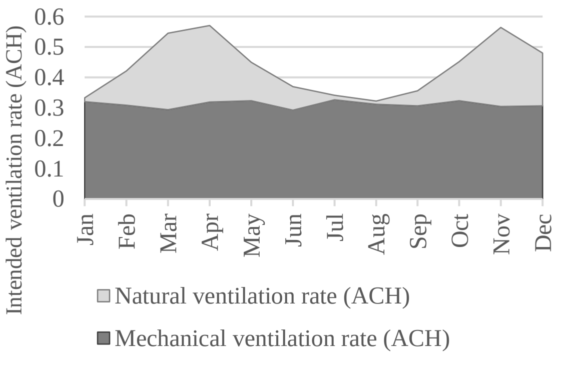

Figure 3: The monthly average values for the combinations of mechanical and natural ventilation air change rates

The results shown in Table 2 indicate that the analytical EMS script used to calculate the concentrations of the generic contaminant has achieved satisfactory margins of error in comparison to the EnergyPlus generated results. Table 2 shows the monthly and hourly error evaluations for all scenarios tested (different infiltration scenarios and different methods for inputting the outdoor GC levels). The table values highlighted in light red have failed to pass the error threshold criteria. The table shows the results for both zones, but only Zone 1 results are shown in the graphs.

Table 2: Percentages of error (monthly and hourly CVRMSE and NMBE) for the GC and CO_2 results generated using the analytical EMS approach in comparison to the EnergyPlus results- red cells failed to meet the acceptable threshold.

Monthly data comparison results (Target: CVRMSE≤ 15%, NMBE≤ ±5%)															
Zone	**Data**	**Error Indicator**	**Infiltration air change rates (ACH)**												
			0.5	**1**	**1.5**	**2**	**2.5**	**3**	**3.5**	**4**	**4.5**	**5**	**10**	**15**	**20**
Zone 1	**GC-Hourly**	**CVRMSE**	6.78%	4.65%	3.49%	2.80%	2.34%	2.00%	1.76%	1.56%	1.41%	1.28%	0.67%	0.46%	0.34%
		NMBE	6.49%	4.46%	3.35%	2.69%	2.24%	1.92%	1.69%	1.50%	1.35%	1.23%	0.65%	0.44%	0.33%
	GC-Mean	**CVRMSE**	6.09%	4.26%	3.23%	2.60%	2.18%	1.88%	1.65%	1.47%	1.32%	1.20%	0.63%	0.43%	0.32%
		NMBE	6.09%	4.26%	3.23%	2.60%	2.18%	1.87%	1.65%	1.46%	1.32%	1.20%	0.63%	0.43%	0.32%
	CO_2	**CVRMSE**	3.09%	1.64%	3.03%	4.20%	5.06%	5.75%	6.31%	6.74%	7.11%	7.42%	9.10%	9.78%	10.13%
		NMBE	2.08%	1.11%	2.90%	4.13%	5.02%	5.71%	6.27%	6.71%	7.08%	7.40%	9.08%	9.76%	10.11%
Zone 2	**GC-Hourly**	**CVRMSE**	4.19%	3.03%	2.31%	1.87%	1.58%	1.35%	1.19%	1.06%	0.96%	0.87%	0.46%	0.31%	0.24%
		NMBE	4.01%	2.91%	2.22%	1.80%	1.51%	1.30%	1.15%	1.02%	0.92%	0.84%	0.45%	0.30%	0.23%
	GC-Mean	**CVRMSE**	3.68%	2.73%	2.12%	1.72%	1.45%	1.25%	1.10%	0.98%	0.89%	0.81%	0.43%	0.29%	0.22%
		NMBE	3.67%	2.73%	2.12%	1.72%	1.45%	1.25%	1.10%	0.98%	0.89%	0.81%	0.43%	0.29%	0.22%
	CO_2	**CVRMSE**	3.18%	1.79%	3.14%	4.26%	5.10%	5.77%	6.33%	6.75%	7.12%	7.43%	9.10%	9.78%	10.13%
		NMBE	2.01%	1.18%	2.98%	4.18%	5.05%	5.73%	6.29%	6.72%	7.09%	7.41%	9.08%	9.76%	10.11%
Hourly data comparison results (Target: CVRMSE≤ 30%, NMBE≤ ±10%)															
Zone	**Data**	**Error Indicator**	**Infiltration air change rates (ACH)**												
			0.5	**1**	**1.5**	**2**	**2.5**	**3**	**3.5**	**4**	**4.5**	**5**	**10**	**15**	**20**
Zone 1	**GC-Hourly**	**CVRMSE**	9.54%	6.22%	4.64%	3.72%	3.10%	2.66%	2.34%	2.08%	1.88%	1.72%	0.94%	0.67%	0.54%
		NMBE	6.50%	4.46%	3.35%	2.69%	2.25%	1.93%	1.69%	1.50%	1.36%	1.24%	0.65%	0.44%	0.34%
	GC-Mean	**CVRMSE**	7.30%	4.54%	3.35%	2.67%	2.22%	1.90%	1.66%	1.48%	1.33%	1.21%	0.64%	0.43%	0.33%
		NMBE	6.09%	4.27%	3.24%	2.61%	2.18%	1.88%	1.65%	1.47%	1.32%	1.21%	0.64%	0.43%	0.33%
	CO_2	**CVRMSE**	10.84%	7.38%	7.50%	8.57%	9.61%	10.57%	11.39%	12.11%	12.70%	13.22%	16.09%	17.26%	17.89%
		NMBE	2.43%	0.88%	2.71%	3.95%	4.85%	5.54%	6.10%	6.56%	6.93%	7.25%	8.95%	9.62%	9.98%
Zone 2	**GC-Hourly**	**CVRMSE**	7.15%	4.68%	3.54%	2.87%	2.41%	2.08%	1.83%	1.64%	1.49%	1.36%	0.76%	0.56%	0.46%
		NMBE	4.02%	2.91%	2.23%	1.80%	1.52%	1.31%	1.15%	1.02%	0.93%	0.84%	0.45%	0.31%	0.23%
	GC-Mean	**CVRMSE**	5.30%	3.06%	2.24%	1.78%	1.49%	1.27%	1.12%	1.00%	0.90%	0.82%	0.43%	0.29%	0.22%
		NMBE	3.67%	2.74%	2.12%	1.72%	1.45%	1.25%	1.10%	0.99%	0.89%	0.81%	0.43%	0.29%	0.22%
	CO_2	**CVRMSE**	11.03%	7.54%	7.70%	8.69%	9.70%	10.63%	11.45%	12.13%	12.73%	13.24%	16.09%	17.26%	17.89%
		NMBE	2.36%	0.96%	2.78%	4.00%	4.88%	5.57%	6.12%	6.56%	6.94%	7.26%	8.95%	9.62%	9.98%

The table results denote that the generic contaminant levels evaluated in both zones- and generated using either the varying outdoor GC data or the fixed GC outdoor annual mean methods- have achieved CVRMSE values that ranged from 0.22% to 6.78% for the monthly data comparison as shown in Figure 4, which is much less than the acceptable threshold of 15%. However, NMBE values for GC levels generated by the script for Zone 1 were around 6% for the 0.5 ACH infiltration rate scenario as shown in Figure 5, which fails to meet the acceptable NMBE criteria for the monthly data comparison of 5%.

Although the error results for both zones are within the same range, Zone 2 have passed the monthly NMBE check for the 0.5 ACH infiltration scenario. This indicates that the zone geometry might have a slight impact on the precision of the results. This can be attributed to the geometry-specific deposition air change rates calculated in each zone based on the zone's total surface areas.

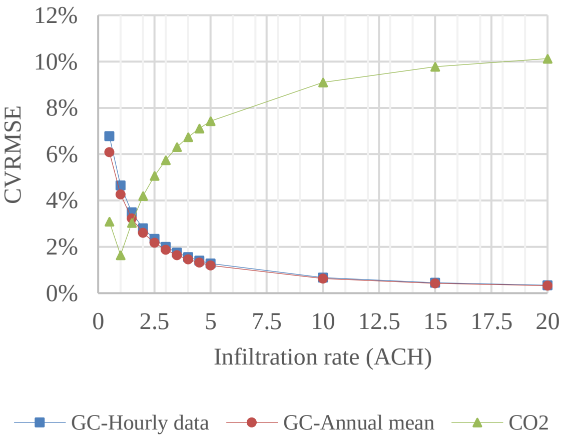

Figure 4: Monthly CVRMSE for GC and CO_2 in Zone 1

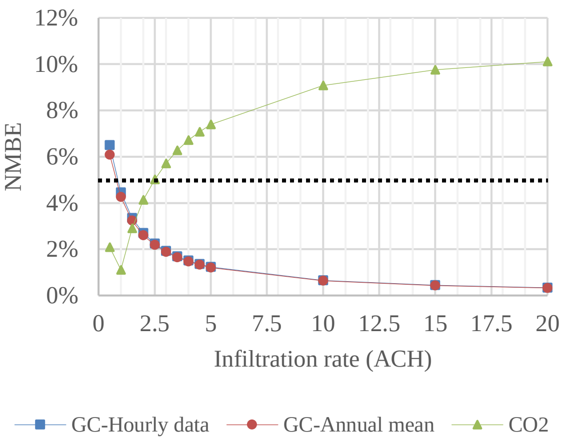

Figure 5: Monthly NMBE for GC and CO_2 in Zone 1

Figures 4-7 all indicate a clear relationship between the error value and the amount of outdoor air flowing into the building. The more the outdoor air flow, the less the error in the GC level estimates, and the higher the error in the CO_2 level estimates. This trend in the results mean that the error value tends to decrease for all contaminants (including CO_2) if the contamination levels are high. High contamination levels for GC of outdoor origin occur when the building allows more outdoor air, while high CO_2 levels (and other GC of indoor origin) occur when the building is not permitting air to escape the building. Although having errors is not good in general, it is a good sign when these errors will only be occurring when the contaminants levels are low which is low risk.

Regarding the CO_2 levels evaluated using the script, all scenarios with infiltration rates higher than 2 ACH have failed to meet the monthly NMBE criteria. It can be noticed that the monthly CVRMSE and NMBE values for CO_2 data are almost equal which means that there is a consistent (monotonic) miscalculation of CO_2 levels (either consistent underestimation or overestimation of CO_2 levels). The positive sign for NMBE indicates that the EMS script tends to overestimate CO_2 consistently, and the error tends to increase when more outdoor air is allowed into the building.

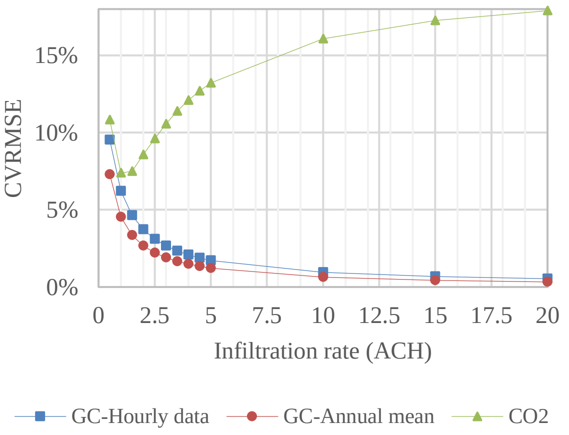

Figure 6: Hourly CVRMSE for GC and CO_2 in Zone 1

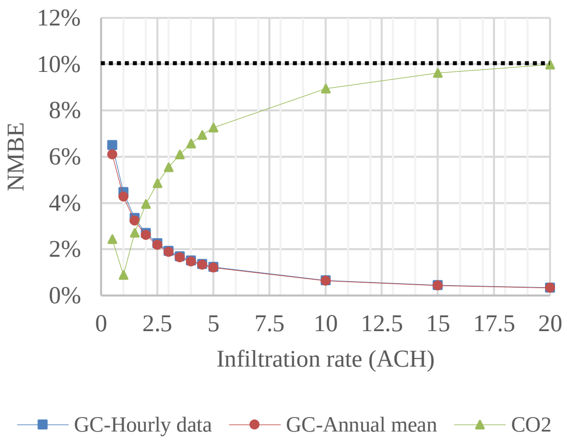

Figure 7: Hourly NMBE for GC and CO_2 in Zone 1

Looking at the error values for the hourly data comparisons shown in Table 2 and Figures 6 and 7, it can be found that all scenarios tested for GC and CO_2 evaluation in both zones have met the CVRMSE and NMBE criteria of ≤30% and ≤±10% respectively. This can be attributed to the higher error threshold permitted for the hourly data comparisons. This means that the EMS script can be reliable since it has passed the hourly data comparison criteria. This is valid especially for the calculations of GC of outdoor origin as the error values were far below the acceptable threshold for hourly data comparison and have almost passed the monthly data comparison as well.

A comparison between the annual simulation for hourly GC values generated using the analytical EMS script vs the EnergyPlus values is shown in Figure 8. The results displayed belong to Zone 1, and the inputs were varying hourly outdoor contaminant concentrations while the infiltration rate was set to an average air change rate in Cairo at near 6.14 ACH (Raafat et al., 2023). Figure 9 shows a zoomed in version of Figure 8 that focuses on one week in January where significant fluctuations in the GC ($PM_{2.5}$) have occurred. Both figures indicate that the EMS script produce almost identical results to EnergyPlus.

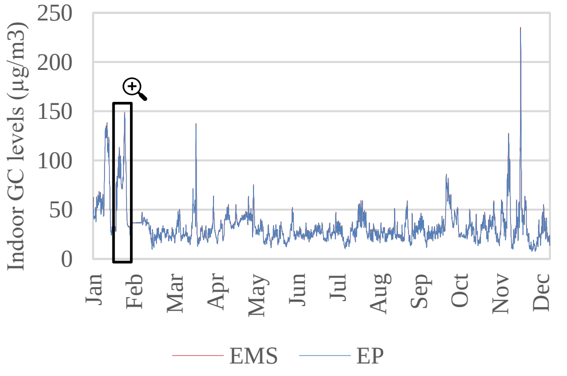

Figure 8: Annual simulation showing hourly GC levels for Zone 1 measured using the analytical approach (EMS) and EnergyPlus (EP), at infiltration rate= 6.14 ACH, input method for outdoor GC level was variable hourly rates

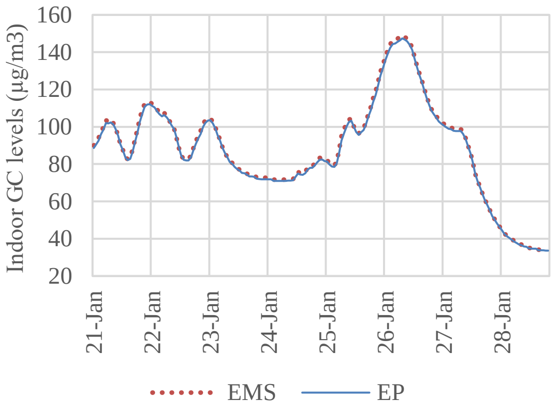

Figure 9: One week simulation showing hourly GC levels for Zone 1 measured using the analytical approach (EMS) and EnergyPlus (EP), at infiltration rate= 6.14 ACH, input method for outdoor GC level was variable hourly rates

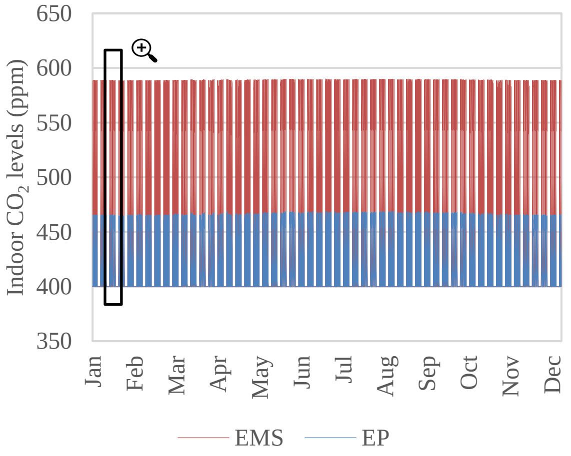

Figure 10: Annual simulation showing hourly CO_2 levels for Zone 1 measured using the analytical approach (EMS) and EnergyPlus (EP), at infiltration rate= 6.14 ACH

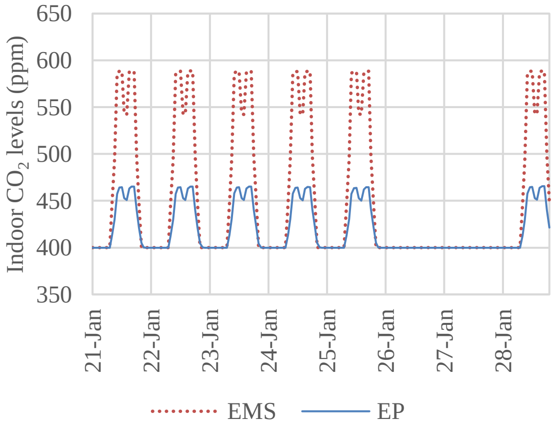

Figure 11: One week simulation showing hourly CO_2 levels for Zone 1 measured using the analytical approach (EMS) and EnergyPlus (EP), at infiltration rate= 6.14 ACH

Figures 8 and 9 show that the GC evaluation using the EMS script was very much following the hourly data simulated using EnergyPlus with a slight tendency to overestimate the GC levels. In contrast, CO_2 estimates using the EMS script seem to be clearly overestimated when compared to the EnergyPlus results shown in the annual simulation results shown in Figure 10 and the week simulation sample illustrated in Figure 11. Both figures are for the CO_2 levels generated in Zone 1 for the 6.14 ACH infiltration scenario. It can be noticed that the CO_2 levels generated by the EMS script have steeper slopes as CO_2 levels increase and decrease quicker in the EMS script than EnergyPlus.

This difference in data slopes can be attributed to one of two reasons, or a combination of both. The first reason is a discrepancy in the way the CO_2 generated from the people is calculated in the EMS script against EnergyPlus. The second potential reason is that EnergyPlus tends to approximate the results for CO_2 levels using one of three algorithms: Euler Method, Third Order Backward Difference, and Analytical Solution. It is understood from the Engineering Manual that the Third Order Backward Difference approximation method will be used by default. This method makes every datapoint (CO_2 level at every timestep) be affected by the previous three datapoints (CO_2 levels in the previous three timesteps) which slows down the rate of change in the values. It is unclear whether the EnergyPlus approximation or systemic discrepancy in the analytical calculations is contributing the most to the error, but holding comparisons to other tools such as CONTAM can help with further investigation.

Conclusion

The analytical approach for indoor air contaminant evaluation scripted using EMS was tested on two zones with different geometries and for multiple infiltration scenarios to see the caveats of the approach suggested. The robustness of the proposed method was measured by comparing the results to the EnergyPlus results generated using the same inputs according to the ASHRAE Guide 14 calibration indexes for CVRMSE and NMBE. The comparison of GC levels was implemented for primary validation of the method proposed, while CO_2 comparisons were carried out for subsidiary validation and further understanding of the caveats of the model.

Following the hourly calibration criteria set by ASHRAE Guide 14, the analytical approach proposed managed to calculate GC and CO_2 levels that could meet the targets for acceptable margin of error when compared to the EnergyPlus generated results. However, trying to satisfy the monthly calibration criteria resulted in the CO_2 calculations failing to meet the NMBE criteria, especially when the infiltration rate is higher than 2 ACH. On the other hand, one GC estimate in one zone failed to meet the monthly NMBE calibration criteria, when the infiltration air change rate was set to 0.5 ACH.

There is a noticeable non-linear correlation between the magnitude of the error and the outdoor air flow air change rate. The correlation is positive when evaluating CO_2 levels and negative when evaluating GC of outdoor origin. It was found that the script gets the GC and CO_2 levels with high precision especially when their levels are high, but the script might be overestimating the contamination levels when they are at their lows. Hence, the proposed method will unlikely be underestimating or overestimating the situations of high risk but might slightly overestimate low risk conditions.

The error values were consistent when outdoor GC levels were inputted as hourly values or a fixed annual mean value. However, the error for GC calculations was slightly impacted by the geometry of the room. This can be attributed to the calculation of the deposition air change rate that is dependent on form factor of the zone.

The calculations for GC of outdoor origin are deemed satisfactory, but further investigation for GC of indoor origin can be followed to examine the correlation of the error to the outdoor air flow rates. It is slightly unclear from this study if the errors can be attributed to the approximation in contaminant levels already embedded into EnergyPlus, or rather to some systemic discrepancies in the calculation methodologies between EnergyPlus and the analytical method proposed. Comparing the results to more tools such as CONTAM can help establish deeper understanding the caveats of the EMS script.

While acknowledging the caveats that might be present in the model, the approach presented can be deployed to evaluate multiple GCs and to implement air quality based control strategies that look at multiple indoor contaminants simultaneously.

Nomenclature

ACH	Air changes per hour
ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers
CO_2	Carbon dioxide
CVRMSE	Coefficient of variance for root mean square error
EMS	Energy management system in the EnergyPlus program
EP	EnergyPlus program
GC	Generic air contaminant
HVAC	Heating, ventilation, and air conditioning
NMBE	Normalised mean bias error
$PM_{2.5}$	Air particulate matter of diameter ≤ 2.5 micrometre

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