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On the Benefits of Whole-building IAQ, Ventilation, Infiltration, and Energy Analysis Using Co-simulation between CONTAM and EnergyPlus

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Abstract. Publicly available tools to perform whole-building simulation of indoor air quality, ventilation, and energy have been available for several decades. Until recently, these tools were developed in isolation, such as the whole-building contaminant transport and airflow analysis tool, CONTAM, developed by the National Institute of Standards and Technology (NIST) and the whole-building energy analysis tool, EnergyPlus, developed by the U.S. Department of Energy (DOE). The ability to couple these tools during runtime has been implemented through co-simulation, enabling improved analysis of the interdependent effects of temperature and airflow on contaminant transport and energy use on a whole-building scale.

This presentation will include the development of a set of coupled reference building models for the purposes of evaluating the potential benefits of using co-simulation between CONTAM and EnergyPlus. A set of Residential Prototype Building Models available from DOE has been modified by NIST and utilized to demonstrate the coupling process and the benefits of this coupling with respect to IAQ and energy analysis, and to evaluate multiple whole-building simulation methods related to infiltration, ventilation, and occupant exposure. These methods include an original EnergyPlus prototype model, the original model with NIST-based infiltration correlations, co-simulation between EnergyPlus and CONTAM, and stand-alone CONTAM simulations. Potential benefits will be explored related to the ability of co-simulation to address the effects of variations in building typology and ventilation system performance on contaminant transport results while leveraging the capabilities of whole-building energy analysis.

1 Introduction

The multizone airflow and contaminant transport analysis software, CONTAM, has been under continuous development at the National Institute of Standards and Technology (NIST) since the 1980s [1-3]. This program is publicly and freely available for download from the NIST website. CONTAM provides the ability to simulate ventilation and indoor air quality (IAQ) on a whole-building scale; however, CONTAM does not perform heat transfer analysis. Therefore, users are required to input indoor building temperatures, which impact airflow rates. While these temperatures may be scheduled, e.g., to conform with thermostatic setpoints, they may not fully capture the heat transfer-related properties associated with building energy-related systems such as envelope construction and heating, ventilating, and air-conditioning (HVAC) systems that affect temperature differences between zones and fan run times. EnergyPlus is also publicly available software developed by the U.S. Department of Energy [4]. EnergyPlus provides the ability to simulate multizone, whole-building heat transfer analysis including the sizing and control of HVAC systems.

These programs are able to address a broad range of important processes but when used alone the capabilities are limited. For example, CONTAM has been used to evaluate the energy costs of infiltration without the direct benefit of energy simulation [5]. EnergyPlus, on the other hand, has been incorporated with the ability to simulate two contaminants: carbon dioxide (CO_2) and a generic contaminant but does not account for particle losses associated with filtration or building envelope penetration. Further, EnergyPlus can implement an Airflow Network model (AFN) to enable multizone airflow analysis. However, these capabilities are largely based on those implemented by CONTAM and its predecessors [6, 7] and can be cumbersome to implement without a graphical user interface as provided with CONTAM. Used together these programs can better capture the often-interdependent transport mechanisms, providing more comprehensive analyses of measures aimed at improving energy and IAQ performance.

1.1 Co-simulation between CONTAM and EnergyPlus
To capture the inter-dependency between temperature and airflow (and hence contaminant transport), CONTAM has been coupled with EnergyPlus [8]. The coupling between EnergyPlus and CONTAM is achieved using quasi-dynamic coupling via the Functional Mock-up Interface for Co-simulation specification as implemented in EnergyPlus [9, 10]. This method of coupling provides for the run-time exchange of data between two separate simulation programs at regular time intervals during co-simulation.

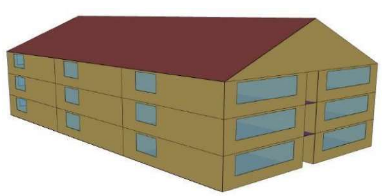
During the co-simulation EnergyPlus acts as the controlling program. Prior to transient simulations for up to one year, EnergyPlus first performs system sizing and then performs warm-up simulations whereby co-simulation occurs repeatedly over a 24-hour period until zone temperatures stabilize. During the warm-up, reversible source-sinks of CONTAM (i.e., deposition-resuspension surfaces and diffusion-based materials) can also be loaded with contaminant via the CONTAM restart file. The data exchanged during co-simulation is outlined below, and details are provided in references [2, 8].

From EnergyPlus to CONTAM
- **Zone Temperatures** and **Relative Humidity**
- **Ventilation system airflow rates** for zone supply and return airflows
- **Outdoor airflow fractions** of outdoor airflow controllers
- **Exhaust fan airflow rates**
- **Outdoor environmental data** including temperature, barometric pressure, wind speed, and wind direction
- **Output variables** user-selected from available EnergyPlus output variables

From CONTAM to EnergyPlus
- **Zone infiltration airflows**
- **Inter-zone airflows**
- **Controls values** user-defined to be exposed via the CONTAM controls network, e.g., a signal calling for ventilation airflow due to an elevated contaminant level

1.2 Residential Building Models
A multi-family building model was selected from a set of prototype building models that were originally developed in EnergyPlus for DOE by the Pacific Northwest National Laboratory (PNNL). This model was used to demonstrate the co-simulation process and to compare the capabilities of and among various simulation tools [11]. These prototype models were intended to inform the decision-making process related to developing building energy codes, i.e., International Energy Conservation Code (IECC), and they have evolved over the years along with the relevant codes and standards [12]. The EnergyPlus model used in this study consisted of slab-on-grade construction with each apartment having a forced-air HVAC system with electric resistance heating and direct-expansion cooling coils and constant exhaust ventilation.

The building model, shown in Figure 1, is a three-story, garden style apartment building with no enclosed stairwells or shafts, and each apartment modeled as a single zone 12.19 m x 9.14 m x 2.59 m high (40 ft x 30 ft x 8.5 ft). Simulations were performed using the IECC 2006 building representation for climate zone 5A (*USA_MA_Boston-Logan.Intl.AP.725090_TMY3.epw*).



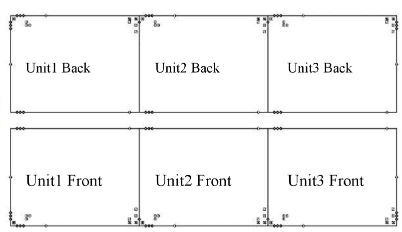


Figure 1. Multi-family building model (left: EnergyPlus model) and floor plan (right: CONTAM model) with apartment names

2 Methods

EnergyPlus version 9.1 and CONTAM 3.4 were used for the simulations, so the original EnergyPlus models were updated using the *IDFVersionUpdater* tool provided with EnergyPlus. CONTAM models were developed with the *ContamW* graphical user interface using the pseudo-geometry mode to create scaled representations of the building floor plans for each level of the building including the attic.

2.1 Coupling Strategy

Coupling of EnergyPlus and CONTAM requires building representations for both programs, i.e., an EnergyPlus input file (IDF) and a CONTAM project file (PRJ). Two NIST-developed tools were utilized to facilitate the EnergyPlus-CONTAM co-simulation: *Contam3DExport* program and *ContamFMU* dynamic link library. *Contam3DExport* creates IDF files from a PRJ file along with the files required to coordinate the co-simulation, and *ContamFMU* provides for control of software execution and the exchange of data with the CONTAM simulation engine, *ContamX*, during co-simulation. A schematic of the coupling process and associated files and software is shown in Figure 2, and details are provided in the CONTAM User Guide [2].

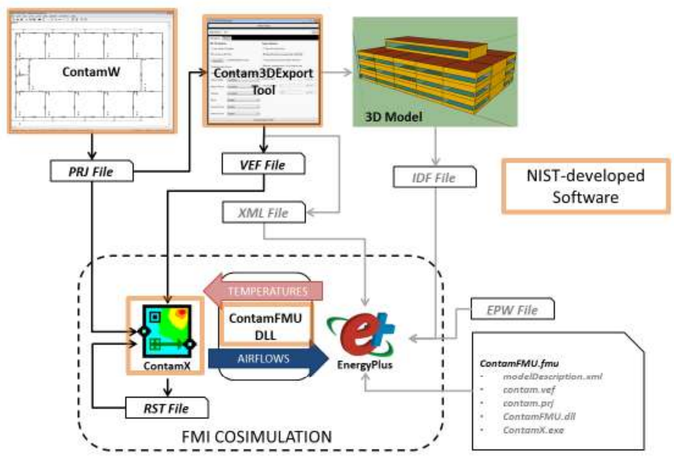


Figure 2. EnergyPlus-CONTAM Coupling Schematic

A scaled version of the building was developed in *ContamW* and extruded to a three-dimensional IDF using *Contam3DExport*. The roof as generated by *Contam3DExport* was cuboidal and required modification to create the gable geometry within the IDF. The model developed herein was within approximately one percent of the building volume of the original IDF. The exported IDF was then modified to align with the original IDF with respect to the following building model properties: internal loads, HVAC system properties (e.g., heating and cooling coils, sizing parameters, and thermostats), demand hot water, schedules, building construction and materials, and shading surfaces. Some of these items were created by *Contam3DExport* and required modification, e.g., cooling and heating coils, and other components were not included in the exported IDF file, e.g., shading surfaces.

2.2 Building Simulations

Inter-model comparisons of the resultant whole-building energy use, infiltration rates, and contaminant concentrations were made using the following simulation methods.

- Original EnergyPlus-only (labeled ***E+*** in results)
- Original EnergyPlus-only with infiltration correlations (labeled ***E+**** in results)
- EnergyPlus-CONTAM co-simulation (labeled ***COSIM*** in results)
- CONTAM-only (labeled ***Cw*** in results)

Explanations for each of these methods and relevant differences between them are provided in the following sections.

2.2.1 Energy Inputs

All the models that utilized EnergyPlus (*E+*, *E+**, and *COSIM*) implemented auto-sizing of the HVAC systems, which determined the supply fan flow rates. The CONTAM-only model (*Cw*) was defined to implement indoor temperatures based on the thermostatic set-points for both heating and cooling modes as per the EnergyPlus thermostatic set-point schedules. These schedules included the cooling season from May 1 through September 30 with a cooling setpoint of 23.88 ºC (75 ºF) and a heating setpoint of 22.22 ºC (72 ºF). Further, the supply airflow rates and an intermittent fan run time schedule (5 minutes ON, 15 minutes OFF) of the *Cw* model were based on the system sizing results and the approximate fan run-time fraction of the *E+* simulation results, respectively. In this manner, the *E+* simulation was utilized to inform inputs to the *Cw* model without direct coupling between them.

2.2.2 Infiltration Inputs
The *E+* model implemented the *ZoneInfiltration:EffectiveLeakageArea* calculation method based on Equation (1) with effective leakage areas (A_L) in cm^2, at a 4 Pa reference pressure and discharge coefficient of 1.0, for each apartment apportioned as shown in Table 1. ΔT is the indoor-outdoor temperature difference in ºC, W_s is the wind speed in m/s, and C_s and C_{ws} are stack and wind speed coefficients: 0.00029 and 0.000231, respectively. The effective leakage area in the CONTAM models (*Cw* and *COSIM*) were calculated based on the values in Table 1 and the surface areas of the *Middle* and *Top* floor apartments to be 1.443 cm^2/m^2 of wall surface area.

$$\text{Infiltration} = \frac{A_L}{1000}\sqrt{C_s\Delta T + C_{ws}\cdot W_s^2} \quad (1)$$

Table 1. Effective Leakage Area of Original EnergyPlus Models

Apartments	*Effective Leakage Area [cm^2]*
Corner apartments (Units 1 & 3) on Bottom and Top floors	286
Center apartments (Unit 2) on Bottom and Top floors	252
Corner apartments (Units 1 & 3) on Middle floor	125
Center apartments (Unit 2) on Middle floor	91

The *E+** model was based on the *E+* model which was then modified to use the infiltration calculation method (referred to in EnergyPlus as *ZoneInfiltration:DesignFlowRate*) presented in Equation (2). The *Cw* model was used to determine whole-building infiltration rates for the entire year for Boston weather. The coefficients A, B, and D in Equation (2) were generated from these *Cw* infiltration results using the method presented in references [13, 14] and determined to be 0.4688, 0.0166, and 0.0174, respectively. The design infiltration rate, I_{design}, was set to 3.72 x 10^{-4} m^3/s per m^2 of exterior building surface area.

$$\text{Infiltration} = I_{design}(A + B|\Delta T| + D\cdot W_s^2) \quad (2)$$

Thus, the *E+** model utilized results of CONTAM simulations to inform required inputs without direct coupling between EnergyPlus and CONTAM.

2.2.3 Ventilation Inputs
The *E+* model utilized the EnergyPlus *ZoneVentilation:DesignFlowRate* method to account for exhaust ventilation in each zone. This ventilation method acts in an additive manner with respect to infiltration to increase outdoor air intake beyond that due to infiltration. This is an empirical method of introducing outdoor air into the building as opposed to the physics-based methods incorporated by multizone or network airflow modeling. The simulations that utilized CONTAM (*Cw* and *COSIM*) incorporated exhaust ventilation via the CONTAM model. This method of incorporating exhaust ventilation acts as a driving force for infiltration as opposed to the additive nature employed by the *E+* models. The EnergyPlus correlation models (*E+**) did not implement the *ZoneVentilation:DesignFlowRate* method, because the correlations were performed with the exhaust systems activated in the CONTAM models.

2.2.4 Contaminant Inputs
To demonstrate contaminant analysis methods, two contaminants were considered: CO_2 and fine particulate matter ($PM_{2.5}$). CO_2 is one of the contaminants that EnergyPlus can simulate directly and is primarily generated by building occupants, thus it is impacted by the building ventilation rate and can be used for demand-controlled ventilation. The outdoor CO_2 concentration was set constant at 731.8 mg/m^3 (400 ppm), and the maximum CO_2 generation rate was set to 4.48 x 10^{-6} m^3/s·person which was based on the activity schedule for two occupants as defined in the original EnergyPlus model with a maximum internal heat gain of 117.28 W/person and assuming an occupant CO_2 emission rate of 3.82 x 10^{-8} m^3/s·W. $PM_{2.5}$ is associated with both internal and external sources. In these simulations, an outdoor $PM_{2.5}$ contaminant time history file was incorporated based on measurements in Boston, MA; an indoor cooking source of 1.56 mg/min was scheduled from 7:00 to 7:10 and 18:00 to 18:20 every day, and particle

deposition occurred in every zone at a rate of 0.19 h^{-1} [15]. CONTAM enables filter models to be used in any airflow path including those associated with HVAC systems, i.e., outdoor air and recirculation air filters, and those associated with envelope openings, i.e., to account for particle removal as they penetrate into the building from outdoors. EnergyPlus does not enable the use of filters. Therefore, only the CONTAM models incorporated recirculation filters within the HVAC systems and an envelope penetration coefficient of 0.72 for $PM_{2.5}$.

3 Results and Discussion

Energy simulation results were evaluated to ensure the coupled model yielded reasonable results compared to the original EnergyPlus model. Comparisons between whole-building and apartment-level infiltration rates are then presented followed by contaminant results.

3.1 Energy

Annual energy usage results are shown in Figure 3 including heating, cooling, fan, and total energy use for the three simulation methods that utilized EnergyPlus (*E+*, *E+**, and *COSIM*). Results indicate that the total energy use for the *COSIM* and *E+** simulations were 12 % and 13 % less than the original results. The difference was due to the means by which exhaust ventilation was implemented in the *E+* model as will be discussed in the next section. As a result of the method used to account for exhaust in the *E+* models, consideration should be given to modifying the PNNL models to better account for infiltration.

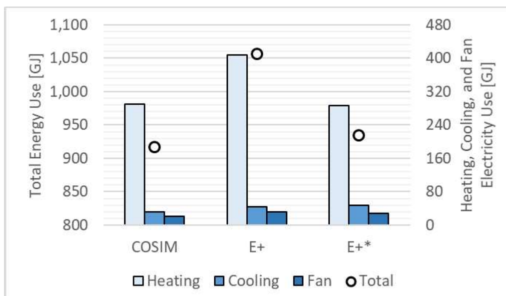


Figure 3. Annual Energy Usage Using Three Different Infiltration Calculation Methods

3.2 Infiltration

Box-whisker plots of the daily average air infiltration rates are presented in Figure 4 for the months of January and July using all four simulation methods. The *E+* results were noticeably higher than those of the other methods due to the additive nature of the exhaust ventilation and infiltration methods implemented in this model. In contrast to the "additive" nature of infiltration and exhaust flow rates in the *E+* model, the exhaust systems in the CONTAM models (*Cw* and *COSIM*) act as a driving force for infiltration, so infiltration will only be greater than the exhaust flow rate if the mass flow rate attributed to natural driving forces are greater than the exhaust ventilation rate. The *E+** results accounted for the exhaust ventilation within the correlations, i.e., the exhaust systems were active in the *Cw* simulations used to generate the correlation coefficients, so additive ventilation was not included in the IDF of the *E+** model.

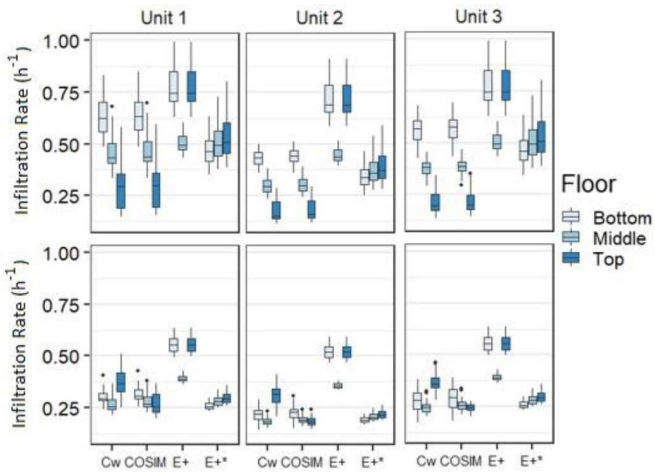


Figure 4. Daily Average Infiltration Rates of *Front* Units for January (top) and July (bottom) using Four Simulation Methods (see Figure 1 and Section 2.2 for explanations of category and zone names)

The differences in the *E+* results for different levels directly reflected the leakage areas as defined in Table 1, i.e., rates for units on the *Bottom* and *Top* floors were the same and higher than those on the *Middle* floor, and the *Front* and *Back* (not shown) units were always the same. The CONTAM-only (*Cw*) and co-simulation (*COSIM*) results were quite similar to each other (minor differences were reflected in the outliers), because the energy model controlled the single-zone temperatures very precisely to match the thermostatic set-points which were also scheduled in the *Cw* models. This reveals the capabilities of CONTAM to predict building infiltration when indoor temperatures are tightly controlled and single-zone representations are warranted. Further, the CONTAM-based calculations are not empirical, i.e., they are physics-based, so they account for pressure-driven airflows and relative leakage areas between zones including inter-floor leakages which is a key benefit of multizone network analysis.

All the simulation methods revealed the expected seasonal differences in infiltration rates, i.e., winter infiltration rates were higher than the summer rates. This difference can be attributed to greater absolute indoor-outdoor temperature differences in January than in July and associated buoyancy effects. Patterns in the relative differences between floors were the same between January (winter) and July (summer) except for the *Cw* results. Infiltration results for the simulation methods that utilized EnergyPlus (*E+*, *E+**, and *COSIM*) were obtained from the EnergyPlus output files while the *Cw* results were obtained from the CONTAM output files, and the CONTAM results included infiltration from the attic that was not accounted for in the EnergyPlus results. Therefore, in the July results, when infiltration is likely to occur from the attic into the *Top* floor zones, the infiltration rates tended to increase in the *Top* floor zones. This is another benefit of using the multizone network analysis. However, it is important to understand the meaning of simulation outputs when evaluating results, for example, when EnergyPlus infiltration rates for the *COSIM* case did not match those determined by the associated CONTAM model. The EnergyPlus simulations with correlations (*E+**) were similar in magnitude with the *Cw* and *COSIM* results, but exhibited infiltration rates that increased from the *Bottom* to the *Top* floor. This is a result of increased wind speed with elevation that is accounted for in EnergyPlus by default and the fact that the *ZoneInfiltration:DesignFlowRate* equation includes a coefficient of the square of the wind speed which dominates the resultant infiltration as presented in Equation (2).

3.3 Contaminant Transport

Contaminant results are shown in Figure 5 for the months of January and July using the four different simulation methods. Box-whisker plots of daily averages are provided for the *Front* units (results for *Back* units were very similar) and the infiltration results for *Unit 1* are repeated here to simplify evaluation of contaminant results as they relate to infiltration.

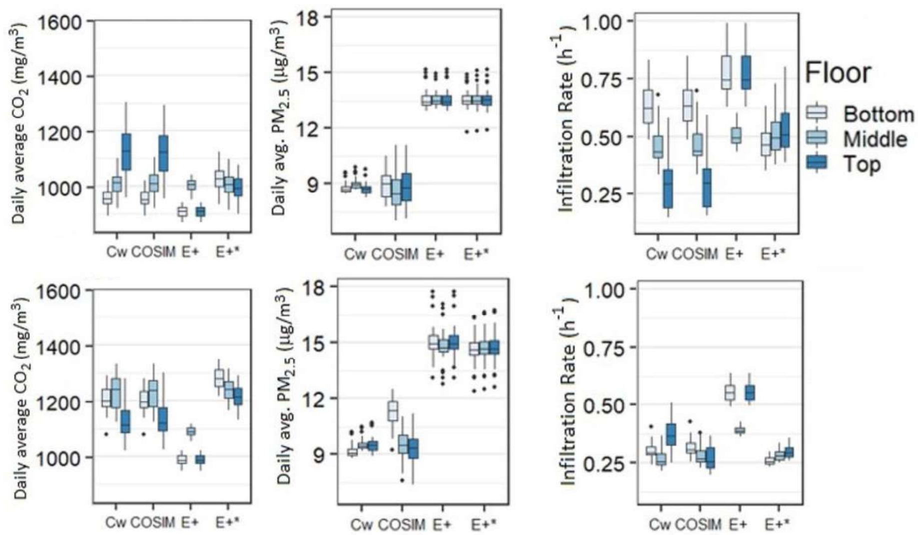


Figure 5. Daily Average Simulation Results (CO_2, $PM_{2.5}$, and Infiltration) of the *Front* in Unit 1 for January (top) and July (bottom) using Four Simulation Methods (see Figure 1 and section 2.2 for explanations of category and unit names).

Carbon Dioxide (CO_2)

CO_2 results generally reflected the infiltration rates because the CO_2 was generated internally, with higher infiltration rates leading to lower CO_2 concentrations. In nearly all cases, the original *E+* CO_2 results were lower, which follows from the additive modeling of ventilation and infiltration of the *E+* discussed previously. The variation in CO_2 concentrations with elevation as captured by the CONTAM methods (*Cw* and *COSIM*) also revealed the benefits of utilizing the physics-based infiltration and ventilation calculations of multizone modeling. This is revealed in *Cw* results wherein the pattern of infiltration rates is reflected in the CO_2 results for the July simulations. As addressed in the infiltration results, the interzone mixing between the attic and the *Top* floor enables CONTAM to capture the contaminant transport due to buoyancy-induced flows which lead to the downward internal airflows when indoor temperatures are lower than outdoors.

Particles ($PM_{2.5}$)

The average outdoor $PM_{2.5}$ concentrations (not shown) for January and July were 13.5 μg/m^3 and 16.4 μg/m^3, respectively. In the *E+* and *E+** models, the dominant removal mechanism was dilution by infiltration, so the average indoor $PM_{2.5}$ concentrations were close to the average ambient concentrations. Detailed plots of $PM_{2.5}$ concentrations for all simulation methods (not shown) revealed that concentrations fell below the ambient concentrations after each cooking event due to the combination of dilution, deposition, and filtration which was also reflected in the daily averages being below the respective outdoor averages. $PM_{2.5}$ results revealed the benefits of using CONTAM for particle analysis. The most apparent differences were the reduced levels of $PM_{2.5}$ concentrations exhibited by the *Cw* and *COSIM* results. While both EnergyPlus and CONTAM accounted for particle removal by deposition, the CONTAM models additionally removed particles via mechanical system filters and envelope penetration coefficients. All the EnergyPlus HVAC systems were auto-sized, leading to variations in system fan flows. For the *Cw* and *COSIM* cases this affected the amount of air moving across the particle filters located within the HVAC returns. This was revealed in the differences between the *COSIM* and *Cw* cases. *Cw* incorporated the fan flow rates of the *E+* results, which were different from the *COSIM* flows in most cases and significantly different in some cases, e.g., *COSIM* flows were lower than the *Cw* flows for *Unit 1* on the *Bottom* floor as shown in Figure 6.

As was the case with the previously presented infiltration rates, both the CO_2 and $PM_{2.5}$ results revealed that the contaminant concentrations in the *Front* and *Back* (not shown) units were nearly identical. This was due to the fact that these two rows of apartment buildings acted as two separate, but similar buildings. Minor differences were exhibited in the *Cw* and *COSIM* results because wind pressure coefficients on the breezeway-facing building surfaces were defined to be lower to account for shielding effects. This detailed treatment of wind pressure variations is another benefit of using multizone airflow modeling.

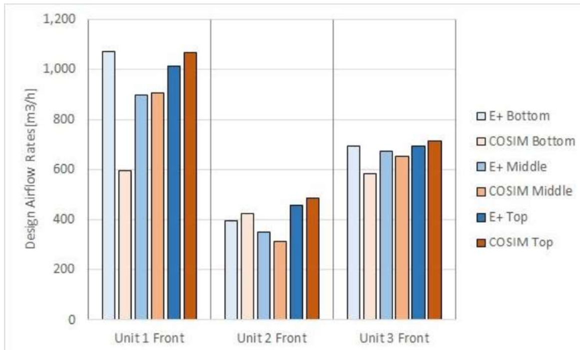


Figure 6. HVAC System Fan Flow Rates of *Front* Units for *E+* and *COSIM* Cases

4 Conclusions

A CONTAM representation of a multi-family residential reference building model was developed and coupled with EnergyPlus. This presentation provided a preliminary inter-model comparison between four different simulation methods including the original EnergyPlus model and fully coupled co-simulation between EnergyPlus and CONTAM. While some differences were revealed between these simulation methods, the benefits of co-simulation depend on the analysis being performed. In the case of these fairly simple, single-zone apartment units, major benefits of utilizing co-simulation were revealed in analyzing the removal of particulates by filtration and envelope penetration. Further, these building models utilized balanced supply and return airflows and exhaust ventilation. The balanced airflows do not drive infiltration or interzone airflow, hence contaminant transport, between apartment units, and the exhaust ventilation drove infiltration, thus reducing the effects of wind and buoyancy.

The coupled models have been shown to better capture overall building energy performance. Future work will address the effects of unbalanced system flows, variations in inter-apartment source strengths, multizone representations of apartment units, and ideally, comparison of model predictions with empirical data.

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