Assessment of occupant-behavior-based indoor air quality and its impacts on human exposure risk: A case study based on the wildfires in Northern California

Na Luo [1, 2, 3], Wenguo Weng [1, 2*], Xiaoyu Xu [1, 2], Tianzhen Hong [3], Ming Fu [4], Kaiyu Sun [3]

[1] Institute of Public Safety Research, Department of Engineering Physics, Tsinghua University, Beijing, 100084, P.R. China

[2] Beijing Key Laboratory of City Integrated Emergency Response Science, Tsinghua University, Beijing, 100084, China.

[3] Building Technology and Urban Systems Division, Lawrence Berkeley National Laboratory, USA

[4] Hefei Institute for Public Safety Research, Tsinghua University, Hefei, Anhui Province, 320601, China.

Abstract: The recent wildfires in California, U.S., have caused not only significant losses to human life and property, but also serious environmental and health issues. Ambient air pollution from combustion during the fires could increase indoor exposure risks to toxic gases and particles, further exacerbating respiratory conditions. This work aims at addressing existing knowledge gaps in understanding how indoor air quality is affected by outdoor air pollutants during wildfires—by taking into account occupant

*Correspondence and requests for materials should be addressed to Prof. Weng (email: wgweng@tsinghua.edu.cn)

behaviors (e.g., movement, operation of windows and air-conditioning) which strongly influence building performance and occupant comfort. A novel modeling framework was developed to simulate the indoor exposure risks considering the impact of occupant behaviours by integrating building energy and occupant behaviour modeling with computational fluid dynamics simulation. Occupant behaviors were found to exert significant impacts on indoor air flow patterns and pollutant concentrations, based on which, certain behaviors are recommended during wildfires. Further, the actual respiratory injury level under such outdoor conditions was predicted. The modeling framework and the findings enable a deeper understanding of the actual health impacts of wildfires, as well as informing strategies for mitigating occupant health risk during wildfires.

Key words: human exposure risk, indoor air quality, occupant behavior, respiratory injury, NAPA wildfire, computational fluid dynamics simulation

Introduction

Climate change is influencing large wildfire frequency and globally widespread disturbance that affect both human and natural systems (Hurteau et al. 2014). The 2013 Rim Fire in California has caused an average PM2.5 concentration of 20 μg/m^3 and ranged from 0 to 450 μg/m^3, which was proved to exert significant adverse health effects to a large population (Navarro et al. 2016). As another one of the worst wildfires recently, several massive wildfires swept Napa and Sonoma counties in the North Bay areas of San Francisco on the western coast of the United States on the night of October 8, 2017 (HST). The fires resulted in the worst air quality that has ever been recorded in the San Francisco Bay Area[1]. The outdoor air quality index[2,3], measured in particulate matter (e.g., PM2.5) exceeded 250 ug/m^3, and a measure of other criteria pollutants[4] (e.g., sulfur dioxide – SO_2) exceeded 200 ppb, indicating that the high level of air pollution could cause serious health effects in most people who breathed in the contaminated air outdoors.

A sudden increase in the number of hospitalizations during the days following the fires could be related to the negative health effects of high gaseous and particulate pollutant levels in the area, which included

[1] Xinhua. Massive wildfires engulf north San Francisco counties. http://news.xinhuanet.com/english/2017-10/10/c_136667925.htm Accessed 2017-10-10

[2] EPA USA. Air Data: Air Quality Data Collected at Outdoor Monitors Across the US. https://www.epa.gov/outdoor-air-quality-data Accessed 2018-06-15

[3] Air Quality Data Query Tool. https://www.arb.ca.gov/aqmis2/aqdselect.php Accessed 2018-806-15

[4] The criteria pollutants (also known as “criteria air contaminants – CAC”) are a set of air pollutants (normally six common pollutants, which are ozone, particulate matter, carbon monoxide, lead, sulfur dioxide, and nitrogen dioxide) that cause smog, acid rain and other health hazards.

increased risk for asthma, and deterioration of pre-existing respiratory diseases (Lewis et al. 2013). A number of recent researches reported effects of the different airborne particle metrics on respiratory diseases, cardiovascular effects, lung cancer, asthma, and lung cancer via human inhalation exposure (You et al. 2017; Haikerwal et al. 2015; Haddrell et al. 2015). In other words, during the past decades, wildfires have exerted a large negative global impact on human health, ecosystems, societies, economies and climate(Jolly et al. 2015; Jaffe et al. 2013). Even worse, according to the California's Fourth Climate Change Assessment Report (Bedsworth et al. 2018), there is no sign of abating in the expansion of wildfires due to the climate variations. There is an urgent need to mitigate the impacts of the adverse air quality on the human health caused by the increasing wildfires (Anderson et al. 2018; West et al. 2013).

Since individuals spend an average of 87% of their time indoors (Klepeis et al. 2001), indoor air quality (IAQ) is probably more indicative of the pollution exposure levels affecting residents' health than the outdoor measures. According to the report by the Institute of Medicine (2011), IAQ is affected by three main factors: occupant behavior (OB), building characteristics, and pollutant properties. Among them, as the most significant factor, OB affects IAQ through occupants' interactions with the outdoor physical environment. Behaviours such as window opening and closing (Stabile et al. 2017), HVAC operation, and walking into or out of a room (Montgomery et al. 2015) will change the boundary conditions of the indoor environment, thus influence

the flow pattern of indoor air, which, ultimately cause the increase or decrease of the indoor pollution levels.

Many previous experimental studies focused on the separate impacts of occupant behaviors and building performances on the indoor airflow patterns and pollutant diffusion process, such as human movements, air-conditioning system-related parameters and window operation-related natural ventilation (Luo et al. 2016; Luongo et al. 2016). Several Computational Fluid Dynamics (CFD) models have also been improved by validating with quantitative measurements (Luo et al. 2018b; Gosselin and Chen 2008). These investigations revealed detailed information about indoor air flow patterns and pollutant concentration levels under different specific conditions. However, in a real office environment, occupant behaviors are always complex and dynamic due to transient indoor conditions such as temperature, humidity, and occupant counts, which are mostly associated with the outdoor environment (Lin et al. 2017). Also, when assessing the impacts of the indoor environment on human health, exposure to air pollution is not only largely determined by pollutant concentrations in the spaces where people spend their time, but also by the amount of time they spend in those spaces. Therefore, the static status of the indoor environment is no longer suitable and appropriate for evaluating the indoor human exposure risks during daily working hours; a set of OB-related dynamic schedules should be first generated to guide the indoor CFD modeling and risk evaluation. Furthermore, for a given indoor environment, the respiratory

injury level is also crucial for assessing adverse health impacts of wildfires, which requires the pollutant concentration near the oro-nasal as the boundary condition for assessment. PM2.5 and ultrafine particles are both considered as the representative pollutants when indicating the indoor air quality level to the public (Ibald-Mulli et al. 2002; Zhao et al. 2009). Several studies recognized that PM2.5 are better related to resuspension phenomena and combustion processes, while quite a high amount of our overall daily dose of ultrafine particles is due to the indoor sources. Considering the access to the measured data for further validation, we selected PM2.5 as the main particle metrics in this work.

Here we used both EnergyPlus and Fluent to co-simulate indoor occupant behaviors as well as the corresponding IAQ and particle deposition inside respiratory systems, respectively. Indoor pollutant concentrations were simulated and used to calculate the IAQ index, which indicated potential adverse health effects. Results of the properties affected by particle concentrations near the mouth and nose of occupants, could be potentially used as the initial and boundary conditions for the assessment of the respiratory injury. Outcomes from the study formulated a framework for modeling (as shown in Figure 1) exposure to indoor pollutants as well as the potential assessment of human health hazards in an office environment—considering occupant movement and behavior, which can inform strategies to mitigate occupant health issues during times of serious outdoor air pollution such as wildfires. For broader application, this co-simulation

framework among Building Energy Modeling (BEM), occupant behavior modeling and CFD builds a bridge in the outdoor-to-indoor penetration process especially considering the indoor occupant behaviors, which thus could be broadly applied in the assessment of indoor quality under many other extreme weather events or use cases such as haze pollution in China, as well as the vehicle exhaust etc.

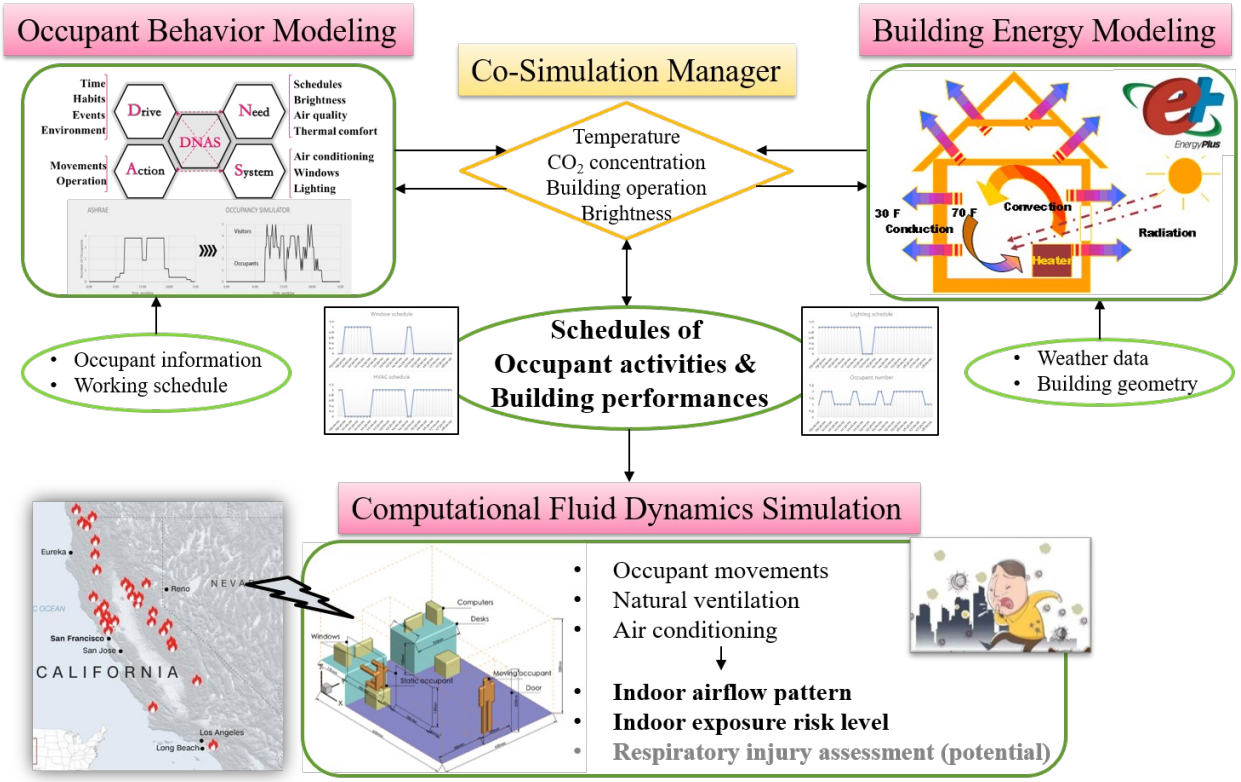

Figure 1 Overview of the modeling framework. The Building Energy Modeling tool (EnergyPlus) was co-simulated with the Occupant Behavior Modeling tool (obFMU – a functional mockup unit of occupant behavior model) to calculate the occupant-related schedules, primarily based on the outdoor environment and the building performance. These modeled activities and building performances were then integrated into the Fluent modeling process as the boundary conditions through a C++ user-defined function (UDF), to further calculate the indoor airflow and contaminant concentration. Eventually, the corresponding indoor exposure risk could be evaluated, as well as the respiratory injury level as one of the potential assessments in the future work.

Materials and Methods

Occupant behavior modeling. Whole building performance simulation, using EnergyPlus coupled with obFMU, has been used to simulate occupant behavior and generate occupant-related schedules in the last decade (Hong et al. 2017). EnergyPlus is an open-source program that models heating, ventilation, cooling, lighting, water use, renewable energy generation, and other building energy flows (Crawley et al. 2001). It is the flagship building simulation engine supported by the United States Department of Energy (DOE). The occupant behavior function mockup unit (obFMU) is an occupant behavior-modeling tool developed by Lawrence Berkeley National Laboratory (T. Hong et al. 2016). It was developed for co-simulation with EnergyPlus, requiring an XML file generated based on the obXML (occupant behavior eXtensible Markup Language) schema (Hong, D'Oca, Taylor-Lange, et al. 2015) and a configuration file. The obXML schema describes the occupant behavior by implementing a DNAS (drivers-needs-actions-systems) framework (Hong, D'Oca, Turner, et al. 2015). The obFMU is the engine for occupant behavior simulation and co-simulates via the functional mockup interface (FMI) with building performance simulation programs, e.g., EnergyPlus and ESP-r.

Occupant behavior activities. In this work, the simulated scenario is designed in an office room with two occupants working as different types. One occupant keeps working on the computer, while the other works as a secretary, who might often walk out of the room to get printed materials or

coordinate with other people. The simulation period is from 9:00am to 6:00pm, which are the working hours for the office workers. According to the weather data on October 13, 2017, the building performance, including the four occupant-related schedules and the operation characteristics of the indoor facilities, were modeled in EnergyPlus. Four categories of occupant behavior models were used in this study: occupant movement, lighting, windows, and HVAC operation. They were used to describe the characteristics of related occupant behaviors, based on which the probability of occupants taking an action is estimated. More specifically, Chen's agent-based stochastic occupant movement model (Chen et al. 2018), Haldi's lighting control models (switch on light at arrival or when it is dark, switch off at departure) (Haldi 2013), and Newsham's window control model (open at arrival or when the outdoor environment is suitable, close at arrival, departure or when the outdoor environment is not suitable) (Newsham 1994) were adopted. HVAC operation is a combination of availability schedule and actual window operation. In other words, when the window is open, the HVAC system will be off; when the window is closed, the HVAC system will be on if occupants feel hot. The occupant behavior models were compiled in an obXML file, which worked as the input to obFMU and was used to co-simulate with EnergyPlus. Occupant-related schedules, including the occupancy schedule, lighting schedule, natural ventilation schedule (namely window schedule), as well as the HVAC schedule were generated in the simulation process, seen in Figure 2. As for the detailed characteristics, the operation

parameters of the windows and HVAC refer to the velocity, temperature, and pollutant concentration of the inlet airflow. The electric power of the lighting and computers was associated with the indoor environment in the modeling process. The changes of occupant count represented the moments when the occupant was entering or leaving the room.

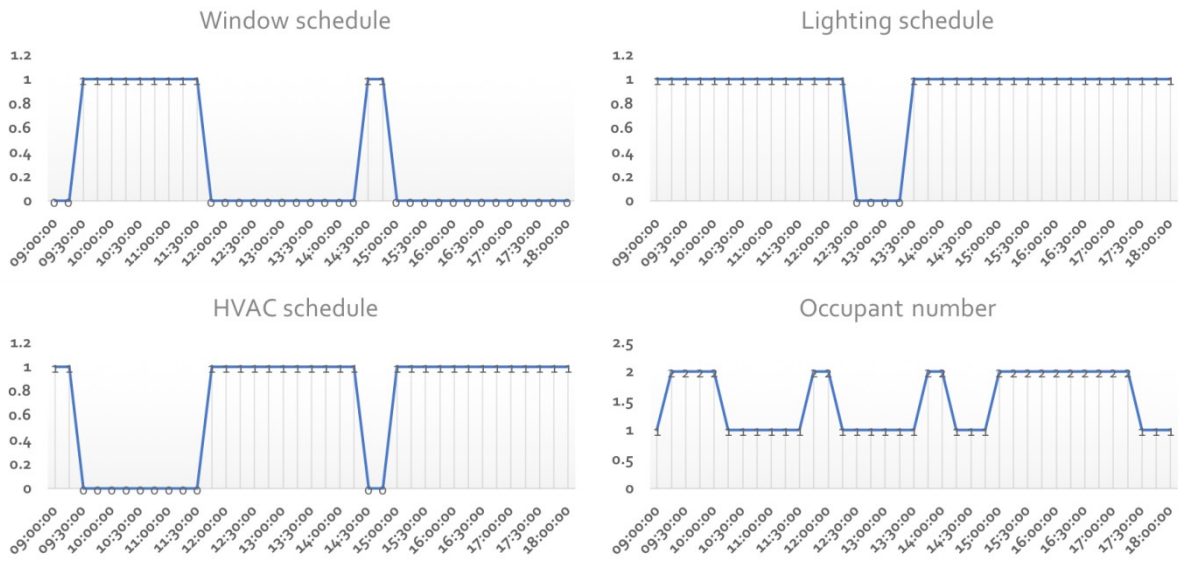

Figure 2. Four occupant-related schedules from the co-simulation of EnergyPlus and obFMU.

Indoor air flow field modeling. The CFD software ANSYS Fluent (Version 20018.0.0) was employed to simulate the transient indoor flow field affected by the occupant behaviors. Gambit (Version 2.4.6) was used to build the geometric model of the office room (Figure 3) and generate the grids for simulation. The total number of grids is 6.7 million. The minimum mesh volume was $2.64 \times 10^{-9} m^3$, located close to the skin of the moving occupant. The method of mesh generation was used in our previous study (Luo et al. 2062018a, 2018b). The transient solver was employed during the calculation. As for representing the turbulence airflow caused by the ventilation and

occupant movements, the RNG k-ε model adopted in this work was validated by previous work (Zhang et al. 2009; Han et al. 2014; Fracastoro et al. 2002), with the overall consideration of accuracy, computing efficiency, and affordability for modeling the indoor flow field. The differential viscosity model and the swirl dominated flow in the RNG options were selected. During the iterative process, the pressure-implicit with splitting of operators (PISO) algorithm was employed to solve the pressure-velocity coupling equations. The second-order upwind scheme was also used to consider the diffusion-convection in the governing equation. The Discrete Element Model (DEM) Collison term and the Brownian Motion term were both applied to include the particle-particle interactions (voidage and collision), which captured the particle resuspension phenomenon of PM2.5. According to the aforementioned schedules and the related parameters, a UDF in the Fluent software has been created to automate the transient changes of the window boundary conditions, HVAC boundary conditions, light conditions, and the human movement status. The gaseous composition and the corresponding concentrations of the inlet airflow were based on the measured outdoor air quality data, seen in Table 1. The time steps during the occupant moving and static process were set to 0.01 s and 1 s, respectively. The calculation is computed in a four-node Linux cluster. Each node of the cluster has 12 processors (2.4 GHz Intel 64). The overall simulation period in this case is nine hours (32400 seconds), which requires 120 hours of the computing time.

Table 1. The daily maximum outdoor air quality of some criteria pollutants (SO_2, CO, and O_3) and the particulate matter (PM2.5) within the following week after the wildfire event in Northern California (October 8 – 14, 2017). The gaseous composition and the corresponding concentrations of the inlet airflow was based on the measured outdoor air quality data.

	Oct. 8	Oct. 9	Oct. 10	Oct. 11	Oct. 12	Oct. 13	Oct. 14
SO_2 (ppb)	65.90	89.49	/	/	248.93	439.05	345.92
CO (ppm)	0.80	1.19	/	1.29	1.83	2.84	2.29
O_3 (ppb)	12.72	25.49	31.40	33.54	76.57	92.08	50.48
PM2.5 (ug/m^3)	86.30	115.30	214.70	/	91.97	212.49	179.40

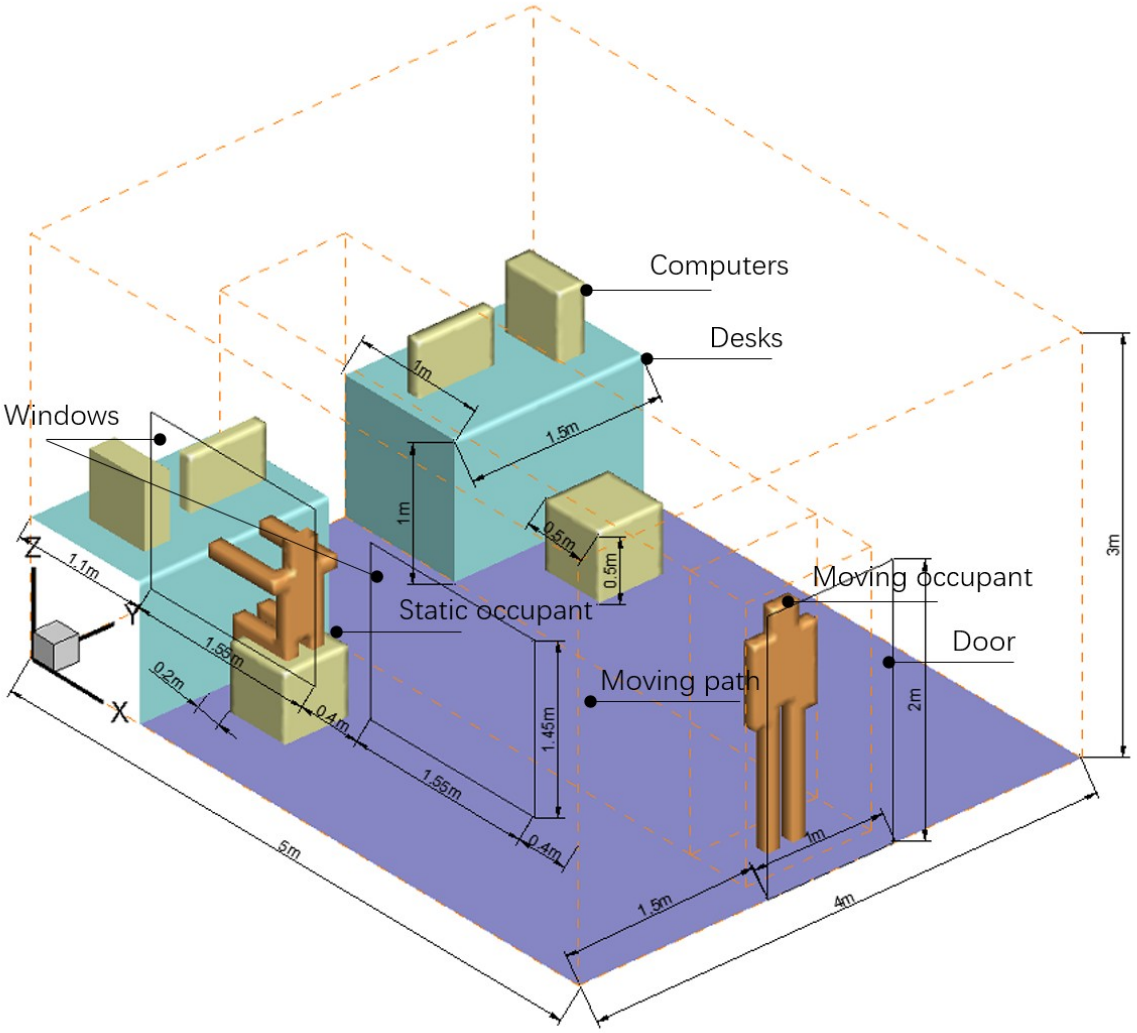

Figure 3. The geometrical features of the office room. There are two desks (1.0 m × 0.5m × 0.7 m in length × width x height) at one side of the room (5 m × 4 m × 3 m in length × width × height). One occupant remains sitting in front of the desk, the other one (1.75 m-height) walks through the door (2 m × 1 m in height × width), which is on the other side of the room. There are two windows (1.55 m × 1.45 m in width × height) on the side wall, which is adjacent to the seated occupant. The diffuser outlet of the HVAC (0.3 m × 0.2 m in width × height) is at the top of the wall towards the door. The lighting fixture is at the center of the celling.

UDF setting. The UDF (user-defined function) setting is a very important link in the overall framework, serving as a “bridge” connecting the outdoor and indoor concentration conditions, as well as taking the occupant behavior into consideration. The aforementioned generated occupant-related schedules determined both the natural and mechanical ventilation strategies (such as opening and closing time, as well as the air flow rate and its temperature etc.), these strategies were implemented in the CFD simulation as “time-series data” through coding the user-defined function. The natural ventilation strategy in Newsham’s research (Newsham 1994) is adopted in this work (open at arrival or when the outdoor environment is suitable, close at arrival, departure or when the outdoor environment is not suitable). Thus, when the windows were opened, the gaseous and particulate pollutants were blown into the room through the windows and the doors, where the velocity and temperature of the inlet airflow were set as the EnergyPlus modeling results. As for the mechanical ventilation strategy, it is a combination of availability schedule and actual window operation (when the window is open, the HVAC system will be off; when the window is closed, the HVAC system will be on if occupants feel hot). While the HVAC system was on, the windows

and the door, as well as the outdoor air system of the HVAC system, were all considered to be closed. The air purification system was assumed to be active in this work, with a removal rate of 50%. Thus, the gaseous composition and the corresponding concentrations of the next timestep's inlet airflow were calculated and input in the UDF code, according to the 50% concentration of reduced pollutants of the last timestep around the HVAC outlet. The air temperature and velocity of the inlet airflow were also set using the EnergyPlus modeling results. As for the movement behavior, the walking speed of the occupant was set to 1 m/s, and it took 5 s walking from the door to his seat (same in the opposite direction).

Calculation of IAQ index. The IAQ index is an index developed by the United States Environmental Protection Agency (EPA) that is used to indicate the indoor air quality in terms of its adverse health effects. On one side, the pollutant concentrations can be converted into the index value based on an empirical piecewise linear function. The breakpoints of specific pollutants are guided in the reports released by WHO in 2005 and 2010 (World Health Organization 2005; 2010). On the other side, the calculated index values are corresponding to different levels of adverse health symptoms based on many previous epidemiological studies and surveys. The IAQ index for each pollutant can be calculated from the modeled pollutant concentration results, as shown in Eq. 1.

$$I_P = \frac{I_{Hi} - I_{Lo}}{BP_{Hi} - BP_{Lo}}(C_P - BP_{Lo}) + I_{Lo} \quad (1)$$

where I_P is the index for pollutant P, C_P is the rounded concentration of pollutant P, BP_{Hi} is the breakpoint that is greater than or equal to C_P, BP_{Lo} is the breakpoint that is less than or equal to C_P, I_{Hi} is the AQI value corresponding to BP_{Hi}, and I_{Lo} is the AQI value corresponding to BP_{Lo}. According to the aforementioned concentration distribution, the average potential inhaled concentration was calculated within the vertical plane in front of the static human. The corresponding air quality level was then calculated based on Eq. 1. While the final AQI is the highest value calculated for each pollutant (Shi et al. 2015).

Results

Verification of the consistency of the two simulations. It was assumed that the occupant-related schedules remained the same in the two simulated environments of EnergyPlus and Fluent, making the process consistent. Due to the model that we employed in the obFMU, decision making regarding the operations of windows and HVAC was largely dependent on the indoor environment, especially room air temperature. Thus, to verify the consistency of the two simulated environments, indoor average temperature was chosen as the parameter for comparison. Figure 4 shows the indoor temperature modeled in EnergyPlus and Fluent, respectively. The occupant-

related schedules generated in EnergyPlus were proved to be reasonable for the indoor environment simulated in Fluent.

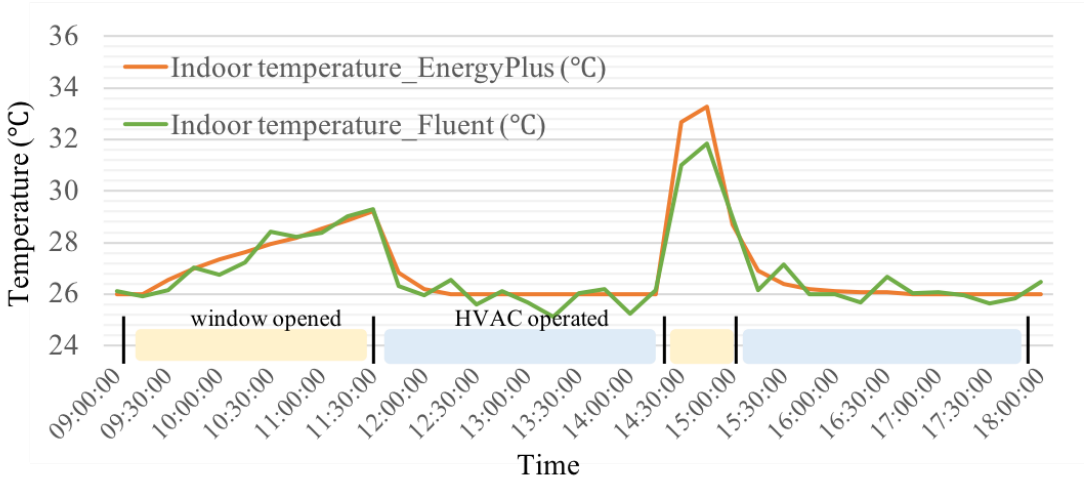

Figure 4. The indoor temperature simulated in EnergyPlus and Fluent. For EnergyPlus and Fluent simulations, indoor temperature both rose slowly till around 29.2 ℃ before 11:30 am, when the windows were opened. Then, the temperature remained at around 26.0 ℃ until 2:30 pm within the duration when the HVAC was turned on. The same phenomenon appeared for such behaviours afterward. Thus, the occupant-related schedules generated in EnergyPlus were reasonable for the indoor environment simulated in Fluent.

IAQ from measured data and simulated results. The indoor and outdoor air qualities before and after this wildfire event were provided by the Indoor Environment Group at Lawrence Berkeley National Laboratory (LBNL). Some office rooms inside the Building 51F in Lawrence Berkeley National Laboratory (LBNL) are serving as a living laboratory to continually monitor the indoor and outdoor carbon dioxide and pollutant concentrations (e.g., ozone, particular matters). Figures 5-6 show the comparisons of IAQ level (namely ozone and PM2.5) between the measured and simulated results. Since more detailed IAQ measurement was not available, we chose the

average and maximum concentration levels as the comparison indexes of the measured and simulated results. From Oct. 8 to Oct. 15, 2017, IAQ worsened after the breakout of the wildfire, and continued for the next whole week (Figure 5 (a)). During this week, the average concentration level of the indoor ozone was 18.11 ppb. The maximum levels of the ozone reached 47.97 ppb on October 12, 2017, when the outdoor quality data was 76 ppb. The simulated average and maximum levels of ozone in Figure 5 (b) were overall consistent with the measured results, except for two details. First, ozone is a highly reactive component that reacts quickly with surfaces when penetrating indoors, which is why the measured ozone levels are generally lower than those modeled levels. Second, the measured indoor ozone level stayed at 10 ppb during the night when all unintentional openings of the building were closed, during which time, the simulated result was almost zero. These differences between the measured and modeled results were supposed to be associated with air infiltration in the building and are further discussed in the discussion section.

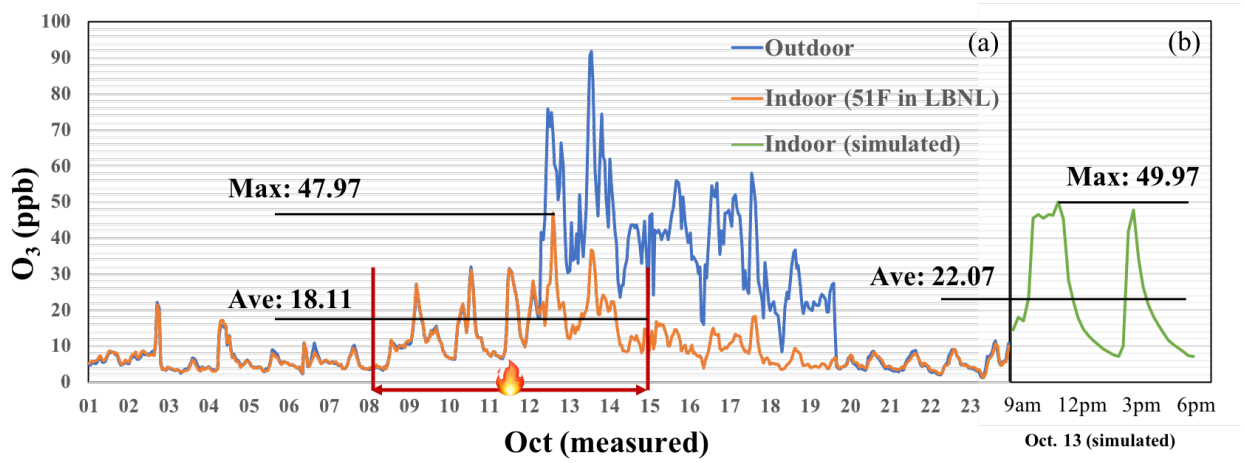

Figure 5 Comparison of the measured and simulated O_3 levels. (**a**) Concentration of Ozone measured indoors and outdoors, before, during and after the wildfire. (**b**) The simulated concentration of the indoor Ozone on Oct. 13.

Measured data of particle levels from October 12 to 14 indicate that the maximum and average levels of PM2.5 were 91.97 ug/m^3 and 51.44 ug/m^3, respectively (Figure 6 (a)), while those of the simulated results were 131.49 ug/m^3 and 53.02 ug/m^3, respectively (Figure 6 (b)). The simulated results were a little higher than the measured data, which might be due to less consideration of the particle interaction. Comparing to the outdoor concentration, the indoor PM was about 65% of the outdoor level on average, under an air exchange rate of 0.7 air changes per hour in this work.

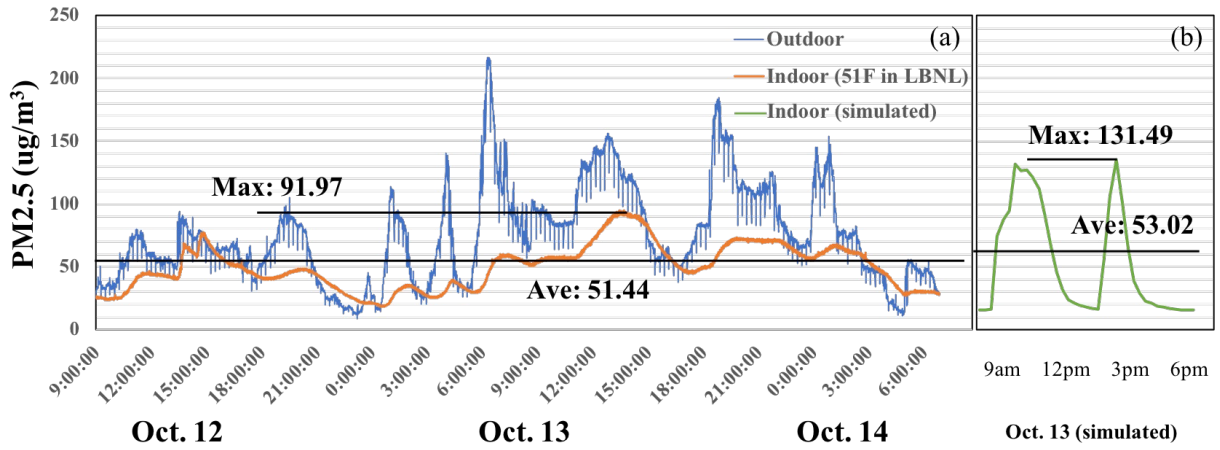

Figure 6 Comparison of the measured and simulated PM2.5 levels. (**a**) Concentration of PM2.5 measured indoors and outdoors during the wildfire. (**b**) The simulated concentration of the indoor PM2.5 on Oct. 13.

The fluctuant simulated results indicated that occupant behaviors exerted a large influence on the indoor pollutant concentration during the working hours. Through the comparison, the fluctuant indoor concentration level was proved to be consistent with the measured data in the actual office environment if the occupant behaviors were considered during the simulation.

Flow pattern and concentration distribution. The plane in front of the oronasal (x=1.25m, see Figure 3) region was chosen as the potential inhalation region. The evolution of the flow structure and the concentrations of different gaseous pollutants in this region may largely influence human inhalation doses, which is significant in assessing exposure risk levels. According to the aforementioned outdoor air quality on that day, the outdoor concentration of sulfur dioxide (SO_2) was much higher than an average day,

and its hazard level was higher than that of carbon monoxide and ozone. Thus, sulfur dioxide was chosen as the representative pollutant to investigate its diffusion characteristics.

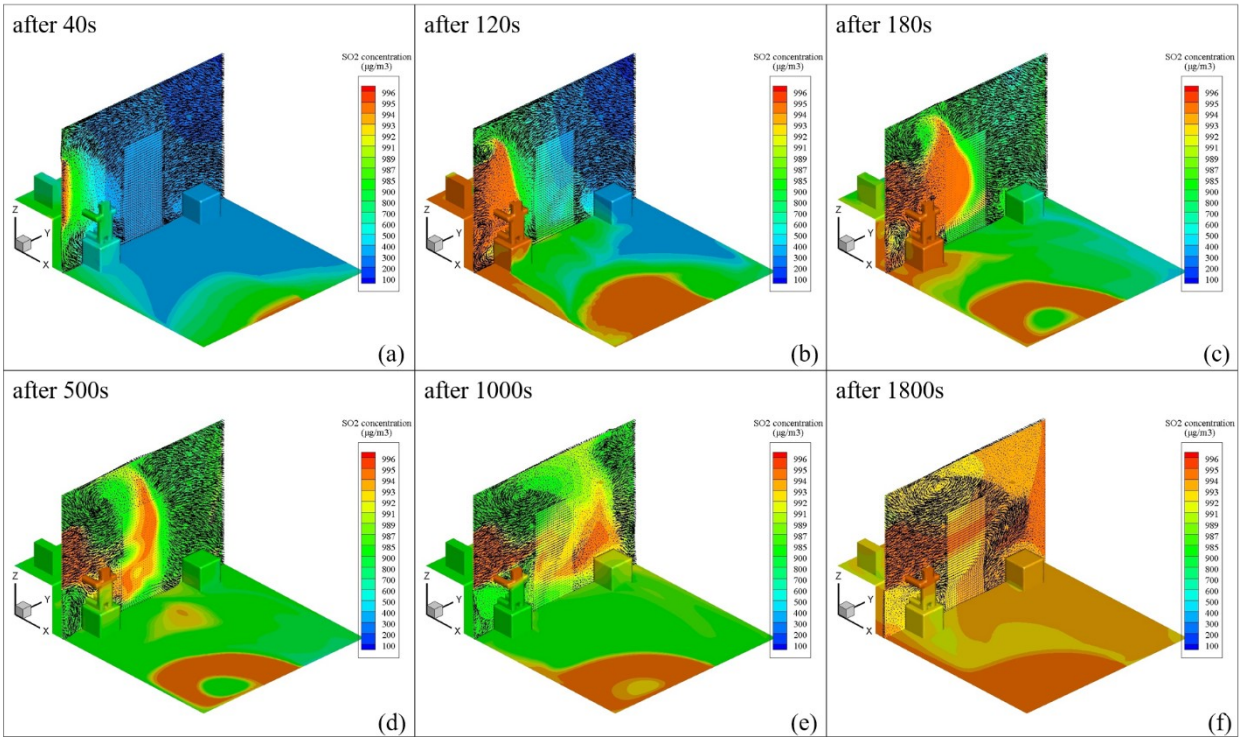

Figure 7 The velocity and concentration fields of SO_2 indoors after the windows were opened. (**a**) At inhalation plane, 40s after the window was opened. (**b**) After 120s. (**c**) After 180s. (**d**) After 500s. (**e**) After 1000s. (**f**) After 1800s.

Operation of windows exerted a significant impact on flow pattern and concentration distribution (Figure 7). Outdoor sulfur dioxide was diffused quickly through the windows. Owing to the short distance between the seated occupant and the windows, the concentration of the sulfur dioxide near the oro-nasal region reached a relatively high level just after 120s (Figure 7 (b)). The inlet airflow was affected by transient outdoor weather

data, such as wind velocity and direction outdoors. Meanwhile, the diffusion of the inlet airflow was also influenced by the existent indoor airflow circulation. Eventually, the concentration of sulfur dioxide remained at a steady state after 30 min, which was around 995 ug/m^3 (348.25 ppb). Due to the same pattern of the velocity field, concentration evolutions for carbon monoxide and ozone were similar to that of the sulfur dioxide. Eventually, after 30 min of opening the windows, concentrations of indoor carbon monoxide and ozone on the inhalation region (x=1.25 m) reached around 1.40 mg/m^3 (1.12 ppm) and 107.08 ug/m^3 (49.97 ppb), respectively.

Flow pattern and concentration distribution caused by other occupant behaviors such as air-conditioning and movement can be found in Figure 8-9. The velocity and concentration fields on the plane near the HVAC outlet 300 s after the HVAC was turned on, indicated the effects of the HVAC operation on the IAQ (Figure 8 (a)). The cold air coming from the HVAC outlet moved downwards during the diffusion (Figure 8 (b-f)). 1300 s after the HVAC operation, the concentration of indoor sulfur dioxide dropped to 500 ug/m^3. And 6000 s after the HVAC operation, the concentration of sulfur dioxide remained at a relatively steady state, which was around 100 ug/m^3. Combined with the aforementioned analysis, occupants are advised to keep the windows closed and run the HVAC systems with the outdoor air dampers shutting off during wildfire to mitigate the indoor exposure risk.

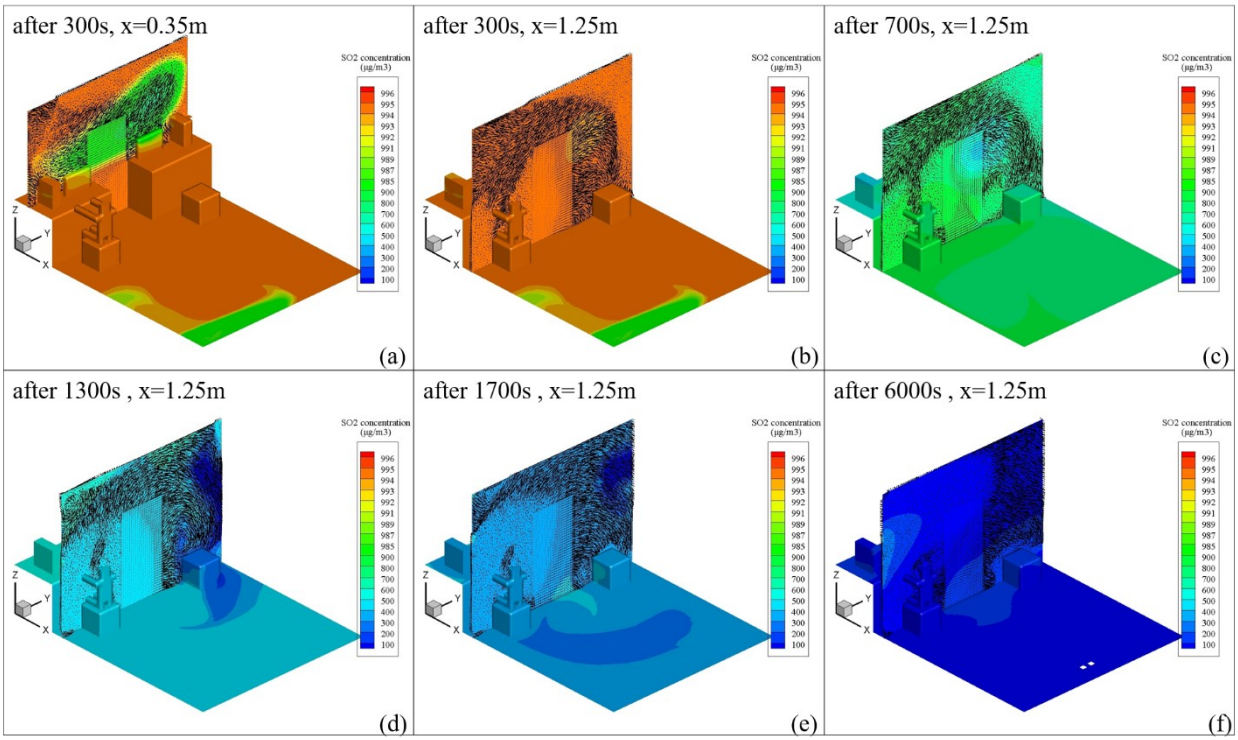

Figure 8 The velocity and concentration fields of SO_2 indoors after the HVAC was turned on. (**a)** At the plane near the HVAC outlet, 300 s after the HVAC was operated. (**b**) At inhalation plane, 300 s after the HVAC was operated. (**c**) After 700 s. (**d**) After 1300 s. (**e**) After 1700 s. (**f**) After 6000 s.

The effects of the occupant movements, i.e. walking out of and into the room, can be found in Figure 9 (a-c) and (d-f), respectively. A strong downward airflow was observed behind its upper body, carrying the gaseous pollutant downwards; while the gap between the lower limbs exerted a horizontal flow between the legs, which enhanced the diffusion speed of the pollutants. The detailed information of the velocity fields evaluated in this study has been verified in a previous PIV experimental study (Luo et al. 2018a). Overall, the movement behavior accelerated the diffusion and mixture of the existed contaminants at different heights, which enhanced the

risk of respiratory exposure. Therefore, occupants are recommended to limit walking activities during the extreme wildfires.

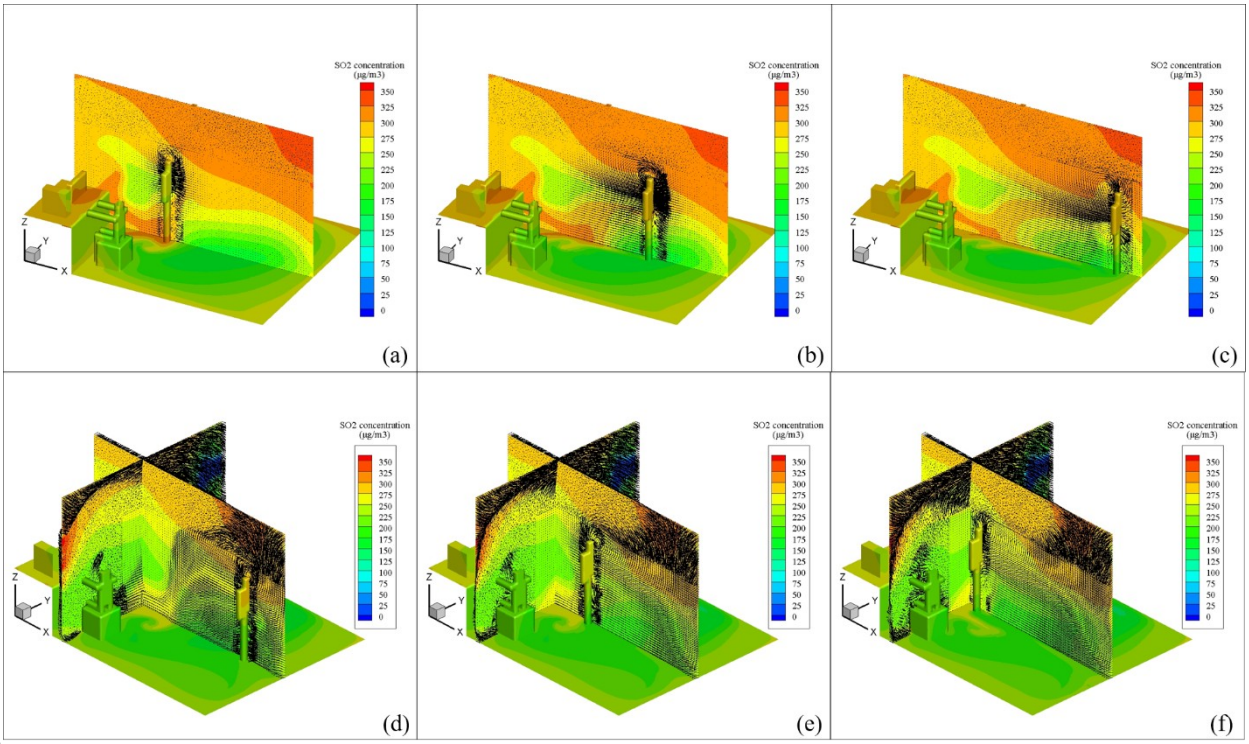

Figure 10 The velocity and concentration fields of SO_2 along the moving. (**a-c**) The occupant was walking out of the office. (**d-f**) The occupant was walking into the room.

Assessment of the daily exposure risk level. Epidemiological studies have linked exposure to indoor air pollution with a wide range of adverse health outcomes. The health effects and the breakpoints of some specific pollutants considered in this study are listed in Table 2 (documented from (WHO 2010; Mintz 2013; World Health Organization 2005)).

Table 2. Pollutant-specific sub-indices and health effects statements for guidance on the AQI. The IAQ index for each pollutant can be calculated from the modeled pollutant concentration results, seen in Methods.

AQI Categories: Index	Ozone (ppb)		Sulfur Dioxide (ppb)		Carbon Monoxide (ppm)	Particulate Matter (ug/m^3) [24-hour]
	[1-hour]	[8-hour]	[1-hour]	[24-		

Values				hour]	[8-hour]	
Good (Up to 50)	-	0-59 None	0-35	0-30	0-4.4 None	0-12.0 None
Moderate (51-100)	-	60-75 Unusually sensitive individuals may experience respiratory symptoms	36-75	>30-140	4.4-9.4 None	12.1-35.4 Respiratory symptoms possible in unusually sensitive individuals; possible aggravation of heart or lung disease in people with cardiopulmonary disease and older adults
			None			
Unhealthy for Sensitive Groups (101-150)	125-164	76-95	76-185	140-220	9.5-12.4 Increasing likelihood of reduced exercise tolerance due to increased cardiovascular symptoms, such as chest pain, in people with heart disease	35.5-55.4 Increasing likelihood or respiratory symptoms in sensitive individuals; aggravation of heart or lung disease and premature mortality in people with cardiopulmonary disease, older adults, and people of lower SES
	Increasing likelihood of respiratory symptoms and breathing discomfort in people with lung disease, such as asthma, children, older adults, and outdoor workers		Increasing likelihood of respiratory symptoms, such as chest tightness and breathing discomfort in people with asthma			
Unhealthy (151-200)	165-204	96-115	186-304	220-300	12.5-15.4 Reduced exercise tolerance due to increased cardiovascular symptoms, such as chest pain, in people with heart disease	55.5-150.4 Increased aggravation of heart or lung disease and premature mortality in people with cardiopulmonary disease, older adults, and people of lower SES; increased respiratory effects in general population
	Greater likelihood of respiratory symptoms and breathing difficulty in people with lung disease, such as asthma, children, older adults, and outdoor workers; possible respiratory effects in general population		Increased respiratory symptoms, such as chest tightness and wheezing in people with asthma; possible aggravation of other lung disease			
Very Unhealthy (201-300)	205-404	116-374	305-604	300-600	15.5-30.4 Significant aggravation of cardiovascular symptoms, such as chest pain, in people with heart disease	150.5-250.4 Significant aggravation of heart or lung disease and premature mortality in people with cardiopulmonary disease, older adults, and people of lower SES; significant increased respiratory effects in general population
	Increasing severe symptoms and impaired breathing likely in people with lung disease, such as asthma, children, older adults, and outdoor workers; increasing likelihood of respiratory effects in general population		Significant increase in respiratory symptoms, such as wheezing and shortness of breath, in people with asthma; aggravation of other lung diseases			
Hazardous (301-500)	405-604	-	605-1004	600-1000	30.5-50.4 Serious aggravation of cardiovascular symptoms, such as chest pain, in people with heart disease; impairment of strenuous activities in general population	250.5-500.4 Serious aggravation of heart or lung disease and premature mortality in people with cardiopulmonary disease, older adults, and people of lower SES; serious risk of respiratory effects in general population

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According to the modeled concentration results, where the 1-hour SO_2 value was 348.25 ppb, CO value was 1.12 ppm, the O_3 value was 47.97 ppb, and the PM2.5 value was 131.49 ug/m^3, the calculated maximum IAQ index was 215, with SO_2 as the responsible pollutant. Qualitative evaluation indicated that this environment would cause an increasing likelihood of respiratory symptoms, such as wheezing, chest tightness and breathing discomfort in people with asthma, as well as an increasing aggravation of other lung diseases. However, to achieve the quantitative evaluation of the injury level, further analyses should be conducted considering an entering path of the particle and gaseous contaminants into the body through breathing. The modeled dynamic indoor contaminant concentration can be served as a boundary condition.

As for the impact of occupant behaviors on the daily exposure risk level, due to the distribution of different indoor occupant behaviors, the indoor pollutant concentration fluctuated obviously during the working hours. Activities such as opening the windows as well as walking into and out of the rooms led to the increase of the pollutant concentration and thus the exposure risk of the human body and respiratory. While turning on the air-conditioning without the function of supplying fresh air decreased the indoor contaminant concentration in a slow but effective way. Therefore, to mitigate indoor exposure risk, occupants are advised to keep windows closed and limit walking activities during the extreme wildfires. Meanwhile, outdoor air dampers should be shutting off when operating the HVAC system to avoid

more purification loads. From another aspect, a proper and accurate set of occupant behavior schedules and the corresponding building boundary conditions are also crucial for enhancing the evaluation and prediction of the indoor risk exposure.

Discussions

This study formulated a framework for the indoor pollutants exposure modeling and the potential human health hazard assessment in an office environment particularly taking into account the actual occupant behaviours. The simulated results under this framework were compared with the actual measured indoor and outdoor data (O_3 and PM2.5), showing great consistency in both the maximum and average levels. The indoor airflow pattern and IAQ fluctuated obviously within working hours, which were largely dependent on specific occupant behaviors. Therefore, comparing to the traditional IAQ and occupant exposure assessments when occupants remained static or the indoor equipment (e.g., HVAC and windows) remained constant running, the framework in this study is proved to provide a more realistic and reliable result aligned with the actual requirement of assessing the health hazard level of the indoor occupants. Furthermore, based on this result as a boundary condition, the deposit fraction and equation can be fitted to predict a more accurate and dynamic respiratory exposure dosage under such outdoor wildfire conditions, which not only indicates the key injury level, but also provides reference for the further physiological stage.

Assessment of the respiratory injury

As aforementioned, the indoor pollutant concentration near the oro-nasal could be considered as the boundary condition for assessing the respiratory deposition. Take nasal inhalation as an example, respiratory injury was mainly caused by the micron particle deposition fraction in nasal cavity, pharynx, larynx and trachea regions for nasal breathing. The detailed modelling method and flow pattern inside the respiratory system were included in another published journal article (Xu et al. 2018).

The simulated particle size range was slightly expanded to allow a wider coverage of the developed deposition equations. For micron-sized particles, deposition fractions were related to the inertial parameter I, which considered particles mass to the square power, and the averaged fluid momentum. The inertial parameter is defined as:

$$I = d_p^2 Q \tag{2}$$

where Q is the volume flow rate (cm^3/s) and d_p (μm) is the particle aerodynamic diameter. Figure 11(a) and (c) show the deposition fraction in human respiratory airways for particles ranging from 0.8 μm to 20 μm against the inertial parameter for oral and nasal inhalation, respectively.

The Stokes number was used to correlate the deposition to length scale, particle density, size and flow rate. It is defined as:

$$St = \frac{\rho_p d_p^2 u C_c}{18 \mu L} \tag{3}$$

where L is the characteristic length of oral and u is the local airflow velocity. The deposition through oral breathing in human airway was related to St and Re.

For the deposition equation in human airway, improved fittings were obtained with $St^{3.271}Re$ and $St^{1.77}Re^{0.145}$ for particle sizes from 0.8 to 20 μm, breathing rate of 10 and 30 L/min for oral and nasal breathing (Figure 11(b) and (d)), with a coefficient of determination $R^2=0.99$. The empirical equations are given as

$$DF_{oral} = [1 - \frac{0.956}{22.701 St^{3.271} \mathrm{Re} + 1}] \times 100\% \quad (4)$$

$$DF_{nasal} = [1 - 0.95 \exp(-7.35 \cdot St^{1.77} \mathrm{Re}^{0.145})] \times 100\% \quad (4)$$

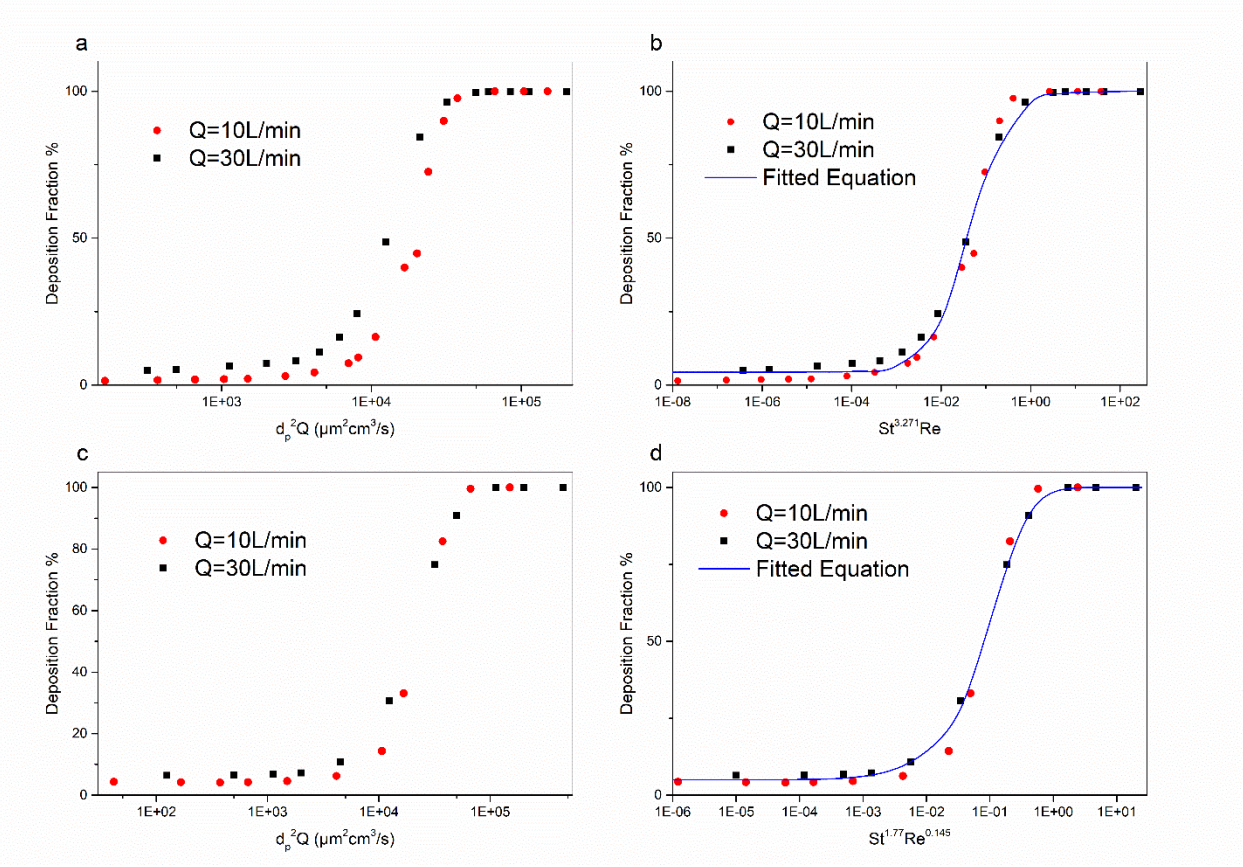

Figure 11 Comparison of micron particles (0.8 – 20 μm). (**a**) deposition fraction for oral inhalation. (**b**) fitted deposition equation for oral inhalation. (**c**) deposition fraction for nasal inhalation. (**d**) fitted deposition equation for nasal inhalation.

The dosimetry (in number, mass, surface area) in human upper airway under various breathing flow rates and breathing pattern was calculated by using the above simulated PM2.5 concentration value, presented in Table 3. The time period of occupants staying indoors was assumed as 8 hours a day (as the working hours from 9am to 5pm). A monotonous growth was obtained in human upper airway dosimetry with the flow rate, which lead to a larger air exchange and particle exposure risk, as well as a higher probability of chronic respiratory diseases.

Table 3 Human upper airway dosages of indoor PM2.5 during a day.

Q (L/min)	Oral inhalation			Nasal inhalation		
	Number (10^6#)	Mass(μg)	Surface area ($10^{-5}m^2$)	Number (10^6#)	Mass(μg)	Surface area ($10^{-5}m^2$)
10	2.93	23.96	5.75	6.41	52.16	12.60
30	36.25	296.6	71.18	31.11	255.3	61.15

Limitations

One limitation of this work is that air infiltration via building permeability (e.g., windows, envelope cracks) was not considered during the CFD simulation. Several previous studies (Shi et al. 2015; G. Hong and Kim 2016; C. Chen and Zhao 2011) have proved the effects of air infiltration on IAQ and verified the infiltration factor as the useful parameter for qualifying the number of indoor particles infiltrating from the outdoor environment. To

549evaluate the potential effect of building permeability on the current results,
550we estimate the average infiltration rate as 0.2 air changes per hour (ACH) in
551summer based on some previous research (Chen and Zhao 2011; G. Hong
552and Kim 2016). According to the volume of the room and the outdoor
553pollutant concentration, the air infiltration process might cause the indoor
554ozone level to raise to 8 ppb during the night. As can be seen in Figure 5, the
555measured indoor ozone concentration stayed around 10 ppm during the
556night when the windows were closed, which was supposed to be associated
557with the air infiltration. Therefore, the actual indoor pollutant concentration
558considering the air infiltration would be 5% higher than the simulated results
559in this work, which results in a higher IAQ index and thus higher exposure
560risk than evaluated.

561 As for the concept of the exposure injury, in the current work, we focus
562more on the indoor air quality and the corresponding respiratory dosage and
563deposition through breathing. As concluded in Table 2, a qualitative
564evaluation indicates the significant potential of wheezing and shortness of
565breath in people with asthma, as well as the increasing of lung disease,
566under the calculated IAQ index. However, quantitative analysis of the
567contaminant penetrating into the blood through layers of skin, stratum
568corneum, viable epidermis and dermal capillaries is also necessary to carry
569out together with the physiological researches in the next step, to determine
570the exact injury level. Recently, a model of transdermal uptake of hazardous
571chemicals has been raised by Morrison et al. in 2017. The final mass of the

gaseous chemicals (e.g., SO_2, CO) entered the blood can be calculated based on the dynamic indoor chemical concentration as a boundary condition. But the key point is to validate the aforementioned model with a set of proper parameters for specific gaseous contaminants.

As for the selection of airborne particle metrics, ultrafine particles also play a non-negligible role in affecting the occupant health, especially to the respiratory system due to its smaller particle size (Ibald-Mulli et al. 2002; Zhao et al. 2009; Nikolova et al. 2011). Plus that the physical diffusion process (origin, dynamic and penetration) between PM2.5 and ultrafine particles are actually different. Therefore, the approach proposed in this work is a simplified approach for not considering the ultrafine particles in the overall framework. To address this problem, accurate measured ultrafine particles data should be collected via carefully designed experiments, to further validate the physical models of their diffusion process.

The methodology in this paper is more targeting at the commercial building types (namely, office buildings) where many indoor pollutant sources such as cooking and incense could be negligible. When it comes to residential building types for a broader application, the simulation of indoor combustion sources should be added to the current methodology, especially the CFD simulation of the origin, dynamics and penetration of such particle metrics (Yang and Ye 2014; Ezzati and Kammen 2001).

Conclusion

This work employed both whole-building simulation (EnergyPlus coupled with obFMU) and computational fluid dynamics (Fluent) to analyze the impacts of occupant behaviors (namely window operation, HVAC operation, and human movements) on indoor airflow patterns and IAQ. The IAQ, especially considering daily occupant behavior schedules, was assessed during the period of a wildfire event in the Northern California, U.S.

The simulated results were compared with the actual measured indoor and outdoor data (O3 and PM2.5). The measured and simulated IAQ were consistent based on the maximum and average levels. The occupant behaviors were proved to exert significant impacts on the indoor air flow pattern and thus the pollutants' concentrations. The indoor airflow pattern and IAQ transformed obviously within working hours, which were largely dependent on occupant behaviors. Thus, to mitigate indoor exposure risk, occupants are advised to keep windows closed and operate HVAC systems without outdoor air. Besides, occupants' movements accelerate the diffusion and mixture of existing contaminants at different heights, which could enhance the risk of respiratory exposure. The daily maximum IAQ index was 215, with SO2 as the responsible pollutant, which might result in significant respiratory symptoms and adverse health effects, such as wheezing and shortness of breath, in children, older adults, and people with asthma. Based on indoor air conditions and considering occupant behaviors, deposit fraction and equation were fitted to predict the respiratory injury level under such outdoor wildfire conditions.

This study formulated a framework for the indoor pollutants exposure modeling and the potential human health hazard assessment in an office environment while taking into account actual occupant behaviors. This co-simulation was conducted by combining the building energy modeling, occupant behavior modeling, CFD modeling, and pollutant modeling, which can be further applied in each IAQ issue where the outdoor-to-indoor pollutant penetration aspect is important (such as wildfire events as demonstrated in this work, haze pollution in China, as well as the vehicle exhaust etc). Results can be used to evaluate and inform strategies to mitigate occupant health conditions during outdoor events of extreme pollution.

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Acknowledgements:

We thank the Indoor Environment Group of Lawrence Berkeley National Laboratory for providing the measured indoor and outdoor air quality data. This study was supported by National Key R&D Program of China (Grant No. 2016YFC0802801 and 2016YFC0802807), National Science Fund for Distinguished Young Scholars of China (Grant No 71725006), National Natural Science Foundation of China (Grant No. 51706123). This work was also supported by the Office of Energy Efficiency and Renewable Energy, the United States Department of Energy under Contract No. DE-AC02-05CH11231. The authors are deeply grateful to these supports.

Author contributions:

N.L., W.W. and T.H. designed the study. N.L., X.X. and K.S. conducted the combined simulation of the OB-based indoor environment. All authors participated in writing and revising the manuscript. All authors read and approved the submitted manuscript.