

# A HYBRID DATA-DRIVEN AND SIMULATION-BASED FRAMEWORK FOR INDOOR AIR QUALITY AND ENERGY MODELING

## Abstract

Natural ventilation can promote comfort, health, and productivity of occupants and, at the same time, reduce the operational energy use of buildings. This strategy, however, is usually applied at the cost of indoor air quality (IAQ) by unintentionally bringing in outdoor air pollutants. Hence, estimation of energy and indoor air quality (IAQ) is essential for the design of naturally ventilated buildings through reliable evaluation of trade-offs between energy-saving potential and human health risks. The primary objective of this paper is to propose a framework for integrated energy and IAQ which enable localizing outdoor conditions, including air pollution and airflows in building site resolution through a hybrid engineering simulation and an artificial intelligence-based approach. CFD, CONTAM, and EnergyPlus applications are used in this framework to calculate airflow, IAQ, and energy-saving potential of the building, respectively. The ML algorithms are also extended into CFD application to help facilitate localizing outdoor airflow, effectively. The results are validated against measured on-site observation data. This framework is tested on the DOE's large-size office buildings located at Federal Campus in downtown Chicago. The outcomes of this research enable designers in an early stage to identify outdoor air determinants and localize them in building site scale, and analyze integrated energy-saving potential and IAQ in a reliable and efficient way.

## Author

Mehdi Ashayeri  
*Illinois Institute of Technology*

## Keywords

Indoor air quality, building energy, natural ventilation, outdoor air pollution, simulation, machine learning

## Introduction

According to the National Human Activity Pattern Survey (NHAPS), Americans spend about 87% of their time indoors (Klepeis et al., 2001). Indoor spaces are to shelter the occupants from severe and uncomfortable weather conditions, as well as the outdoor air contaminants. Heating, ventilating, and air conditioning (HVAC) systems are used to provide thermally comfortable conditions and protect IAQ for the health of building occupants (Dutton et al., 2013). Mechanical systems in buildings have the most significant contributions (39%) to overall energy consumption in the US (U.S. Department of Energy, 2012). Due to recent efforts in reducing energy use and greenhouse gas emissions, NV is being proposed as a means of saving energy and improving the IAQ for office buildings, with respect to “green building” goals. Of all uncertainties in the design of NV systems, the localized methodological, air pollution, and airflow uncertainties regarding the building site are overlooked areas of studies.

Cooling and ventilation systems account for 35% of the end-use energy in the US office stock. NV has the potential to reduce the energy loads during temperature suitable times as well as to lower the psychological distress and sick building syndrome (SBS) prevalence (Mendell et al., 2015; Preziosi, 2004) in the workplace. However, improper design of naturally ventilated systems results in certain acute and chronic diseases (Suh et al., 2000) of occupants in terms of unintentionally bringing in the ambient pollutants. It should be noted that the SBS symptoms are seen where a building is ventilated by conventional mechanical means (with no cooling and humidifiers) or by natural ventilation strategies with insufficient ventilation rates.

Naturally ventilated buildings are often blamed for outdoor environmental conditions and inconsistent performance in providing higher indoor environmental quality (IEQ) for occupants. The inconsistent wind speed and direction (Rong et al., 2015; Yang & Zhao, 2012), seasonal and severe weather variations (Shi et al., 2018), and outdoor air pollution are the most critical variables for designing the NV systems. On the other hand, airflow and air quality simulations are time-consuming and extensive in cases where the CFD simulation or experimental study are applied. Data-driven methods can be applied to help facilitate airflow and air quality analysis for NV studies. Yi et al. (2012) developed a framework which integrates the data-driven and simulation procedures for NV predictions. With applying the artificial neural network (ANN) model (Abbasabadi & Ashayeri, 2019) for estimating the wind speed and direction, the CFD-based simulation results were captured 400 times faster relative to the conventional methods. Meanwhile, through utilizing a stochastic Monte Carlo analysis, the hourly thermal boundary conditions were also obtained faster for calculating building envelope temperature. Chen et al. (2018) proposed a framework which calculates the NV potentials in hybrid operated buildings (small- to medium-size offices) and plots the NV suitable hours for cities within the ASHRAE climatic zones. The results illustrate that May, August, and September are the three suitable months for NV operation in Chicago, which exceeds the mean annual NV suitable hours (11.30%) nationwide. Regarding the literature, the localized ambient air quality in analyzing NV systems is an overlooked area of study.

There is a limited number of research works to analyze the IAQ in naturally ventilated buildings in an integrated manner. However, these models have methodological uncertainties and limitations which stem from oversimplification of data and system, relying on generalized data, a lack of a robust approach to localize the meteorological and outdoor air pollution data in building site scale, and conventional approaches for simulating IAQ and energy use in an integrated way that are less efficient, timely, and computationally.

For airflow studies, the application of CFD simulation is unavoidable to solve the turbulence problems around buildings, which needs a significant amount of time. Also, experimental studies on outdoor air quality need a long-time on-site observation effort. Artificial intelligence-based techniques can be applied to help facilitate the implementation of both in a timely effective way (Challoner et al., 2015; Losada et al., 2016; Tong et al., 2016; Y. Wang & Malkawi, 2014). The main objectives of this research are to:

- Develop an integrated framework for effectively analyzing IAQ and Energy Saving Potentials (IAQ-ES) in NV operated office buildings through the application of hybrid simulation and an artificial intelligence-based approach
- Identify and predict the impacts of local outdoor conditions on an NV-operated office building
- Execute the system in computational and time-efficient ways

## Methodology and Preliminary Results

This section elaborates on the proposed framework, which localizes the meteorological, air pollution, building gas usage, and traffic datasets for IAQ-EU estimation and how the proposed framework was tested on an office building in a city-grid in downtown Chicago. The DOE’s large-size reference model building is placed within the Federal Campus site bounded between State, Dearborn, Jackson, and Adams Streets (Figure 2) for the test. The following four steps summarize the execution process: synthesize data, validation, ambient airflow simulation and prediction, and indoor IAQ-energy simulations (Figure 1).

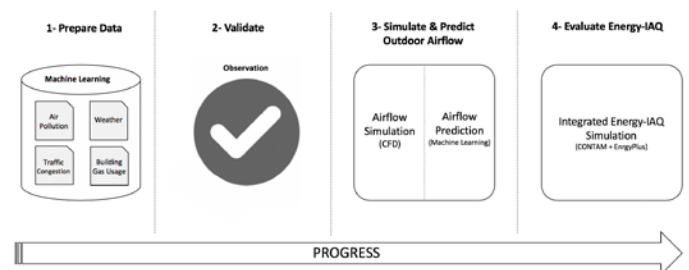


Figure 1: Workflow of IAQ-EU modeling.

This research uses data from four sources: meteorological data taken from the 'Synaptic Data' website, EPA's background air pollution data, traffic congestion data, and building gas usage data. The local air pollution emission rates are estimated using building gas usage, traffic congestion, and emission factors. The prepared dataset is also validated via one-week observation data. A meteorological station which captures the weather conditions, including wind speed, wind direction, temperature, and humidity, may not realistically represent the actual microclimate of a building site, and then reduces the accuracy of the simulation results.

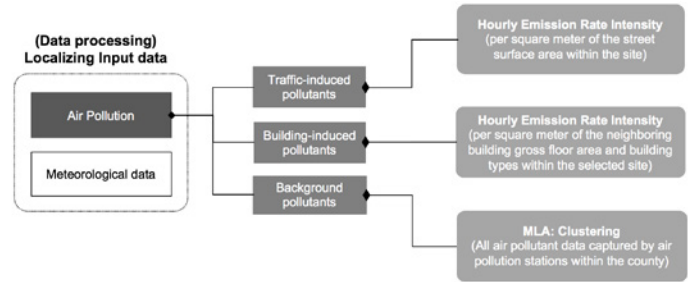


Figure 3: Workflow of localizing outdoor air pollution.

In localizing the outdoor air pollution data, the following three steps were carried out:

In NV studies, using the mean air pollution concentration data is the more common procedure for capturing the background air pollution regimes. This research studied pollutant concentrations including NO<sub>2</sub>, CO, SO<sub>2</sub>, PM<sub>2.5</sub>, and PM<sub>10</sub> through utilizing the clustering approach. In clustering, the actual data is not labeled with class information. The purpose is to partition data into several (more than one) homogeneous groups where the within-group and between group object distance object dissimilarity are optimized. This study used eight consecutive years of air pollution historical data (2010–2017) in capturing the background air pollution regime for the city of Chicago. To generalize the data for the entire period and reduce the calculation loads, those months that provide thermally NV suitable conditions for occupants were only studied. Hence, May through October was selected in this research. It was found that there is no significant oscillation in dividing the data into workdays and weekends (Figure 4), while the concentration of the traffic-induced pollutants highly depends on weekdays as well as the hours during the days (Figure 6).

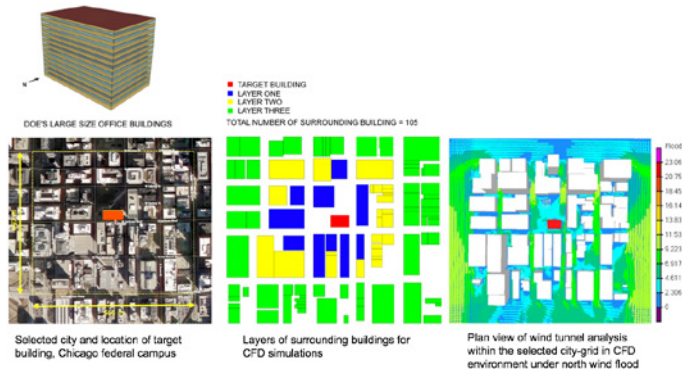


Figure 2: Spatial patterns and airflow analysis.

This study models three layers of surrounding buildings in CFD simulation (Tong et al., 2016) to investigate the airflow analysis around the target building (Figure 2). The weather data from May through October during the eight consecutive years (2010–2017) were aggregated using the O'Hare International Airport station's weather data. For localizing the outdoor airflows, wind direction was set to the cardinal (North, East, South, and West), Intermediate (NE, NW, SE, SW), and secondary intermediate directions (NNE, ENE, ESE, SSE, SSW, WSW, WWW, and NNW) which are given to the CFD model. Then, the provided data was combined with the hourly air pollution dispersion (for local pollutants) and background air pollution concentration to be used in the ANN model for prediction. With applying the CFD engine, the wind pressure coefficient ( $C_p$ ) and the contaminant concentration coefficient ( $C_c$ ) per opening across the building façade were then captured. This procedure is also able to differentiate the airflow variation on building orifice based on the building height. It should be noted that this research carried out CFD analysis only for airflow calculations, while the thermal boundary condition was attained utilizing the EnergyPlus engine.

Insufficient air pollution monitoring stations limits analyzing the impacts of outdoor air quality on IAQ-ES simulation with higher uncertainties. To estimate the local congestion of air pollutants, this research broke down the local air pollution into background, building-induced and traffic-induced pollutants, and combined them with the localized meteorological data to be used in IAQ-ES simulations. Figure 3 illustrates the summarized workflow of ambient air pollution data processing, which is described separately within the next sections.

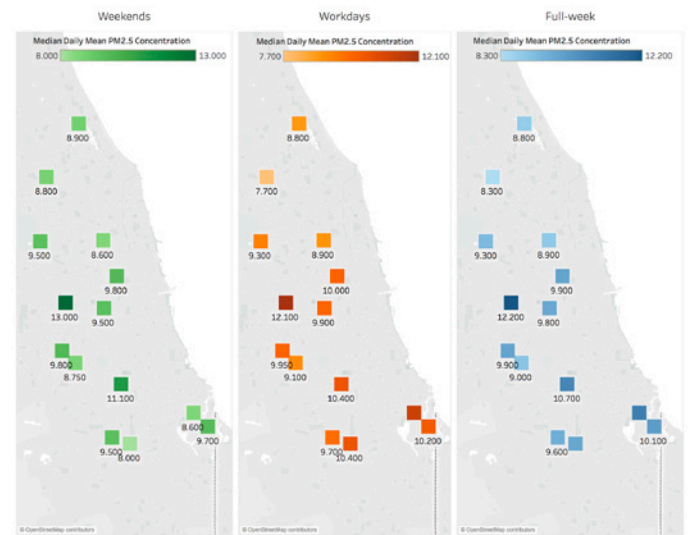


Figure 4: Mean daily PM<sub>2.5</sub> concentration per air monitoring station based on Workdays, Weekends, and Full-week in Cook County during May-October 2010-2017.

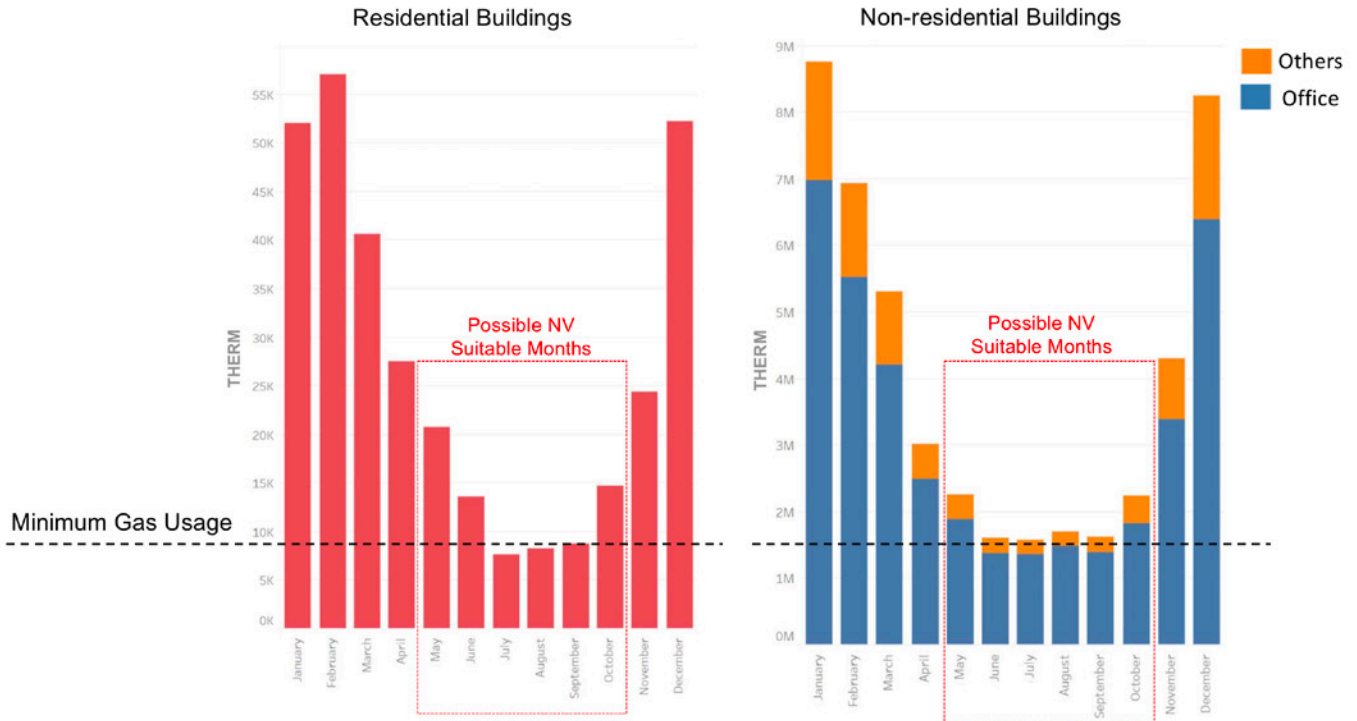


Figure 5: Monthly natural gas usage in Chicago Loop neighborhood for residential and non-residential buildings.

Emissions from building combustions depend on various determinants including the equipment and their maintenance as well as the fuel composition. The National Renewable Energy Laboratory (NERL) has collected the source and on-site fuel combustion emission factors, which are used as the baseline emissions from uncontrolled combustion sources (Deru & Torcellini, 2007). This research used the building-induced air pollutants, which captured the volume of fuel use from the Chicago Energy Usage (2010) dataset (“Energy Usage 2010 | City of Chicago | Data Portal,” n.d.) in the neighborhood scale. Then, by using the Fossil-Fuel-Cycle (FFC) conversion factors (Leslie, 2013) (Table 1) for each of the fuels, the real volume of fuel use was calculated. Pollutants emission rates were drawn from the Source Energy and Emission Factors for Energy Use in Buildings (Deru & Torcellini, 2007).

Fuel type	FFC Factors	Emission factor (Kg/.m3) <sup>a</sup>					
		VOCs	CO	NOx	SO <sub>2</sub>	PM <sub>2.5</sub> <sup>b</sup>	PM <sub>10</sub>
Natural Gas <sup>c</sup>	1.19	2.16E+00	3.30E+01	3.92E+01	2.22E-01	2.97E+00	2.97E+00

a. In 1000m<sup>3</sup>  
 b. PM<sub>10</sub> = PM<sub>2.5</sub> (US EPA, 2016)  
 c. Gas volume at 15.6°C and 101325Pa

Table 1: US average fuel FFC energy factors by fuel type (Leslie, 2013) and emission factors for on-site combustion of commercial boilers. (Source: Deru & Torcellini, 2007.)

The emission rates were calculated for those months that the heating system in buildings is nearly off since NV accrues when the outdoor temperature is suitable enough in bringing in the outdoor air. Figure 5 illustrates the gas usage for the entire year 2010 in which the usage within May to October are in a similar pattern in non-residential buildings, while the residential buildings used more energy in May. Because of the lack of hourly gas usage data, this research assumed that the extra usage in residential buildings was accrued during night hours. Then, for weighting data hourly, those extra usages were excluded. As mentioned earlier, the air pollution studies during similar thermal conditions reduce the level of uncertainty in calculations. As the emission factors depend on temperature and outdoor air pressure, generalizing the emission rates for the NV suitable hours can increase the accuracy and reliability of air quality analysis.

This research captured the traffic information including the number of passenger cars and buses from the Chicago Traffic Tracker, Historical Congestion Estimates by Region 2013–2018 (“Chicago Traffic Tracker - Congestion Estimates by Regions | City of Chicago | Data Portal,” n.d.). The traffic data was divided in two parts: workdays (Monday–Friday) and weekends (Saturday–Sunday) for hourly data (Figure 6).



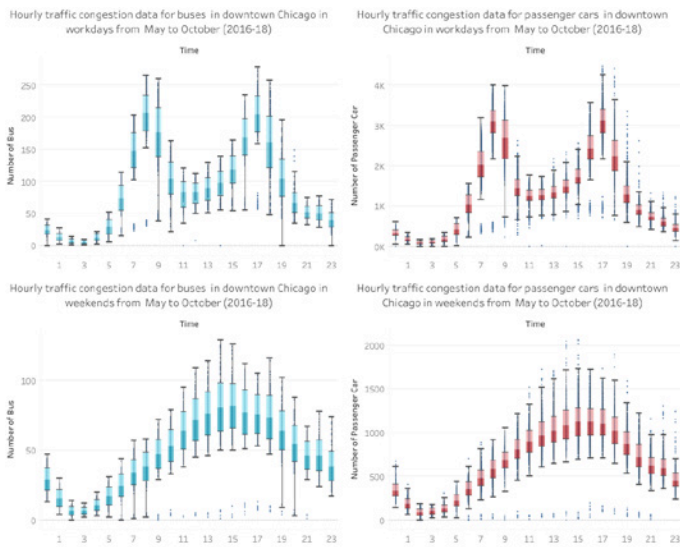


Figure 6: Box-plot and whisker of hourly traffic profiles based on workdays and weekends for cars and buses in the Chicago Loop.

**External Link for CFD0 Editor™ and CONTAM™ Co-Simulation.** Figure 7 illustrates the workflow of CFD and CONTAM co-simulation for outdoor airflow and air pollution analysis. The selected city-grid was bound to 1446mx1577mx480m, then, discretized to 180x197x60 finite volumes.

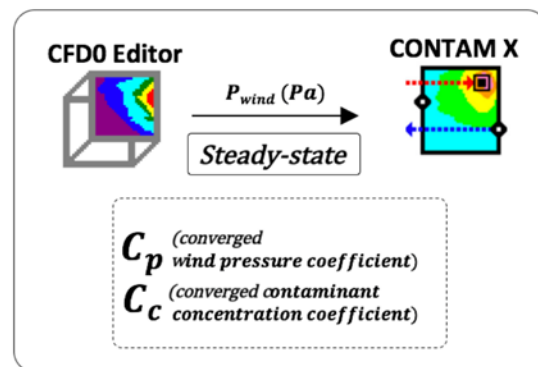


Figure 7: Workflow of external CFD0 Editor and CONTAM co-simulation.

CONTAM is a multizone indoor air quality (IAQ) and ventilation analysis software which is used to determine airflow rates, contaminant concentrations, and personal exposures (Dols & Polidoro, 2015). Airflows are comprised of infiltration, exfiltration, and air movement between internal zones, which are driven by natural or mechanical forces (Ng et al., 2018). CONTAM was used in this research due to its ability to capture dynamic interaction between HVAC systems and real-time weather and airflows in a quick manner (Ng et al., 2018). For coupling the multi-zone model to CFD0, three different methods exist [23]; the pressure-pressure coupling procedure was used in this research in which pressure is exchanged between CFD0 and CONTAM, and is considered as the most stable approach among all (L. Wang & Chen, 2007). Apart from co-simulation methods, the coupling is implemented in two different ways based on airflow impacts on internal or external surfaces. Thus, the external link is used for performing external airflow impacts on building enclosure air-paths, and the internal link is designated for embedding the CFD code to the interior airflow and contaminant transport network using CONTAM. It should be noted that the internal link could only be coupled for a single zone as well as the external link in which the ambient environment is considered as a sole zone, and building model is added within the zone as blockage object. Both models were employed in this research, which is described in the following two sub-sections:

**Internal Link for CFD0 Editor™ and CONTAM™ Co-Simulation.** In order to investigate the non-uniform concentration of outdoor-sourced air contaminants indoors, it was determined to embed the CFD0 zone within the CONTAM airflow network. In the internal coupling model, the boundary condition is initially assigned by CONTAM, then exported into the CFD0 Editor. This research assumed that each floor consists of a single zone to reduce the calculation loads and compensate for the limitation of the tool. Each zone bounded to 73.2mx48.8mx2.74m (LxWxH) with CFD mesh of 183x122x68. Figure 8 illustrates the workflow of internal co-simulation between CFD0 Editor™ and CONTAM™.

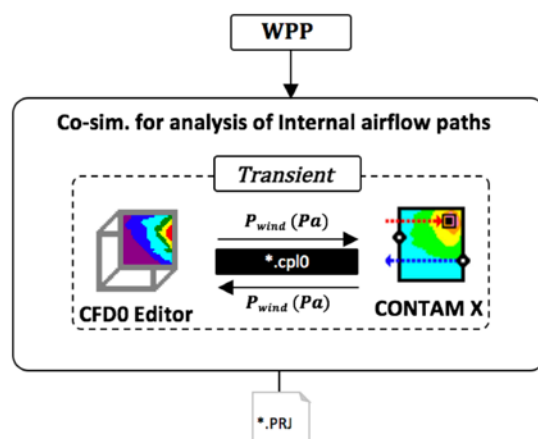


Figure 8: Workflow of internal CFD0 Editor and CONTAM co-simulation.

**Energy Modeling Procedure Using FMI Platform.** CONTAM and EnergyPlus can be coupled in order to implement combined airflow and heat transfer calculations (Dols & Polidoro, 2015). With the calculated inter-zonal airflow rates by CONTAM and CFD0, EnergyPlus was used to simulate hourly energy saving potentials (cooling and ventilation) during NV suitable hours. Figure 9 illustrates the workflow of coupled CONTAM and EnergyPlus for simulating IAQ and energy usage for the studied building.

## Coupled CONTAM and EnergyPlus Workflow

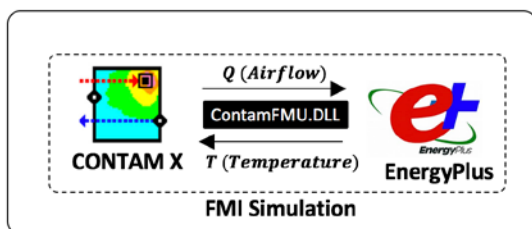


Figure 9: Workflow of IAQ and energy co-simulation.

## Conclusion

In this article, a novel framework was proposed for an integrated indoor air quality and energy modeling under different outdoor conditions through using a hybrid data-driven and simulation-based approach. The framework focuses on naturally ventilated office buildings in an urban context. The article presents the research background, followed by identifying gaps, objectives, methodology, and workflow of the framework. The initial results reveal that the impacts of traffic-induced emission rates are significantly higher than those obtained from gas combustion in buildings across the neighborhood. An initial test on the ANN model predicting the outdoor CFD simulation show a time-effectiveness of the procedure following the proposed framework.

## References

Abbasabadi, N., & Ashayeri, M. (2019). Urban energy use modeling methods and tools: A review and an outlook. *Building and Environment*, 161, 106270. <https://doi.org/10.1016/j.buildenv.2019.106270>

Challoner, A., Pilla, F., & Gill, L. (2015). Prediction of Indoor Air Exposure from Outdoor Air Quality Using an Artificial Neural Network Model for Inner City Commercial Buildings. *International Journal of Environmental Research and Public Health*, 12(12), 15233–15253. <https://doi.org/10.3390/ijerph121214975>

Chen, J., Augenbroe, G., & Song, X. (2018). Evaluating the potential of hybrid ventilation for small to medium sized office buildings with different intelligent controls and uncertainties in US climates. *Energy and Buildings*, 158, 1648–1661. <https://doi.org/10.1016/j.enbuild.2017.12.004>

Chicago Traffic Tracker, "Congestion Estimates by Regions | City of Chicago | Data Portal. (n.d.). Retrieved October 17, 2018, from <https://data.cityofchicago.org/Transportation/Chicago-Traffic-Tracker-Congestion-Estimates-by-Region/t2qc-9pjd>

Deru, M., & Torcellini, P. (2007). *Source Energy and Emission Factors for Energy Use in Buildings (Revised)* (No. NREL/TP-550-38617, 884990). <https://doi.org/10.2172/884990>

Dols, W. S., & Polidoro, B. J. (2015). *CONTAM User Guide and Program Documentation Version 3.2* (No. NIST TN 1887). <https://doi.org/10.6028/NIST.TN.1887>

Dutton, S. M., Banks, D., Brunswick, S. L., & Fisk, W. J. (2013). Health and economic implications of natural ventilation in California offices. *Building and Environment*, 67, 34–45. <https://doi.org/10.1016/j.buildenv.2013.05.002>

Energy Usage 2010 | City of Chicago | Data Portal. (n.d.). Retrieved October 15, 2018, from <https://data.cityofchicago.org/Environment-Sustainable-Development/Energy-Usage-2010/8yq3-m6wp>

Gómez-Losada, Á., Pires, J. C. M., & Pino-Mejías, R. (2018). Modelling background air pollution exposure in urban environments: Implications for epidemiological research. *Environmental Modelling & Software*, 106, 13–21. <https://doi.org/10.1016/j.envsoft.2018.02.011>

He, H., Lu, W.-Z., & Xue, Y. (2014). Prediction of particulate matter at street level using artificial neural networks coupling with chaotic particle swarm optimization algorithm. *Building and Environment*, 78, 111–117. <https://doi.org/10.1016/j.buildenv.2014.04.011>

Klepeis, N. E., Nelson, W. C., Ott, W. R., Robinson, J. P., Tsang, A. M., Switzer, P., ... Engelmann, W. H. (2001). The National Human Activity Pattern Survey (NHAPS): A resource for assessing exposure to environmental pollutants. *Journal of Exposure Science & Environmental Epidemiology*, 11(3), 231–252. <https://doi.org/10.1038/sj.jea.7500165>

Leslie, N. (2013). *American Gas Association 400 N. Capitol St., NW Washington, DC 2000. 72.*

Losada, Á. G., Pires, J. C. M., & Mejías, R. P. (2016). Characterization of background air pollution exposure in urban environments using a metric based on Hidden Markov Models. *Atmospheric Environment*, 127, 255–261. <https://doi.org/10.1016/j.atmosenv.2015.12.046>

Mendell, M. J., Eliseeva, E. A., Spears, M., Chan, W. R., Cohn, S., Sullivan, D. P., & Fisk, W. J. (2015). A longitudinal study of ventilation rates in California office buildings and self-reported occupant outcomes including respiratory illness absence. *Building and Environment*, 92, 292–304. <https://doi.org/10.1016/j.buildenv.2015.05.002>

Ng, L. C., Ojeda Quiles, N., Dols, W. S., & Emmerich, S. J. (2018). Weather correlations to calculate infiltration rates for U. S. commercial building energy models. *Building and Environment*, 127, 47–57. <https://doi.org/10.1016/j.buildenv.2017.10.029>

Preziosi, P. (2004). Workplace air-conditioning and health services attendance among French middle-aged women: A prospective cohort study. *International Journal of Epidemiology*, 33(5), 1120–1123. <https://doi.org/10.1093/ije/dyh136>

Rong, L., Liu, D., Pedersen, E. F., & Zhang, G. (2015). The effect of wind speed and direction and surrounding maize on hybrid ventilation in a dairy cow building in Denmark. *Energy and Buildings*, 86, 25–34. <https://doi.org/10.1016/j.enbuild.2014.10.016>

Shi, Z., Qian, H., Zheng, X., Lv, Z., Li, Y., Liu, L., & Nielsen, P. V. (2018). Seasonal variation of window opening behaviors in two naturally ventilated hospital wards. *Building and Environment*, 130, 85–93. <https://doi.org/10.1016/j.buildenv.2017.12.019>

Suh, H. H., Bahadori, T., Vallarino, J., & Spengler, J. D. (2000). Criteria Air Pollutants and Toxic Air Pollutants. *Environmental Health Perspectives*, 108, 9.

Tong, Z., Chen, Y., & Malkawi, A. (2016). Defining the Influence Region in neighborhood-scale CFD simulations for natural ventilation design. *Applied Energy*, 182, 625–633. <https://doi.org/10.1016/j.apenergy.2016.08.098>

Tong, Z., Chen, Y., Malkawi, A., Adamkiewicz, G., & Spengler, J. D. (2016). Quantifying the impact of traffic-related air pollution on the indoor air quality of a naturally ventilated building. *Environment International*, 89–90, 138–146. <https://doi.org/10.1016/j.envint.2016.01.016>

U.S. Department of Energy. (2012). *Annual Energy Review 2011* (No. 0384). Retrieved from <https://www.eia.gov/totalenergy/data/annual/pdf/aer.pdf>

U.S. EPA, O. (2016, September 26). AP-42: Compilation of Air Emissions Factors [Policies and Guidance]. Retrieved October 16, 2018, from U.S. EPA website: <https://www.epa.gov/air-emissions-factors-and-quantification/ap-42-compilation-air-emissions-factors>

Wang, L., & Chen, Q. (2007). Theoretical and numerical studies of coupling multizone and CFD models for building air distribution simulations. *Indoor Air*, 17(5), 348–361. <https://doi.org/10.1111/j.1600-0668.2007.00481.x>

Wang, L. L., Dols, W. S., & Chen, Q. (2010). Using CFD Capabilities of CONTAM 3.0 for Simulating Airflow and Contaminant Transport in and around Buildings. *HVAC&R Research*, 16(6), 749–763. <https://doi.org/10.1080/10789669.2010.10390932>

Wang, Y., & Malkawi, A. (2014). Annual hourly CFD simulation: New approach—An efficient scheduling algorithm for fast iteration convergence. *Building Simulation*, 7(4), 401–415. <https://doi.org/10.1007/s12273-013-0156-1>

Yang, Y., & Zhao, Y. (2012). Prevailing Wind Direction Forecasting for Natural Ventilation Adjustment in Greenhouses Based on LE-SVM. *Energy Procedia*, 16, 252–258. <https://doi.org/10.1016/j.egypro.2012.01.042>

Yi, Y. K., & Malkawi, A. M. (2012). Site-specific optimal energy form generation based on hierarchical geometry relation. *Automation in Construction*, 26, 77–91. <https://doi.org/10.1016/j.autcon.2012.05.004>