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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

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16**Abstract:** The recent wildfires in California, U.S., have caused not only 17significant losses to human life and property, but also serious environmental 18and health issues. Ambient air pollution from combustion during the fires 19could increase indoor exposure risks to toxic gases and particles, further 20exacerbating respiratory conditions. This work aims at addressing existing 21knowledge gaps in understanding how indoor air quality is affected by 22outdoor air pollutants during wildfires—by taking into account occupant

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23behaviors (e.g., movement, operation of windows and air-conditioning) which 24strongly influence building performance and occupant comfort. A novel 25modeling framework was developed to simulate the indoor exposure risks 26considering the impact of occupant behaviours by integrating building 27energy and occupant behaviour modeling with computational fluid dynamics 28simulation. Occupant behaviors were found to exert significant impacts on 29indoor air flow patterns and pollutant concentrations, based on which, 30certain behaviors are recommended during wildfires. Further, the actual 31respiratory injury level under such outdoor conditions was predicted. The 32modeling framework and the findings enable a deeper understanding of the 33actual health impacts of wildfires, as well as informing strategies for 34mitigating occupant health risk during wildfires.

35

36**Key words:** human exposure risk, indoor air quality, occupant behavior, 37respiratory injury, NAPA wildfire, computational fluid dynamics simulation 38

39Introduction

40Climate change is influencing large wildfire frequency and globally 41widespread disturbance that affect both human and natural systems 42(Hurteau et al. 2014). The 2013 Rim Fire in California has caused an average 43PM2.5 concentration of 20 µg/m³ and ranged from 0 to 450 µg/m³, which was 44proved to exert significant adverse health effects to a large population 45(Navarro et al. 2016). As another one of the worst wildfires recently, several 46massive wildfires swept Napa and Sonoma counties in the North Bay areas of 47San Francisco on the western coast of the United States on the night of 48October 8, 2017 (HST). The fires resulted in the worst air quality that has 49ever been recorded in the San Francisco Bay Area¹. The outdoor air guality 50index^{2,3}, measured in particulate matter (e.g., PM2.5) exceeded 250 ug/m³, 51and a measure of other criteria pollutants⁴ (e.g., sulfur dioxide – SO_2) 52exceeded 200 ppb, indicating that the high level of air pollution could cause 53serious health effects in most people who breathed in the contaminated air 54outdoors.

55A sudden increase in the number of hospitalizations during the days 56following the fires could be related to the negative health effects of high 57gaseous and particulate pollutant levels in the area, which included

^{3&}lt;sup>1</sup> Xinhua. Massive wildfires engulf north San Francisco counties.

⁴http://news.xinhuanet.com/english/2017-10/10/c_136667925.htm Accessed 2017-10-10

^{5&}lt;sup>2</sup> EPA USA. Air Data: Air Quality Data Collected at Outdoor Monitors Across the US.

⁶https://www.epa.gov/outdoor-air-quality-data Accessed 2018-06-15

^{7&}lt;sup>3</sup> Air Quality Data Query Tool. https://www.arb.ca.gov/aqmis2/aqdselect.php Accessed 2018-806-15

^{9&}lt;sup>4</sup> The criteria pollutants (also known as "criteria air contaminants – CAC") are a set of air 10pollutants (normally six common pollutants, which are ozone, particulate matter, carbon 11monoxide, lead, sulfur dioxide, and nitrogen dioxide) that cause smog, acid rain and other 12health hazards.

58increased risk for asthma, and deterioration of pre-existing respiratory 59diseases (Lewis et al. 2013). A number of recent researches reported effects 60of the different airborne particle metrics on respiratory diseases, 61cardiovascular effects, lung cancer, asthma, and lung cancer via human 62inhalation exposure (You et al. 2017; Haikerwal et al. 2015; Haddrell et al. 632015). In other words, during the past decades, wildfires have exerted a 64large negative global impact on human health, ecosystems, societies, 65economies and climate(Jolly et al. 2015; Jaffe et al. 2013). Even worse, 66according to the California's Fourth Climate Change Assessment Report 67(Bedsworth et al. 2018), there is no sign of abating in the expansion of 68wildfires due to the climate variations. There is an urgent need to mitigate 69the impacts of the adverse air quality on the human health caused by the 70increasing wildfires (Anderson et al. 2018; West et al. 2013).

Since individuals spend an average of 87% of their time indoors (Klepeis et 72al. 2001), indoor air quality (IAQ) is probably more indicative of the pollution 73 exposure levels affecting residents' health than the outdoor measures. 74 According to the report by the Institute of Medicine (2011), IAQ is affected by 75 three main factors: occupant behavior (OB), building characteristics, and 76 pollutant properties. Among them, as the most significant factor, OB affects 77 IAQ through occupants' interactions with the outdoor physical environment. 78 Behaviours such as window opening and closing (Stabile et al. 2017), HVAC 79 operation, and walking into or out of a room (Montgomery et al. 2015) will 80 change the boundary conditions of the indoor environment, thus influence

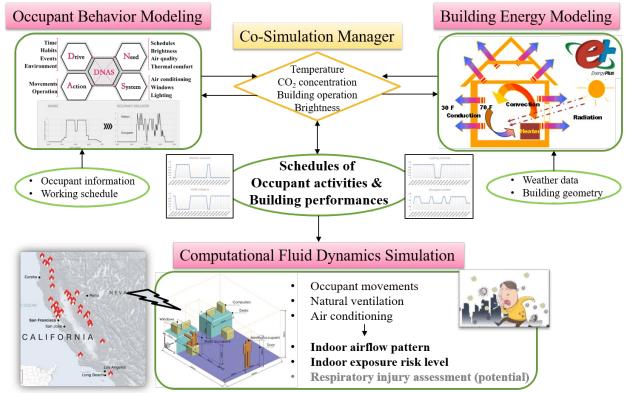
81the flow pattern of indoor air, which, ultimately cause the increase or 82decrease of the indoor pollution levels.

83 Many previous experimental studies focused on the separate impacts of 84occupant behaviors and building performances on the indoor airflow patterns 85and pollutant diffusion process, such as human movements, air-conditioning 86system-related parameters and window operation-related natural ventilation 87(Luo et al. 2016; Luongo et al. 2016). Several Computational Fluid Dynamics 88(CFD) models have also been improved by validating with quantitative 89measurements (Luo et al. 2018b; Gosselin and Chen 2008). These 90 investigations revealed detailed information about indoor air flow patterns 91and pollutant concentration levels under different specific conditions. 92However, in a real office environment, occupant behaviors are always 93complex and dynamic due to transient indoor conditions such as 94temperature, humidity, and occupant counts, which are mostly associated 95 with the outdoor environment (Lin et al. 2017). Also, when assessing the 96impacts of the indoor environment on human health, exposure to air 97 pollution is not only largely determined by pollutant concentrations in the 98spaces where people spend their time, but also by the amount of time they 99spend in those spaces. Therefore, the static status of the indoor environment 100is no longer suitable and appropriate for evaluating the indoor human 101exposure risks during daily working hours; a set of OB-related dynamic 102schedules should be first generated to guide the indoor CFD modeling and 103risk evaluation. Furthermore, for a given indoor environment, the respiratory

104injury level is also crucial for assessing adverse health impacts of wildfires, 105which requires the pollutant concentration near the oro-nasal as the 106boundary condition for assessment. PM2.5 and ultrafine particles are both 107considered as the representative pollutants when indicating the indoor air 108quality level to the public (Ibald-Mulli et al. 2002; Zhao et al. 2009). Several 109studies recognized that PM2.5 are better related to resuspension phenomena 110and combustion processes, while quite a high amount of our overall daily 111dose of ultrafine particles is due to the indoor sources. Considering the 112access to the measured data for further validation, we selected PM2.5 as the 113main particle metrics in this work.

114 Here we used both EnergyPlus and Fluent to co-simulate indoor occupant 115behaviors as well as the corresponding IAQ and particle deposition inside 116respiratory systems, respectively. Indoor pollutant concentrations were 117simulated and used to calculate the IAQ index, which indicated potential 118adverse health effects. Results of the properties affected by particle 119concentrations near the mouth and nose of occupants, could be potentially 120used as the initial and boundary conditions for the assessment of the 121respiratory injury. Outcomes from the study formulated a framework for 122modeling (as shown in Figure 1) exposure to indoor pollutants as well as the 123potential assessment of human health hazards in an office environment— 124considering occupant movement and behavior, which can inform strategies 125to mitigate occupant health issues during times of serious outdoor air 126pollution such as wildfires. For broader application, this co-simulation

127framework among Building Energy Modeling (BEM), occupant behavior 128modeling and CFD builds a bridge in the outdoor-to-indoor penetration 129process especially considering the indoor occupant behaviors, which thus 130could be broadly applied in the assessment of indoor quality under many 131other extreme weather events or use cases such as haze pollution in China, 132as well as the vehicle exhaust etc.



133

134**Figure 1 Overview of the modeling framework.** The Building Energy 135Modeling tool (EnergyPlus) was co-simulated with the Occupant Behavior Modeling 136tool (obFMU – a functional mockup unit of occupant behavior model) to calculate the 137occupant-related schedules, primarily based on the outdoor environment and the 138building performance. These modeled activities and building performances were 139then integrated into the Fluent modeling process as the boundary conditions 140through a C++ user-defined function (UDF), to further calculate the indoor airflow 141and contaminant concentration. Eventually, the corresponding indoor exposure risk 142could be evaluated, as well as the respiratory injury level as one of the potential 143assessments in the future work.

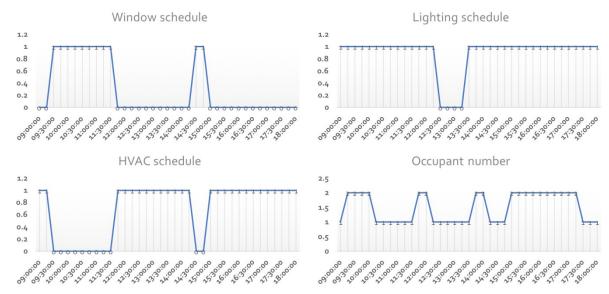
145 Materials and Methods

146**Occupant behavior modeling**. Whole building performance simulation, 147using EnergyPlus coupled with obFMU, has been used to simulate occupant 148behavior and generate occupant-related schedules in the last decade (Hong 149et al. 2017). EnergyPlus is an open-source program that models heating, 150ventilation, cooling, lighting, water use, renewable energy generation, and 151other building energy flows (Crawley et al. 2001). It is the flagship building 152simulation engine supported by the United States Department of Energy 153(DOE). The occupant behavior function mockup unit (obFMU) is an occupant 154behavior-modeling tool developed by Lawrence Berkeley National Laboratory 155(T. Hong et al. 2016). It was developed for co-simulation with EnergyPlus, 156 requiring an XML file generated based on the obXML (occupant behavior 157eXtensible Markup Language) schema (Hong, D'Oca, Taylor-Lange, et al. 1582015) and a configuration file. The obXML schema describes the occupant 159behavior by implementing а DNAS (drivers-needs-actions-systems) 160framework (Hong, D'Oca, Turner, et al. 2015). The obFMU is the engine for 161occupant behavior simulation and co-simulates via the functional mockup 162interface (FMI) with building performance simulation programs, e.g., 163EnergyPlus and ESP-r.

164**Occupant behavior activities.** In this work, the simulated scenario is 165designed in an office room with two occupants working as different types. 166One occupant keeps working on the computer, while the other works as a 167secretary, who might often walk out of the room to get printed materials or

168coordinate with other people. The simulation period is from 9:00am to 1696:00pm, which are the working hours for the office workers. According to the 170weather data on October 13, 2017, the building performance, including the 171 four occupant-related schedules and the operation characteristics of the 172indoor facilities, were modeled in EnergyPlus. Four categories of occupant 173behavior models were used in this study: occupant movement, lighting, 174windows, and HVAC operation. They were used to describe the 175characteristics of related occupant behaviors, based on which the probability 176of occupants taking an action is estimated. More specifically, Chen's agent-177based stochastic occupant movement model (Chen et al. 2018), Haldi's 178lighting control models (switch on light at arrival or when it is dark, switch off 179at departure) (Haldi 2013), and Newsham's window control model (open at 180arrival or when the outdoor environment is suitable, close at arrival, 181departure or when the outdoor environment is not suitable) (Newsham 1994) 182were adopted. HVAC operation is a combination of availability schedule and 183actual window operation. In other words, when the window is open, the HVAC 184system will be off; when the window is closed, the HVAC system will be on if 185occupants feel hot. The occupant behavior models were compiled in an 186obXML file, which worked as the input to obFMU and was used to co-simulate 187 with EnergyPlus. Occupant-related schedules, including the occupancy 188schedule, lighting schedule, natural ventilation schedule (namely window 189schedule), as well as the HVAC schedule were generated in the simulation 190process, seen in Figure 2. As for the detailed characteristics, the operation

191parameters of the windows and HVAC refer to the velocity, temperature, and 192pollutant concentration of the inlet airflow. The electric power of the lighting 193and computers was associated with the indoor environment in the modeling 194process. The changes of occupant count represented the moments when the 195occupant was entering or leaving the room.



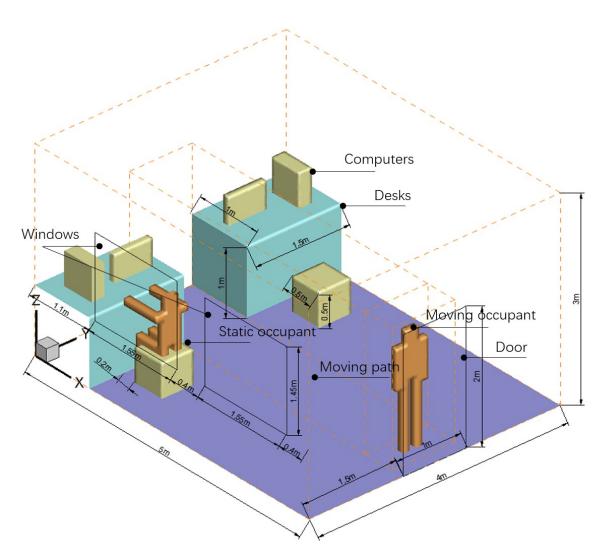
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197**Figure 2.** Four occupant-related schedules from the co-simulation of 198**EnergyPlus and obFMU.** 199**Indoor air flow field modeling.** The CFD software ANSYS Fluent (Version

20018.0.0) was employed to simulate the transient indoor flow field affected by 201the occupant behaviors. Gambit (Version 2.4.6) was used to build the 202geometric model of the office room (Figure 3) and generate the grids for 203simulation. The total number of grids is 6.7 million. The minimum mesh 204volume was $2.64 \times 10^{.9}$ m³, located close to the skin of the moving occupant. 205The method of mesh generation was used in our previous study (Luo et al. 2062018a, 2018b). The transient solver was employed during the calculation. As 207for representing the turbulence airflow caused by the ventilation and 208occupant movements, the RNG k- ϵ model adopted in this work was validated 209by previous work (Zhang et al. 2009; Han et al. 2014; Fracastoro et al. 2002), 210 with the overall consideration of accuracy, computing efficiency, and 211affordability for modeling the indoor flow field. The differential viscosity 212model and the swirl dominated flow in the RNG options were selected. 213During the iterative process, the pressure-implicit with splitting of operators 214(PISO) algorithm was employed to solve the pressure-velocity coupling 215 equations. The second-order upwind scheme was also used to consider the 216 diffusion-convection in the governing equation. The Discrete Element Model 217(DEM) Collison term and the Brownian Motion term were both applied to 218include the particle-particle interactions (voidage and collision), which 219captured the particle resuspension phenomenon of PM2.5. According to the 220aforementioned schedules and the related parameters, a UDF in the Fluent 221software has been created to automate the transient changes of the window 222boundary conditions, HVAC boundary conditions, light conditions, and the 223human movement status. The gaseous composition and the corresponding 224concentrations of the inlet airflow were based on the measured outdoor air 225quality data, seen in Table 1. The time steps during the occupant moving and 226static process were set to 0.01 s and 1 s, respectively. The calculation is 227computed in a four-node Linux cluster. Each node of the cluster has 12 228processors (2.4 GHz Intel 64). The overall simulation period in this case is 229nine hours (32400 seconds), which requires 120 hours of the computing 230time.

Table 1. The daily maximum outdoor air quality of some criteria 232pollutants (SO₂, CO, and O₃) and the particulate matter (PM2.5) 233within the following week after the wildfire event in Northern 234**California (October 8 - 14, 2017).** The gaseous composition and the 235corresponding concentrations of the inlet airflow was based on the measured 236outdoor air quality data.

	eacaeer an quai							
		Oct. 8	Oct. 9	Oct.	Oct.	Oct.	Oct.	Oct.
				10	11	12	13	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
	O₃ (ppb)	12.72	25.49	31.40	33.54	76.57	92.08	50.48
	PM2.5 (ug/m ³)	86.30	115.3	214.70	/	91.97	212.49	179.40
			0					



239**Figure 3. The geometrical features of the office room.** There are two 240desks (1.0 m × 0.5m × 0.7 m in length × width × height) at one side of the 241room (5 m × 4 m × 3 m in length × width × height). One occupant remains 242sitting in front of the desk, the other one (1.75 m-height) walks through the 243door (2 m × 1 m in height × width), which is on the other side of the room. 244There are two windows (1.55 m × 1.45 m in width × height) on the side wall, 245which is adjacent to the seated occupant. The diffuser outlet of the HVAC 246(0.3 m × 0.2 m in width × height) is at the top of the wall towards the door. 247The lighting fixture is at the center of the celling. 248

249**UDF setting.** The UDF (user-defined function) setting is a very important 250link in the overall framework, serving as a "bridge" connecting the outdoor 251and indoor concentration conditions, as well as taking the occupant behavior consideration. aforementioned 252into The generated occupant-related 253schedules determined both the natural and mechanical ventilation strategies 254(such as opening and closing time, as well as the air flow rate and its 255temperature etc.), these strategies were implemented in the CFD simulation 256as "time-series data" through coding the user-defined function. The natural 257ventilation strategy in Newsham's research (Newsham 1994) is adopted in 258this work (open at arrival or when the outdoor environment is suitable, close 259at arrival, departure or when the outdoor environment is not suitable). Thus, 260when the windows were opened, the gaseous and particulate pollutants were 261blown into the room through the windows and the doors, where the velocity 262and temperature of the inlet airflow were set as the EnergyPlus modeling 263 results. As for the mechanical ventilation strategy, it is a combination of 264availability schedule and actual window operation (when the window is open, 265the HVAC system will be off; when the window is closed, the HVAC system 266 will be on if occupants feel hot). While the HVAC system was on, the windows 267and the door, as well as the outdoor air system of the HVAC system, were all 268considered to be closed. The air purification system was assumed to be 269active in this work, with a removal rate of 50%. Thus, the gaseous 270composition and the corresponding concentrations of the next timestep's 271inlet airflow were calculated and input in the UDF code, according to the 50% 272concentration of reduced pollutants of the last timestep around the HVAC 273outlet. The air temperature and velocity of the inlet airflow were also set 274using the EnergyPlus modeling results. As for the movement behavior, the 275walking speed of the occupant was set to 1 m/s, and it took 5 s walking from 276the door to his seat (same in the opposite direction).

Calculation of IAQ index. The IAQ index is an index developed by the 278United States Environmental Protection Agency (EPA) that is used to indicate 279the indoor air quality in terms of its adverse health effects. On one side, the 280pollutant concentrations can be converted into the index value based on an 281empirical piecewise linear function. The breakpoints of specific pollutants are 282guided in the reports released by WHO in 2005 and 2010 (World Health 283Organization 2005; 2010). On the other side, the calculated index values are 284corresponding to different levels of adverse health symptoms based on many 285previous epidemiological studies and surveys. The IAQ index for each 286pollutant can be calculated from the modeled pollutant concentration results, 287as shown in Eq. 1.

288
$$I_{P} = \frac{I_{Hi} - I_{Lo}}{BP_{Hi} - BP_{Lo}} (C_{P} - BP_{Lo}) + I_{Lo}$$
(1)

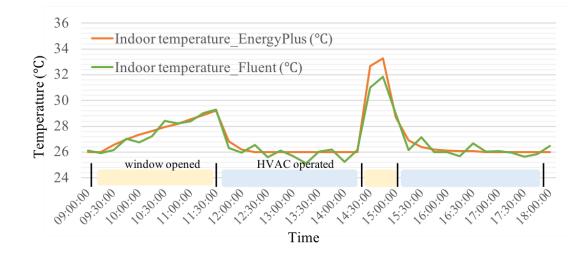
289where I_{P} is the index for pollutant P, C_{P} is the rounded concentration of 290pollutant P, BP_{Hi} is the breakpoint that is greater than or equal to C_{P} , BP_{Lo} is 291the breakpoint that is less than or equal to C_{P} , I_{Hi} is the AQI value 292corresponding to BP_{Hi} , and I_{Lo} is the AQI value corresponding to BP_{Lo} . 293According to the aforementioned concentration distribution, the average 294potential inhaled concentration was calculated within the vertical plane in 295front of the static human. The corresponding air quality level was then 296calculated based on Eq. 1. While the final AQI is the highest value calculated 297for each pollutant (Shi et al. 2015).

298

299Results

300**Verification of the consistency of the two simulations.** It was assumed 301that the occupant-related schedules remained the same in the two simulated 302environments of EnergyPlus and Fluent, making the process consistent. Due 303to the model that we employed in the obFMU, decision making regarding the 304operations of windows and HVAC was largely dependent on the indoor 305environment, especially room air temperature. Thus, to verify the 306consistency of the two simulated environments, indoor average temperature 307was chosen as the parameter for comparison. Figure 4 shows the indoor 308temperature modeled in EnergyPlus and Fluent, respectively. The occupant309related schedules generated in EnergyPlus were proved to be reasonable for

310the indoor environment simulated in Fluent.



311

312**Figure 4. The indoor temperature simulated in EnergyPlus and** 313**Fluent.** For EnergyPlus and Fluent simulations, indoor temperature both 314rose slowly till around 29.2 °C before 11:30 am, when the windows were 315opened. Then, the temperature remained at around 26.0 °C until 2:30 pm 316within the duration when the HVAC was turned on. The same phenomenon 317appeared for such behaviours afterward. Thus, the occupant-related 318schedules generated in EnergyPlus were reasonable for the indoor 319environment simulated in Fluent.

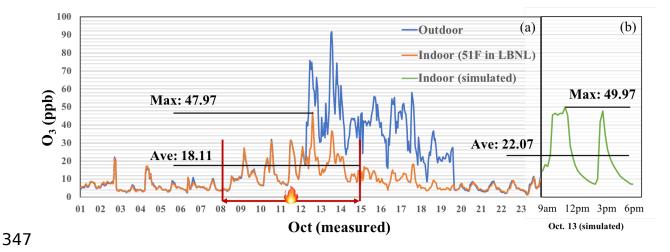
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321IAQ from measured data and simulated results. The indoor and outdoor

322air qualities before and after this wildfire event were provided by the Indoor

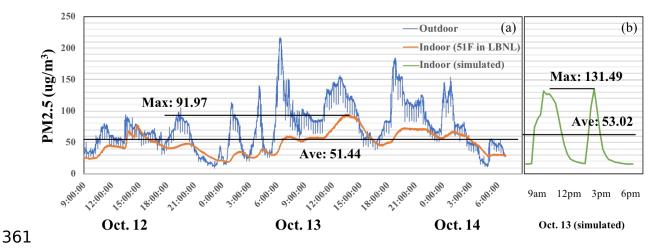
323Environment Group at Lawrence Berkeley National Laboratory (LBNL). Some 324office rooms inside the Building 51F in Lawrence Berkeley National 325Laboratory (LBNL) are serving as a living laboratory to continually monitor 326the indoor and outdoor carbon dioxide and pollutant concentrations (e.g., 327ozone, particular matters). Figures 5-6 show the comparisons of IAQ level 328(namely ozone and PM2.5) between the measured and simulated results. 329Since more detailed IAQ measurement was not available, we chose the 330average and maximum concentration levels as the comparison indexes of 331the measured and simulated results. From Oct. 8 to Oct. 15, 2017, IAO 332worsened after the breakout of the wildfire, and continued for the next whole 333week (Figure 5 (a)). During this week, the average concentration level of the 334indoor ozone was 18.11 ppb. The maximum levels of the ozone reached 33547.97 ppb on October 12, 2017, when the outdoor quality data was 76 ppb. 336The simulated average and maximum levels of ozone in Figure 5 (b) were 337 overall consistent with the measured results, except for two details. First, 338ozone is a highly reactive component that reacts guickly with surfaces when 339penetrating indoors, which is why the measured ozone levels are generally 340 lower than those modeled levels. Second, the measured indoor ozone level 341stayed at 10 ppb during the night when all unintentional openings of the 342building were closed, during which time, the simulated result was almost 343zero. These differences between the measured and modeled results were 344supposed to be associated with air infiltration in the building and are further 345 discussed in the discussion section.

346



348**Figure 5 Comparison of the measured and simulated O**₃ **levels.** (a) 349Concentration of Ozone measured indoors and outdoors, before, during and after 350the wildfire. (b) The simulated concentration of the indoor Ozone on Oct. 13. 351

Measured data of particle levels from October 12 to 14 indicate that the Measured data of particle levels of PM2.5 were 91.97 ug/m³ and 51.44 ug/m³, S54respectively (Figure 6 (a)), while those of the simulated results were 131.49 Measured measured data, which might be due to less Measured a little higher than the measured data, which might be due to less S57consideration of the particle interaction. Comparing to the outdoor Measured data, which measured of the outdoor level on average, Measured an air exchange rate of 0.7 air changes per hour in this work.



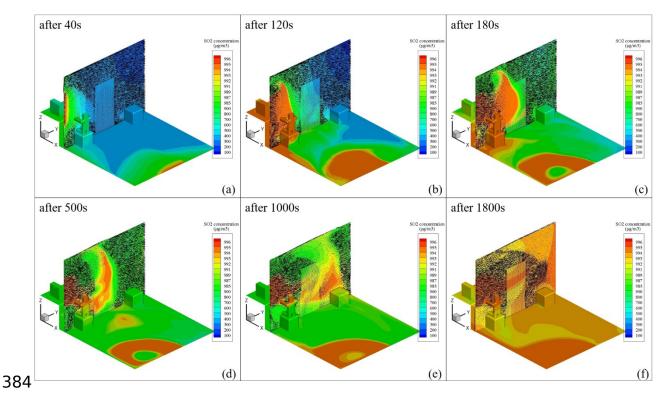
362**Figure 6 Comparison of the measured and simulated PM2.5 levels.** 363(**a**) Concentration of PM2.5 measured indoors and outdoors during the wildfire. (**b**) 364The simulated concentration of the indoor PM2.5 on Oct. 13. 365

366 The fluctuant simulated results indicated that occupant behaviors exerted 367a large influence on the indoor pollutant concentration during the working 368hours. Through the comparison, the fluctuant indoor concentration level was 369proved to be consistent with the measured data in the actual office 370environment if the occupant behaviors were considered during the 371simulation.

372

373**Flow pattern and concentration distribution.** The plane in front of the 374oronasal (x=1.25m, see Figure 3) region was chosen as the potential 375inhalation region. The evolution of the flow structure and the concentrations 376of different gaseous pollutants in this region may largely influence human 377inhalation doses, which is significant in assessing exposure risk levels. 378According to the aforementioned outdoor air quality on that day, the outdoor 379concentration of sulfur dioxide (SO₂) was much higher than an average day, 380and its hazard level was higher than that of carbon monoxide and ozone. 381Thus, sulfur dioxide was chosen as the representative pollutant to 382investigate its diffusion characteristics.

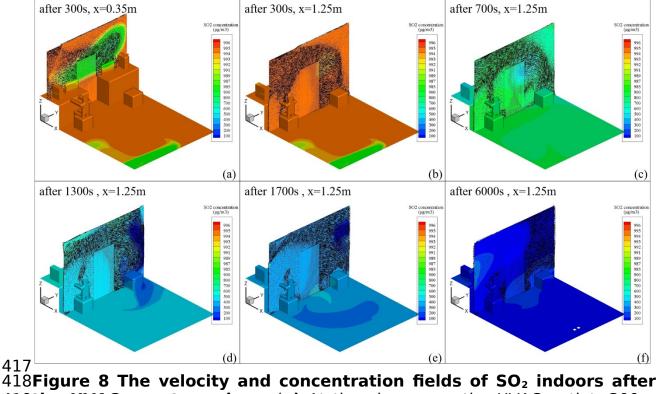




385**Figure 7 The velocity and concentration fields of SO₂ indoors after** 386**the windows were opened.** (a) At inhalation plane, 40s after the window was 387opened. (b) After 120s. (c) After 180s. (d) After 500s. (e) After 1000s. (f) After 3881800s. 389

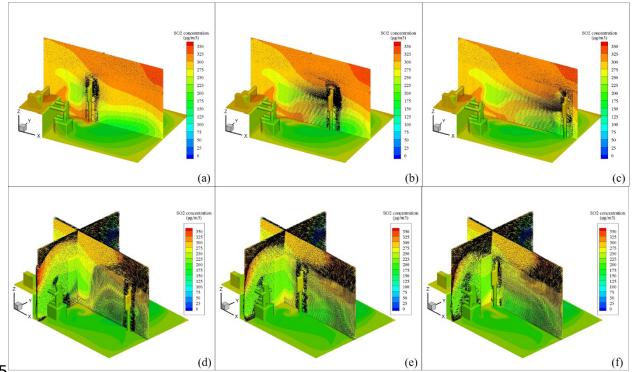
390 Operation of windows exerted a significant impact on flow pattern and 391concentration distribution (Figure 7). Outdoor sulfur dioxide was diffused 392quickly through the windows. Owing to the short distance between the 393seated occupant and the windows, the concentration of the sulfur dioxide 394near the oro-nasal region reached a relatively high level just after 120s 395(Figure 7 (b)). The inlet airflow was affected by transient outdoor weather 396data, such as wind velocity and direction outdoors. Meanwhile, the diffusion 397of the inlet airflow was also influenced by the existent indoor airflow 398circulation. Eventually, the concentration of sulfur dioxide remained at a 399steady state after 30 min, which was around 995 ug/m³ (348.25 ppb). Due to 400the same pattern of the velocity field, concentration evolutions for carbon 401monoxide and ozone were similar to that of the sulfur dioxide. Eventually, 402after 30 min of opening the windows, concentrations of indoor carbon 403monoxide and ozone on the inhalation region (x=1.25 m) reached around 4041.40 mg/m³ (1.12 ppm) and 107.08 ug/m³ (49.97 ppb), respectively.

405 Flow pattern and concentration distribution caused by other occupant 406behaviors such as air-conditioning and movement can be found in Figure 8-9. 407The velocity and concentration fields on the plane near the HVAC outlet 300 408s after the HVAC was turned on, indicated the effects of the HVAC operation 409on the IAQ (Figure 8 (a)). The cold air coming from the HVAC outlet moved 410downwards during the diffusion (Figure 8 (b-f)). 1300 s after the HVAC 411operation, the concentration of indoor sulfur dioxide dropped to 500 ug/m³. 412And 6000 s after the HVAC operation, the concentration of sulfur dioxide 413remained at a relatively steady state, which was around 100 ug/m³. 414Combined with the aforementioned analysis, occupants are advised to keep 415the windows closed and run the HVAC systems with the outdoor air dampers 416shutting off during wildfire to mitigate the indoor exposure risk.



419**the HVAC was turned on. (a)** At the plane near the HVAC outlet, 300 s 420after the HVAC was operated. (b) At inhalation plane, 300 s after the HVAC 421was operated. (c) After 700 s. (d) After 1300 s. (e) After 1700 s. (f) After 4226000 s. 423

424 The effects of the occupant movements, i.e. walking out of and into the 425room, can be found in Figure 9 (a-c) and (d-f), respectively. A strong 426downward airflow was observed behind its upper body, carrying the gaseous 427pollutant downwards; while the gap between the lower limbs exerted a 428horizontal flow between the legs, which enhanced the diffusion speed of the 429pollutants. The detailed information of the velocity fields evaluated in this 430study has been verified in a previous PIV experimental study (Luo et al. 4312018a). Overall, the movement behavior accelerated the diffusion and 432mixture of the existed contaminants at different heights, which enhanced the 433risk of respiratory exposure. Therefore, occupants are recommended to limit 434walking activities during the extreme wildfires.



435 436**Figure 10 The velocity and concentration fields of SO₂ along the** 437**moving**. (**a-c**) The occupant was walking out of the office. (**d-f**) The 438occupant was walking into the room. 439

440Assessment of the daily exposure risk level. Epidemiological studies

441have linked exposure to indoor air pollution with a wide range of adverse

442health outcomes. The health effects and the breakpoints of some specific

443pollutants considered in this study are listed in Table 2 (documented from

444(WHO 2010; Mintz 2013; World Health Organization 2005)).

445**Table 2. Pollutant-specific sub-indices and health effects statements** 446**for guidance on the AQI.** The IAQ index for each pollutant can be 447calculated from the modeled pollutant concentration results, seen in 448Methods.

AQI Categorie	Ozone	e (ppb)	Sulfur D (pp		Carbon Monoxide	Particulate Matter (ug/m ³)
s: Index	[1-hour]	[8-hour]	[1-hour]	[24-	(ppm)	[24-hour]

Values				hour]	[9 bour]		
Good	_	0-59	0-35 0-30 None		[8-hour]	0-12.0	
(Up to 50)		None			None	None	
Moderate (51-100)	-	60-75 Unusually sensitive individuals may experience respiratory symptoms	36-75 No	>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	
	125-164	76-95	76-185	140- 220	9.5-12.4	35.5-55.4 Increasing likelihood	
Unhealthy for Sensitive Groups (101-150)	for Sensitive Groups		Increasing likelihoo of respiratory symptoms, such a		Increasing likelihood of reduced exercise tolerance due to increased cardiovascular symptoms, such as chest pain, in people with heart disease	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	
	165-204	96-115	186- 304	220- 300	12.5-15.4	55.5-150.4 Increased aggravation	
Unhealthy (151-200)	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		Reduced exercise tolerance due to increased cardiovascular symptoms, such as chest pain, in people with heart disease	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	
	205-404	116-374	305- 604	300- 600		150.5-250.4 Significant	
Very Unhealthy (201-300)	symptoms a breathing lik with lung d as asthma older adults workers; likelihood o effects i	kery in people lisease, such a, children, a, and outdoor increasing f rospiratory aggrav		increase in symptoms, eezing and f breath, in h asthma; on of other seases	15.5-30.4 Significant aggravation of cardiovascular symptoms, such as chest pain, in people with heart disease	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	
Hazardou s (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	

450 According to the modeled concentration results, where the 1-hour SO₂ 451value was 348.25 ppb, CO value was 1.12 ppm, the O₃ value was 47.97 ppb, 452and the PM2.5 value was 131.49 ug/m³, the calculated maximum IAQ index 453was 215, with SO₂ as the responsible pollutant. Qualitative evaluation 454indicated that this environment would cause an increasing likelihood of 455respiratory symptoms, such as wheezing, chest tightness and breathing 456discomfort in people with asthma, as well as an increasing aggravation of 457other lung diseases. However, to achieve the quantitative evaluation of the 458injury level, further analyses should be conducted considering an entering 450path of the particle and gaseous contaminants into the body through 460breathing. The modeled dynamic indoor contaminant concentration can be 461served as a boundary condition.

462 As for the impact of occupant behaviors on the daily exposure risk level, 463due to the distribution of different indoor occupant behaviors, the indoor 464pollutant concentration fluctuated obviously during the working hours. 465Activities such as opening the windows as well as walking into and out of the 466rooms led to the increase of the pollutant concentration and thus the 467exposure risk of the human body and respiratory. While turning on the air-468conditioning without the function of supplying fresh air decreased the indoor 469contaminant concentration in a slow but effective way. Therefore, to mitigate 470indoor exposure risk, occupants are advised to keep windows closed and 471limit walking activities during the extreme wildfires. Meanwhile, outdoor air 472dampers should be shutting off when operating the HVAC system to avoid

473more purification loads. From another aspect, a proper and accurate set of 474occupant behavior schedules and the corresponding building boundary 475conditions are also crucial for enhancing the evaluation and prediction of the 476indoor risk exposure.

477**Discussions**

478This study formulated a framework for the indoor pollutants exposure 479modeling and the potential human health hazard assessment in an office 480environment particularly taking into account the actual occupant behaviours. 481The simulated results under this framework were compared with the actual 482measured indoor and outdoor data (O_3 and PM2.5), showing great 483consistency in both the maximum and average levels. The indoor airflow 484pattern and IAQ fluctuated obviously within working hours, which were 485largely dependent on specific occupant behaviors. Therefore, comparing to 486the traditional IAQ and occupant exposure assessments when occupants 487 remained static or the indoor equipment (e.g., HVAC and windows) remained 488constant running, the framework in this study is proved to provide a more 489 realistic and reliable result aligned with the actual requirement of assessing 490the health hazard level of the indoor occupants. Furthermore, based on this 491 result as a boundary condition, the deposit fraction and equation can be 492 fitted to predict a more accurate and dynamic respiratory exposure dosage 493under such outdoor wildfire conditions, which not only indicates the key 494injury level, but also provides reference for the further physiological stage.

495Assessment of the respiratory injury

496As aforementioned, the indoor pollutant concentration near the oro-nasal 497could be considered as the boundary condition for assessing the respiratory 498deposition. Take nasal inhalation as an example, respiratory injury was 499mainly caused by the micron particle deposition fraction in nasal cavity, 500pharynx, larynx and trachea regions for nasal breathing. The detailed 501modelling method and flow pattern inside the respiratory system were 502included in another published journal article (Xu et al. 2018).

503 The simulated particle size range was slightly expanded to allow a wider 504coverage of the developed deposition equations. For micron-sized particles, 505deposition fractions were related to the inertial parameter *I*, which 506considered particles mass to the square power, and the averaged fluid 507momentum. The inertial parameter is defined as:

$$508 \quad I = d_p^2 Q \tag{2}$$

509 where Q is the volume flow rate (cm³/s) and d_p (µm) is the particle 510aerodynamic diameter. Figure 11(a) and (c) show the deposition fraction in 511human respiratory airways for particles ranging from 0.8 µm to 20 µm 512against the inertial parameter for oral and nasal inhalation, respectively. 513 The Stokes number was used to correlate the deposition to length scale, 514particle density, size and flow rate. It is defined as:

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

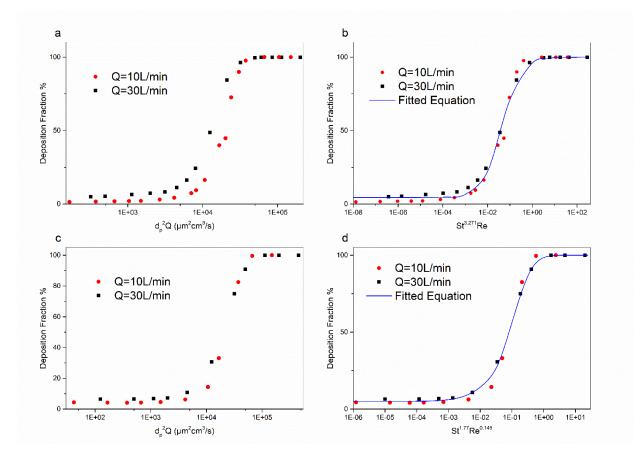
. .

516 where *L* is the characteristic length of oral and *u* is the local airflow 517velocity. The deposition through oral breathing in human airway was related 518to *St* and *Re*.

519 For the deposition equation in human airway, improved fittings were 520obtained with $St^{3.271}Re$ and $St^{1.77}Re^{0.145}$ for particle sizes from 0.8 to 20 µm, 521breathing rate of 10 and 30 L/min for oral and nasal breathing (Figure 11(b) 522and (d)), with a coefficient of determination R^2 =0.99. The empirical 523equations are given as

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

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



527**Figure 11 Comparison of micron particles (0.8 – 20 \mum).** (**a**) deposition 528fraction for oral inhalation. (**b**) fitted deposition equation for oral inhalation. 529(**c**) deposition fraction for nasal inhalation. (**d**) fitted deposition equation for 530nasal inhalation.

531

532 The dosimetry (in number, mass, surface area) in human upper airway 533under various breathing flow rates and breathing pattern was calculated by 534using the above simulated PM2.5 concentration value, presented in Table 3. 535The time period of occupants staying indoors was assumed as 8 hours a day 536(as the working hours from 9am to 5pm). A monotonous growth was 537obtained in human upper airway dosimetry with the flow rate, which lead to 538a larger air exchange and particle exposure risk, as well as a higher 539probability of chronic respiratory diseases.

-					<u> </u>			
	0		Oral in	halation	Nasal inhalation			
	Q (L/mi n)	Numbe r (10 ⁶ #)	Mass(µ g)	Surface area (10 ⁻ ⁵ m ²)	Numb er (10 ⁶ #)	Mass(µ g)	Surface area (10 ⁻ ⁵m²)	
	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	

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

541

542Limitations

543 One limitation of this work is that air infiltration via building permeability 544(e.g., windows, envelope cracks) was not considered during the CFD 545simulation. Several previous studies (Shi et al. 2015; G. Hong and Kim 2016; 546C. Chen and Zhao 2011) have proved the effects of air infiltration on IAQ and 547verified the infiltration factor as the useful parameter for qualifying the 548number 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

572gaseous chemicals (e.g., SO_2 , CO) entered the blood can be calculated based 573on the dynamic indoor chemical concentration as a boundary condition. But 574the key point is to validate the aforementioned model with a set of proper 575parameters for specific gaseous contaminants.

576 As for the selection of airborne particle metrics, ultrafine particles also play 577a non-negligible role in affecting the occupant health, especially to the 578respiratory system due to its smaller particle size (Ibald-Mulli et al. 2002; 579Zhao et al. 2009; Nikolova et al. 2011). Plus that the physical diffusion 580process (origin, dynamic and penetration) between PM2.5 and ultrafine 581particles are actually different. Therefore, the approach proposed in this 582work is a simplified approach for not considering the ultrafine particles in the 583overall framework. To address this problem, accurate measured ultrafine 584particles data should be collected via carefully designed experiments, to 585further validate the physical models of their diffusion process.

586 The methodology in this paper is more targeting at the commercial 587building types (namely, office buildings) where many indoor pollutant 588sources such as cooking and incense could be negligible. When it comes to 589residential building types for a broader application, the simulation of indoor 590combustion sources should be added to the current methodology, especially 591the CFD simulation of the origin, dynamics and penetration of such particle 592metrics (Yang and Ye 2014; Ezzati and Kammen 2001).

593

594 Conclusion

595This work employed both whole-building simulation (EnergyPlus coupled with 596obFMU) and computational fluid dynamics (Fluent) to analyze the impacts of 597occupant behaviors (namely window operation, HVAC operation, and human 598movements) on indoor airflow patterns and IAQ. The IAQ, especially 599considering daily occupant behavior schedules, was assessed during the 600period of a wildfire event in the Northern California, U.S.

601The simulated results were compared with the actual measured indoor and 602outdoor data (O3 and PM2.5). The measured and simulated IAQ were 603 consistent based on the maximum and average levels. The occupant 604behaviors were proved to exert significant impacts on the indoor air flow 605pattern and thus the pollutants' concentrations. The indoor airflow pattern 606and IAQ transformed obviously within working hours, which were largely 607dependent on occupant behaviors. Thus, to mitigate indoor exposure risk, 608occupants are advised to keep windows closed and operate HVAC systems 609 without outdoor air. Besides, occupants' movements accelerate the diffusion 610and mixture of existing contaminants at different heights, which could 611enhance the risk of respiratory exposure. The daily maximum IAQ index was 612215, with SO2 as the responsible pollutant, which might result in significant 613 respiratory symptoms and adverse health effects, such as wheezing and 614 shortness of breath, in children, older adults, and people with asthma. Based 615on indoor air conditions and considering occupant behaviors, deposit fraction 616and equation were fitted to predict the respiratory injury level under such 617outdoor wildfire conditions.

618This study formulated a framework for the indoor pollutants exposure 619modeling and the potential human health hazard assessment in an office 620environment while taking into account actual occupant behaviors. This co-621simulation was conducted by combining the building energy modeling, 622occupant behavior modeling, CFD modeling, and pollutant modeling, which 623can be further applied in each IAQ issue where the outdoor-to-indoor 624pollutant penetration aspect is important (such as wildfire events as 625demonstrated in this work, haze pollution in China, as well as the vehicle 626exhaust etc). Results can be used to evaluate and inform strategies to 627mitigate occupant health conditions during outdoor events of extreme 628pollution.

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788Author contributions:

789N.L., W.W. and T.H. designed the study. N.L., X.X. and K.S. conducted the combined 790simulation of the OB-based indoor environment. All authors participated in writing 791and revising the manuscript. All authors read and approved the submitted 792manuscript.