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1 **Exploring the Feasibility of Predicting Contaminant Transport Using a Stand-Alone**
2 **Markov Chain Solver Based on Measured Airflow in Enclosed Environments**

3

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15 **Abstract:**

16 Correctly predicting contaminant transport in enclosed environments is crucial for improving
17 interior layouts to reduce infection risks. Using the measured airflow field as input to predict
18 the contaminant transport may overcome the challenges of measuring complex boundary
19 conditions and inaccurate turbulence modeling in the existing methods. Therefore, this study
20 numerically explored the feasibility of predicting contaminant transport from the measured
21 airflow field. A stand-alone Markov chain solver was developed so that the calculations need
22 not rely on commercial software. Airflow information from CFD simulation results, including
23 the three-dimensional velocity components and turbulence kinetic energy, was used as
24 surrogate for experimental measurement based on the spatial resolution of ultrasonic
25 anemometers. Three cases were used to assess the feasibility of the proposed method, and the
26 calculation results were compared with the benchmark calculated by the commercial CFD
27 software. The results show that, when the airflow was simple, such as that in an isothermal
28 ventilated chamber, the stand-alone Markov chain solver based on the measured airflow field
29 predicted the trend of contaminant transport and peak concentrations reasonably well. However,
30 for complex airflow, such as that in non-isothermal chambers with heat sources or occupants,
31 the solver can reasonably predict only the general trend of contaminant transport.

32

33 **Keywords:**

34 Markov chain model; Airflow measurement; Contaminant; Computational fluid dynamics
35 (CFD); Enclosed environment.

36 1. Introduction

37 In recent decades, transmission of airborne infectious diseases has become a major public
38 concern. For example, outbreaks of measles [1], severe acute respiratory syndrome (SARS) [2],
39 influenzas [3], and coronavirus disease 2019 (COVID-19) [4] have severely threatened human
40 life and health. All these pandemics have been found to be related to the airflow patterns in
41 enclosed environments [5], [6], [7]. If an infected person shares a living space with other
42 occupants, the virus-containing droplets generated through talking, breathing, coughing, and
43 sneezing can be transported by the airflow and inhaled by other occupants, resulting in cross-
44 infection [8], [9]. In modern society, staying indoors at close proximity to other people is very
45 common in daily life [10], and increases the chance of airborne diseases transmission.
46 Therefore, correctly predicting contaminant transport in enclosed environments is important
47 for improving interior layouts to reduce the risk of infection.

48

49 To predict contaminant transport in an existing indoor environment, a popular approach is to
50 first conduct on-site measurements of the boundary conditions, then employ computational
51 fluid dynamics (CFD) to calculate the airflow distribution, and finally use a contaminant
52 transport model to make the prediction. For example, Zhang and Chen [11] first measured the
53 boundary conditions, such as the supply air velocity, temperature and the rate of heat generation
54 by occupants and equipment, in a ventilated room, and then used the renormalized group (RNG)
55 $k-\epsilon$ model for airflow simulation and the Eulerian model to calculate the particle transport. Pan
56 et al. [12] first measured boundary conditions such as supply air velocity in a laboratory
57 chamber, and then used large eddy simulation (LES) to calculate the airflow and the Lagrangian
58 model to predict the particle transport and deposition. Zhang et al. [13] first measured the air
59 velocity from supply air diffusers and the temperatures in the boundary areas in an aircraft
60 cabin mockup, and then calculated the airflow field using the RNG $k-\epsilon$ model and the particle
61 dispersion with the Lagrangian model. These studies have provided great insight into
62 approaches for predicting contaminant transport in existing indoor environments.

63

64 However, the accuracy of the methods above depends strongly on accurate calculation of the
65 airflow distribution, which is challenging in practical applications. One challenge is the
66 measurement of boundary conditions in some cases. For example, Zhang et al. [13] observed
67 that it was not feasible to obtain detailed measurements of the three-dimensional air velocity
68 distribution at inlets with the use of ultrasonic anemometers due to their large size. Chen et al.
69 [14] ascribed significant discrepancies between simulation results and experimental data to
70 inaccurate measurement of boundary conditions. Vidal et al. [15] found it difficult to determine
71 and quantify boundary conditions in practice as it was extremely time consuming to measure
72 all variables such as temperature, air velocity, and pressure drop. In addition, the existing
73 turbulence models are not always accurate, especially for prediction of three-dimensional air
74 velocity components and turbulence quantities. For example, although the RNG $k-\epsilon$ model was
75 found to have the best overall performance in calculating the airflow distribution in indoor
76 environments [16], Wang and Chen [17] found that the error in the model's predictions could
77 reach 30% for air velocity and turbulence kinetic energy in complex airflows such as forced or

78 mixed convection.

79

80 The above challenges could be overcome through direct measurement of the whole airflow
81 field, followed by the use of an appropriate model to predict the contaminant transport. For
82 airflow measurements, a possible approach is particle image velocimetry (PIV), which is
83 widely used for 2-D airflow measurements, [18], [19], [20]. A recently proposed volumetric
84 PIV technique is the tomographic PIV system, which employs four or more cameras to measure
85 the 3-D air velocity distribution [21]. Although 3-D airflow field measurements for a whole
86 space are still challenging, the rapid development of advanced sensing technologies may
87 facilitate such measurements in the near future. Therefore, it is worthwhile to explore the
88 feasibility of predicting contaminant transport from the measured airflow field in an enclosed
89 environment.

90

91 Furthermore, in light of the challenges in airflow field measurements, an appropriate
92 contaminant transport model that can accommodate relatively low-resolution airflow inputs
93 should be identified. Currently, the Eulerian and Lagrangian models are the most popular for
94 prediction of contaminant transport. The Eulerian model solves the contaminant transport
95 equation, while the Lagrangian model tracks each particle by solving its momentum equation
96 [22]. Normally, these two models require the detailed airflow field as input to calculate the
97 contaminant transport [23]. It would be challenging to use the Eulerian and Lagrangian models
98 with relatively low-resolution or even zonal airflow input. Recently, the Markov chain model
99 was proposed for the prediction of transient contaminant transport [24]. This model is based
100 on the transition probabilities between zones instead of solving the contaminant transport
101 equation. The transition probabilities are determined by the rate of airflow from the current
102 zone to a neighboring zone. Hence, theoretically, the Markov chain model can accommodate
103 relatively low-resolution or zonal airflow inputs [25]. Furthermore, the Markov chain model
104 does not require iterations in each time step, and is thus more computationally efficient than
105 the Eulerian or Lagrangian model. Therefore, this study hypothesizes that it is feasible to
106 predict contaminant transport using the Markov chain model based on the measured airflow
107 field in an enclosed environment.

108

109 This study first developed a stand-alone solver for the Markov chain model in MATLAB 2020a
110 [26] that can use airflow field data as input and calculate the transient contaminant transport.
111 An advantage of the solver is that it does not rely on any commercial software, which would
112 facilitate future practical applications. This study applied the stand-alone Markov chain solver
113 to three cases in which the input of the airflow field was obtained by virtual measurements
114 based on CFD simulation. The resolution for the sampling of the virtually measured air
115 velocities was based on the available experimental technique. The feasibility of using the
116 Markov chain model to predict the contaminant transport from the measured airflow field was
117 then explored by means of a case study.

118

119 **2. Methods**

120 **2.1 Markov chain model**

121 This study used the first-order homogenous Markov chain technique, in which the future state
122 is determined by the current state and the probability that the state will change [27]. The whole
123 airflow field is divided into $n - 1$ zones, and the n^{th} zone is defined as the space where the
124 contaminants exhaust. The contaminant quantity (mass or number) at a certain state (denoted
125 N_k) is stored in the following vector:

126

127
$$N_k = (N_{k,1} \ N_{k,2} \ \dots \ N_{k,n}) \quad (1)$$

128

129 where $N_{k,i}$ is the quantity of contaminant in zone i at state k . Note that it is assumed that in
130 one time step, the contaminant in a certain zone can only enter the neighboring zones. Therefore,
131 after one time step, for state $k + 1$, the contaminant number in zone i can be calculated by:

132

133
$$N_{k+1,i} = N_{k,i} \cdot p_{i,i} + \sum_{nb} N_{k,nb} \cdot p_{nb,i} \quad (2)$$

134

135 where the subscript nb represents the neighboring zones to zone i . Here $p_{i,i}$ and $p_{nb,i}$ are
136 the transition probabilities. In this work, $p_{i,i}$ is the probability that the contaminant stays in
137 the current zone, and $p_{i,j}$ represents the transport probability that the contaminant will move
138 from zone i to zone j . At state k , the contaminant concentration in zone i ($C_{k,i}$) can be
139 computed by:

140

141
$$C_{k,i} = \frac{N_{k,i}}{V_i} \quad (3)$$

142

143 where V_i is the volume of zone i . The $p_{i,i}$ can be computed in accordance with the mass
144 balance equation [28]:

145

146
$$p_{i,i} = \exp\left(-\sum_{nb} \frac{Q_{i,nb}}{V_i} \Delta t\right) \quad (4)$$

147

148 where $Q_{i,nb}$ represents the rate of airflow from zone i to the neighboring zone. Assuming
149 that zone j is one of the neighboring zones to zone i , the $p_{i,j}$ can then be calculated by [28]:

150

151
$$p_{i,j} = \frac{Q_{i,j}}{\sum_{nb} Q_{i,nb}} (1 - p_{i,i}) \quad (5)$$

152

153 Note that within a time step (Δt), the maximum distance (s_{max}) by which the contaminant can
 154 move is the distance between the center of zone i and the furthest boundary of zone j .
 155 Assuming that the air velocity (v) from zone i to zone j is $v_{i,j}$, the maximum time step
 156 (Δt_{max}) can then be estimated by:

157

158
$$\Delta t_{max} = \frac{s_{max}}{v_{i,j}} \quad (6)$$

159

160 The time step used in this study was smaller than the Δt_{max} , in order to comply with the
 161 requirements of the first-order homogenous Markov chain model.

162

163 A mathematical solver was constructed in MATLAB 2020a [26] to execute the Markov chain
 164 model. Note that the solver developed in this study is stand-alone and does not rely on any
 165 commercial software, thus facilitating future practical applications. The input was the measured
 166 airflow field data, and the output was the transient contaminant concentration distributions,
 167 since the Markov chain model is based on the airflow and contaminant transport between zones.
 168 The rate of airflow from zone i to the neighboring zone j , $Q_{i,j}$, consists of the mean airflow
 169 rate ($Q_{mean,i,j}$) and the turbulent fluctuating airflow rate ($Q_{fluctuating,i,j}$):

170

171
$$Q_{i,j} = Q_{mean,i,j} + Q_{fluctuating,i,j} \quad (7)$$

172

173 Fig. 1 depicts the relationship between the airflow measurements and the $Q_{mean,i,j}$ and
 174 $Q_{fluctuating,i,j}$ in the Markov chain model. The three-dimensional air velocity components
 175 (u, v, w) and the turbulence kinetic energy (k) are measured at the center of each zone. The
 176 mean airflow rate from the current zone i to the neighboring zone j , $Q_{mean,i,j}$, is calculated
 177 by:

178

179
$$Q_{mean,i,j} = \frac{v_i + v_j}{2} \cdot A_{ij} \quad (8)$$

180

181 where v_i and v_j are the measured mean air velocity in the y direction in zones i and j ,
 182 respectively, and A_{ij} is the area of the connecting face between zones i and j . The turbulent
 183 fluctuating airflow rate from the current zone i to the neighboring zone j , $Q_{fluctuating,i,j}$,
 184 can be calculated from the measured turbulence kinetic energy in zone i (k_i):

185

186

$$Q_{fluctuating,i,j} = \alpha_{i,j} \sqrt{2k_i/3} \cdot A_{ij} \quad (9)$$

187

188 where the coefficient $\alpha_{i,j}$ is used to characterize the influence of the distance between the two
189 adjacent zones and the time step on the turbulent dispersion of contaminants, which can be
190 calculated by [24]:

191

$$\alpha_{i,j} = 2 \cdot \left(1 - \phi \left(\frac{\Delta s_{i,j} / \Delta t}{\sqrt{2k_i/3}} \right) \right) \quad (10)$$

193

194 where $\Delta s_{i,j}$ is the distance from the centroid of zone i to that of zone j , $\phi()$ is the
195 cumulative distribution function of a standard normal distribution:

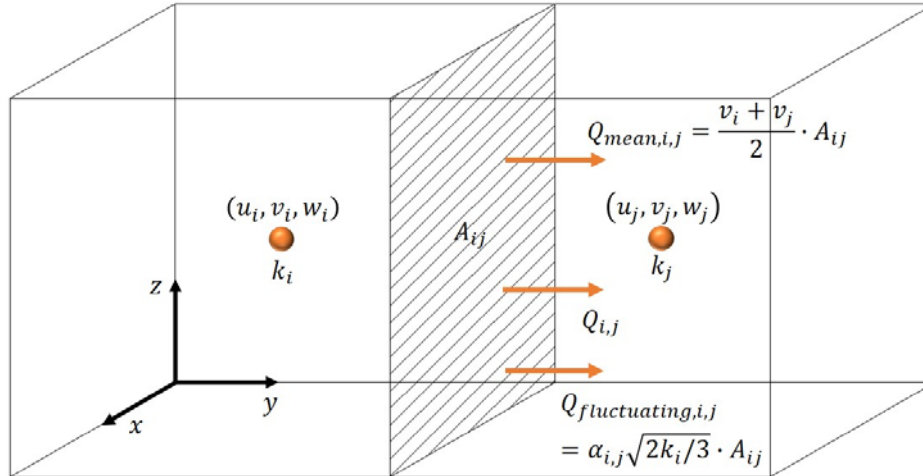
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$$\phi(x) = \frac{1}{2} \left(1 + \operatorname{erf} \left(\frac{x}{\sqrt{2}} \right) \right) \quad (11)$$

198

199 where $\operatorname{erf}()$ is the error function.

200



201

202 Fig. 1. Relationship between the airflow measurements and the airflow rates $Q_{mean,i,j}$ and
203 $Q_{fluctuating,i,j}$ in the Markov chain model.

204

205 2.2 Measured airflow field

206 2.2.1 Possible measuring technique

207 Various techniques can be employed to measure the airflow field in an enclosed environment.
208 For example, ultrasonic anemometers can be used for three-dimensional air velocity
209 measurements. However, the size of an ultrasonic anemometer is around 0.15 m, and it may be
210 too bulky to obtain the airflow distribution with a very high resolution. Nevertheless, since the
211 Markov chain model can accommodate relatively low-resolution or zonal airflow inputs, the
212 airflow field data with a resolution of 0.15 m obtained by ultrasonic anemometers may be
213 sufficient as the input for the Markov chain model. Another potential issue is the time needed
214 to conduct the measurements for the whole space. The traditional manual operation is not
215 practical. However, with the rapid development of robotic technologies, automated
216 measurements with ultrasonic anemometers, like using cable-driven robots with routing design
217 [29] or robotic arms equipped with probes [30] will significantly reduce the time cost and
218 enable whole-space measurements in the near future.

219

220 A number of other techniques can be potentially used for whole-space airflow measurements
221 in a rapid and non-invasive manner. For example, particle image velocimetry can be employed
222 to characterize the airflow in an enclosed environment. The most frequently used PIV system
223 can only measure the two-dimensional airflow field [20], which is insufficient as the input for
224 the Markov chain model. To obtain the three-dimensional airflow field, volumetric PIV systems
225 such as the tomographic PIV system can be used. However, since volumetric PIV systems
226 require four or more cameras [21], they are expensive and complicated, and therefore may not
227 be suitable for practical applications. Light detection and ranging (LIDAR) is another potential
228 technique for whole-space airflow measurements in the future. LIDAR is a remote sensing
229 technology that has been widely used in atmospheric physics to measure parameters such as
230 temperature, pressure, humidity, and wind, and to detect substances such as trace gases, clouds,
231 and aerosols [31]. In the future, if volumetric PIV systems have advanced to affordable and
232 portable instruments or if the LIDAR technique is further developed for indoor applications,
233 the proposed method for predicting contaminant transport from the measured airflow field
234 would become easier and more practical.

235

236 **2.2.2 Virtually measured airflow field**

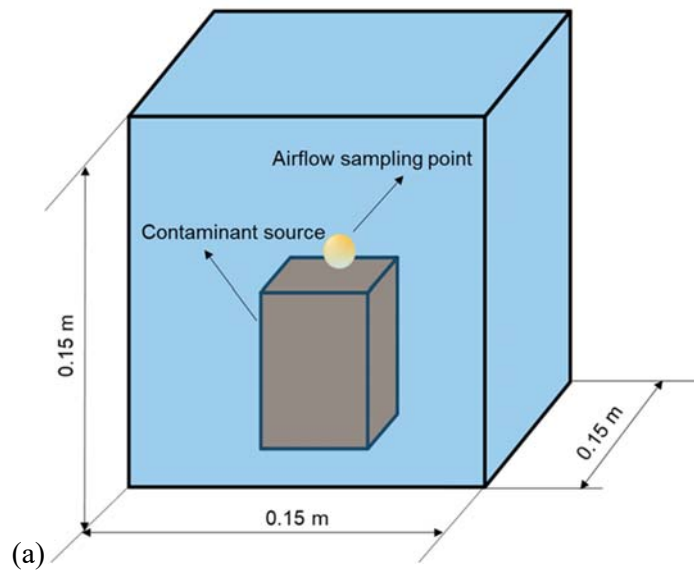
237 Currently, the feasibility of predicting contaminant transport from the measured airflow fields
238 with relatively low resolution is unclear. To preliminarily explore this hypothesis, this study
239 conducted computer experiments based on CFD simulations by commercial software code
240 ANSYS Fluent [32]. Namely, the high-resolution airflow field calculated by CFD with fine
241 grids was treated as the “true” airflow. To mimic whole-space airflow measurements using
242 ultrasonic anemometers, the airflow data, including the three-dimensional air velocity
243 components and turbulence kinetic energy, were sampled virtually on the basis of a 0.15-m
244 resolution. The virtually measured airflow data were then used as input for the Markov chain
245 model to predict contaminant transport in the space using the MATLAB stand-alone solver
246 developed in this study. The RNG k - ϵ model was used to calculate the airflow and turbulence,
247 as recommended for enclosed environments [16]. The equations for the model can be found in
248 the ANSYS Fluent manual [33].

249

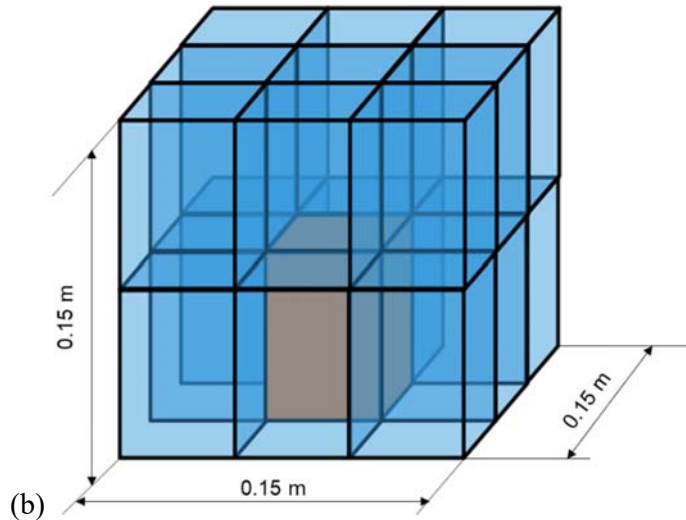
250 2.3 Grid strategy for Markov chain calculation

251 The grid used for Markov chain calculation in this study was hexahedral, and it was determined
252 from both the airflow sampling points and the geometric properties of the boundary zones. The
253 grid was constructed with the air sampling points taken as the centroid of each cell. The airflow
254 field inside each cell was assumed to be uniform, and the airflow properties on a cell face were
255 determined by its two connecting cells. However, the size of the boundary zones might be
256 smaller than that of the constructed corresponding cells. For accurate set-up of the boundary
257 conditions, the cells required further refinement. An example of the grid refinement strategy is
258 provided in Fig. 2. Here, Fig. 2(a) shows a cell constructed according to the airflow sampling
259 point with a sampling resolution of 0.15 m; thus, the cell size is 0.15 m × 0.15 m × 0.15 m. The
260 size of the contaminant source is smaller than the cell size. Fig. 2(b) shows the refined cell
261 based on the size of the contaminant source, and the division of the original cell into 18 cells.
262 The airflow data in the 18 cells were set the same as that of the original cell. With this effort,
263 the grid can truly reflect the sizes of the boundaries and improve the performance of the model.

264



265



266

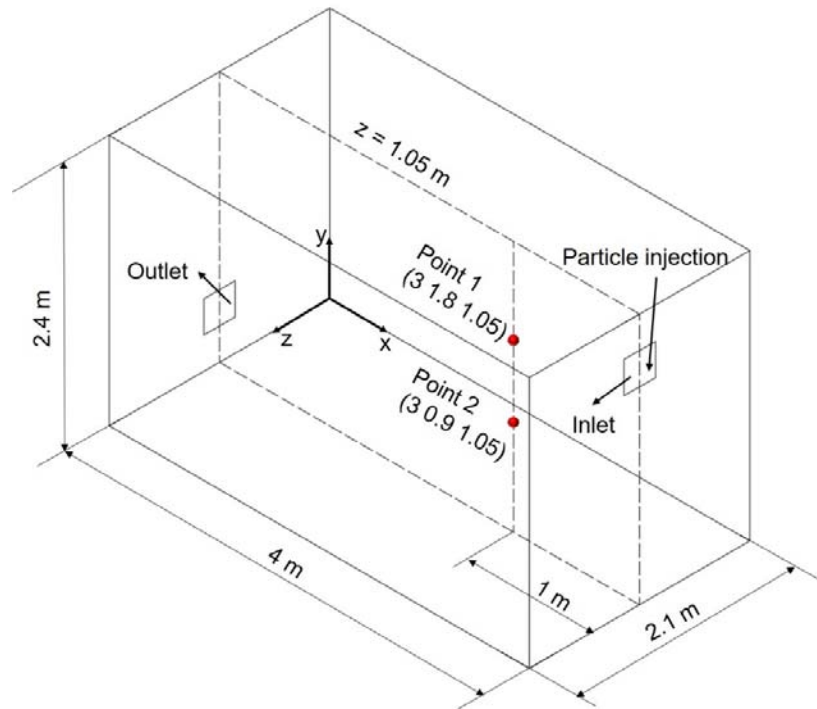
267 Fig. 2. Example of grid refinement for Markov chain calculation: (a) a cell constructed
 268 according to the airflow sampling point with a sampling resolution of 0.15 m, and (b) the
 269 refined cell based on the size of the contaminant source.

270

271 3. Benchmark for contaminant transport

272 Ideally, the benchmark for evaluating the stand-alone Markov chain solver should be obtained
 273 by means of high-quality airflow and contaminant transport measurements. For preliminary
 274 analysis, this study conducted computer experiments as a proof of concept. Calculated
 275 contaminant transport results based on CFD simulations were used as the benchmark. The CFD
 276 simulation in this study employed the Fluent-based Markov chain solver developed by Chen et
 277 al. [24] for calculating contaminant transport. To ensure that the benchmark results were
 278 reasonably accurate, the CFD program was validated by experimental data from Zhang et al.
 279 [34]. Fig. 3 shows the chamber used by Zhang et al. [34], of which the dimensions were 4 m
 280 (L) \times 2.1 m (W) \times 2.4 m (H). A supply air inlet was installed on one of the side walls at a
 281 distance of 0.3 m from the ceiling. The outlet was installed on the opposite side wall, at a height
 282 of 0.3 m above the floor. Both the inlet and outlet had dimensions of 0.3 m \times 0.3 m. The average
 283 velocity of the supply air was 0.84 m/s; the supply air angle was 10° downward; and the
 284 turbulence intensity was 20%. Particles with diameter of 1 μ m were injected into the chamber
 285 through the inlet. The transient particle concentrations were measured by Zhang et al. [34] at
 286 two positions as shown in Fig. 3, and were used for model validation.

287



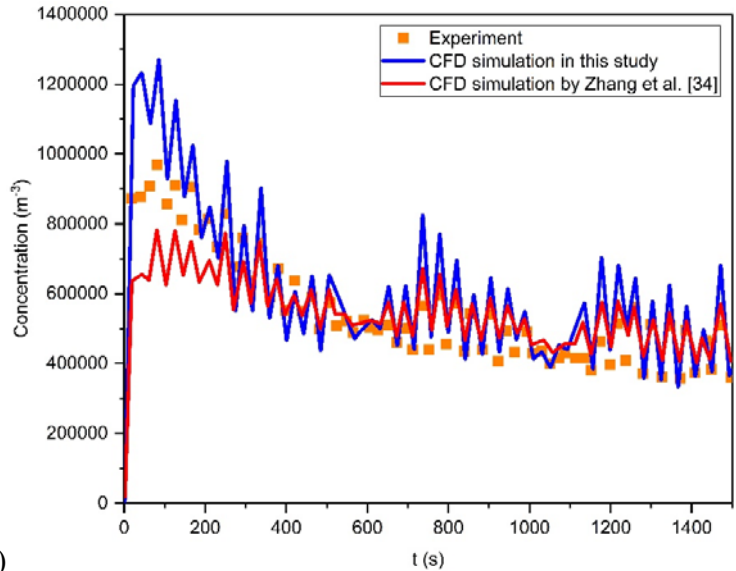
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289 Fig. 3. Schematic of the chamber for the particle transport experiment by Zhang et al. [34].

290

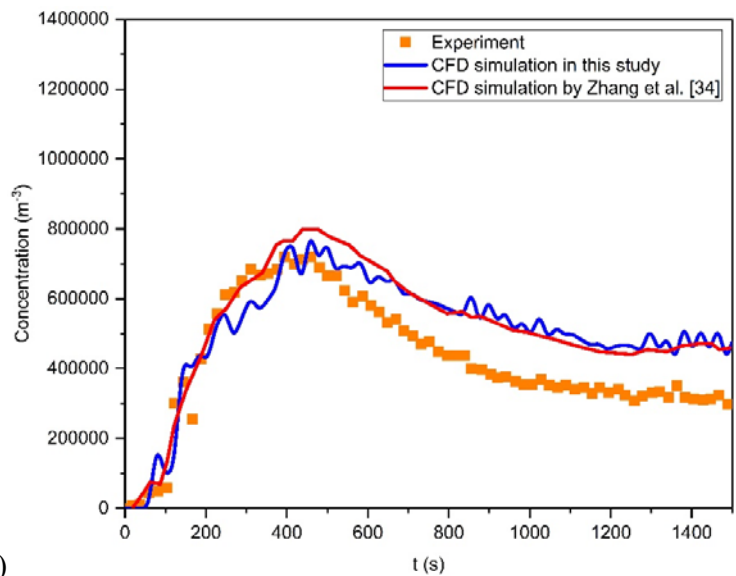
291 The airflow field was obtained with the use of the RNG $k-\varepsilon$ model. A grid independence test
 292 was conducted, and the grid resolution of 32,480 was found to be sufficiently fine. The time
 293 step size for calculating the transient transport was set at 0.01 s. Fig. 4 compares the transient
 294 particle concentrations obtained by the CFD simulations and the experimental data. In general,
 295 the calculated results from the CFD simulations captured the peaks of the contaminant transport.
 296 Although there were some discrepancies between the calculated results and the experimental
 297 data, the calculated results from the CFD simulations in this study were close to those
 298 calculated by Zhang et al. [34]. Note that in Fig. 4 (b), the results simulated by Zhang et al. [34]
 299 was smoother than the calculated results in this study. The reason is the time step was set at
 300 0.01 s in this study, while that used by Zhang et al. [34] was 1 s. Therefore, the CFD models in
 301 this study predicted the trend of transient contaminant transport reasonably well, and could be
 302 used as the benchmark for comparison.

303



304

(a)



305

(b)

306 Fig. 4. Comparison of transient particle concentrations calculated by the CFD-Markov chain
 307 model based on commercial CFD software and the experimental data at the two measuring
 308 locations: (a) height = 1.8 m and (b) height = 0.9 m.

309

310 **4. Case study**

311 In this study, three cases were used to explore the feasibility of predicting contaminant transport
 312 from the measured airflow field. The three cases focused on the transient contaminant transport
 313 in ventilated chambers under isothermal conditions, with one heat source, and with two
 314 occupants seated face to face, respectively. For all the cases, the benchmark results were the
 315 transient contaminant transport calculated by the validated Fluent-based Markov chain solver
 316 with a high-resolution grid. Based on the “true” airflow field calculated by CFD, the three-
 317 dimensional air velocity components and turbulence kinetic energy with a 0.15-m resolution
 318 (the highest resolution that can be achieved when using ultrasonic anemometers) were virtually
 319 sampled. With the virtually measured airflow data as input, the MATLAB stand-alone Markov

320 chain solver developed in this study was used to calculate the contaminant transport. The results
321 were normalized by the maximum concentrations at the initial state:

322

$$323 \quad C_k^* = \frac{C_k}{C_{0(max)}} \quad (12)$$

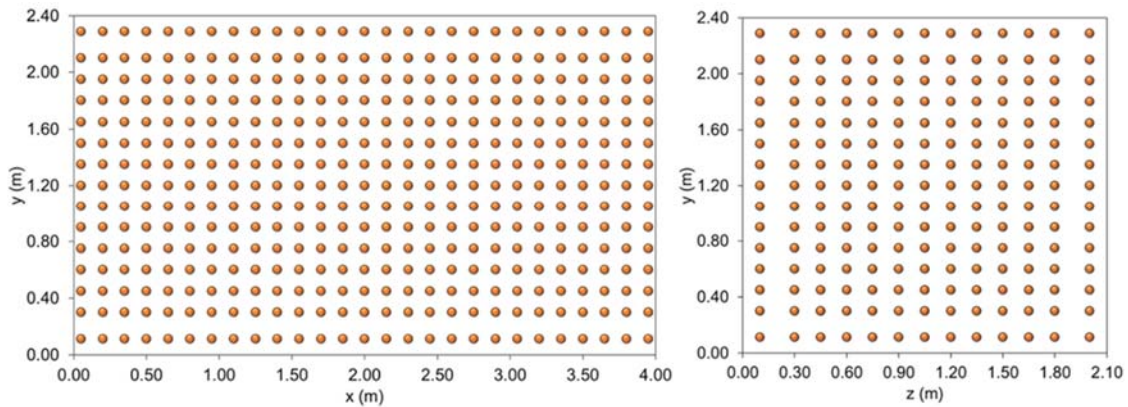
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325 where C_k and C_k^* respectively represent the calculated and normalized concentrations at state
326 k , and $C_{0(max)}$ is the maximum concentration at the initial state. The normalized results were
327 then compared with the benchmark to assess the feasibility of predicting contaminant transport
328 from the measured airflow field.

329

330 4.1 Case 1: Contaminant transport in an isothermal ventilated chamber

331 The configuration of the chamber in Case 1 is shown in Fig. 3. The thermo-fluid boundary
332 conditions were the same as those in the validation case. The benchmark CFD calculation was
333 based on a total grid number of 32,480. Fig. 5 shows the distribution of the airflow sampling
334 points based on a 0.15 m resolution. Note that due to geometric constraints, some of the
335 sampling points close to the walls may not be exactly at the interval of 0.15 m. In total, the
336 airflow measurements were conducted at 5,265 points. The Markov chain grid was constructed
337 on the basis of the airflow sampling points and the geometric characteristics of boundary zones,
338 as described in Section 2.2.3. The final Markov chain grid number was 7,695. The
339 contaminants were injected into the chamber through the supply air inlet for 0.1 s. The time
340 step size was set at 0.1 s.



341

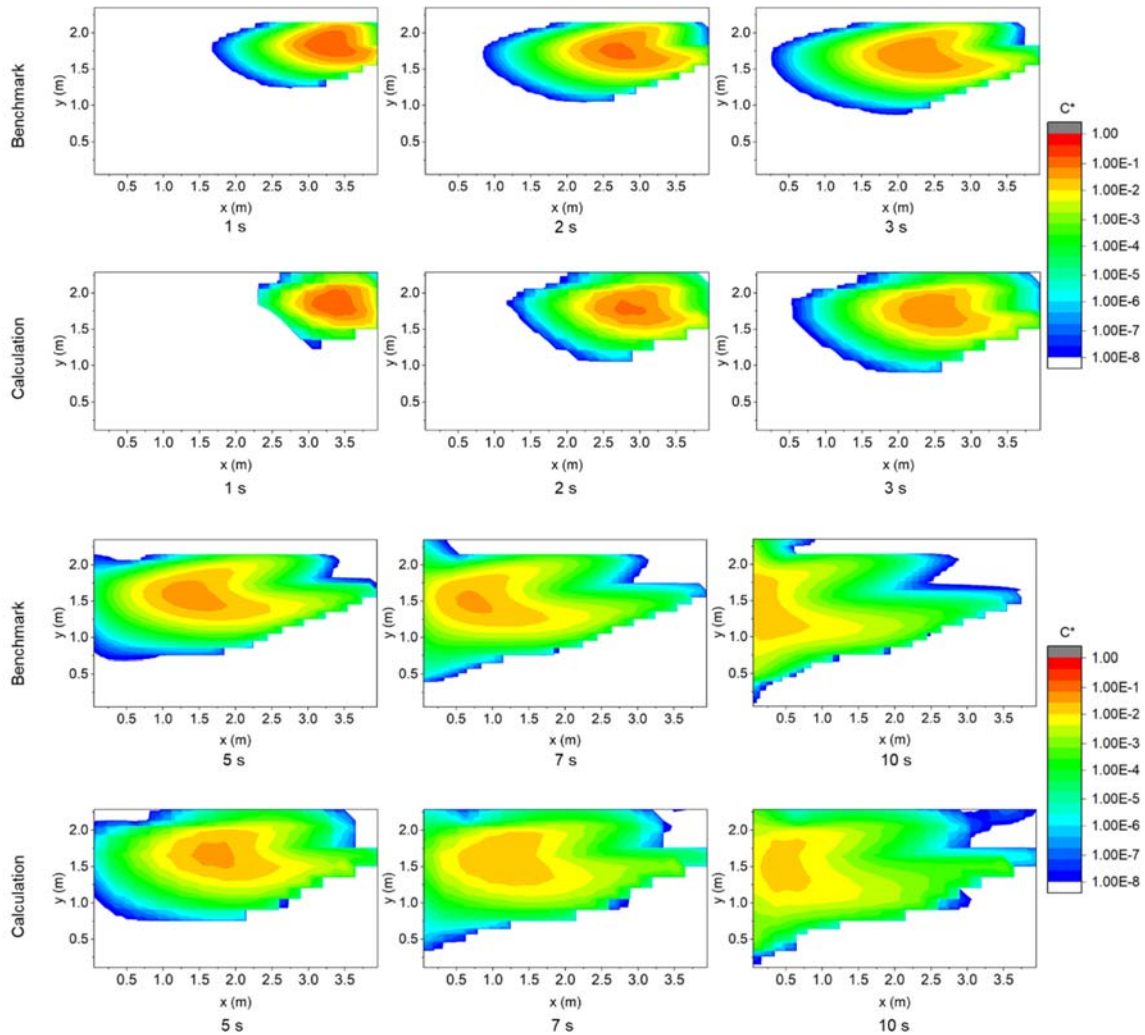
342 Fig. 5. Distribution of the airflow sampling points with a resolution of 0.15 m for Case 1.

343

344 Fig. 6 depicts the transient contaminant transport in the first 10 s at the cross-section of the
345 central z-plane. The general trend of the contaminant transport calculated using the stand-alone
346 Markov chain solver based on the measured airflow field was in good agreement with the
347 benchmark. Furthermore, the location and time at which the maximum contaminant
348 concentration occurred were also correctly predicted. Therefore, the computer experiment for

349 Case 1 partially demonstrated the feasibility of using the stand-alone Markov chain solver to
 350 predict contaminant transport from the three-dimensional air velocity components and
 351 turbulence kinetic energy in the whole chamber measured by ultrasonic anemometers.

352



353

354 Fig. 6. Comparison of the contaminant transport between the benchmark and the results
 355 calculated from the measured airflow field at a 0.15-m resolution using the stand-alone Markov
 356 chain solver for Case 1.

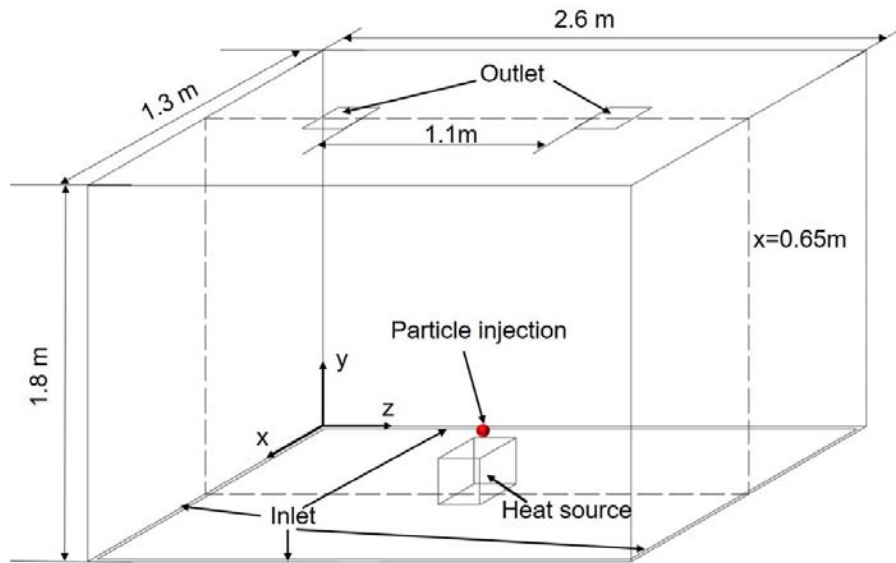
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358 4.2 Case 2: Contaminant transport in a ventilated chamber with a heat source

359 A schematic of the ventilated chamber for Case 2 [35] is shown in Fig. 7. The dimensions of
 360 the chamber were 2.6 m, 1.3 m and 1.8 m in length, width and height, respectively. Four 2.5-
 361 cm wide slots were installed at the edges of the floor to supply cool air at 20 °C with a velocity
 362 of 0.08 m/s and turbulence intensity of 10%. Two outlets with dimensions of 0.2 m × 0.2 m
 363 were located on the ceiling. Meanwhile, a 0.2 m (L) × 0.2 m (W) × 0.22 m (H) heat source at
 364 the center of the floor had a heat generation rate of 65 W. The contaminant source was located
 365 above the heat source, and it was set as a pulse source within the duration of 0.2 s. A grid

366 resolution of 53,740 was used for the airflow calculation in accordance with a grid
 367 independence test. Fig. 8 shows the distribution of the airflow measuring points based on a
 368 resolution of 0.15 m. There was a total of 1,155 points for the airflow measurements. The
 369 Markov chain grid was then constructed on the basis of the airflow sampling points and the
 370 sizes of boundary zones, and the total grid number was 1,683. The time step size for
 371 contaminant transport calculation was set at 0.2 s for Case 2.

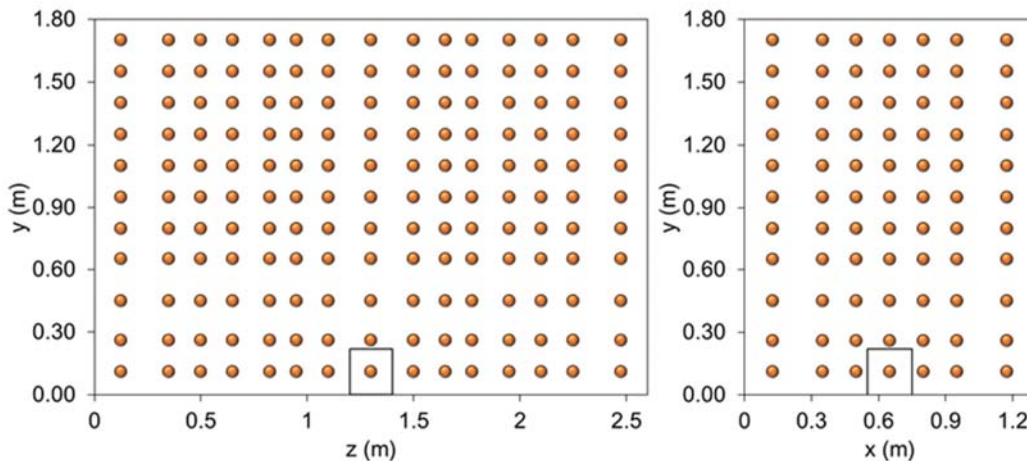
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373

374 Fig. 7. Schematic of the chamber for Case 2 studied by Bolster and Linden [35].

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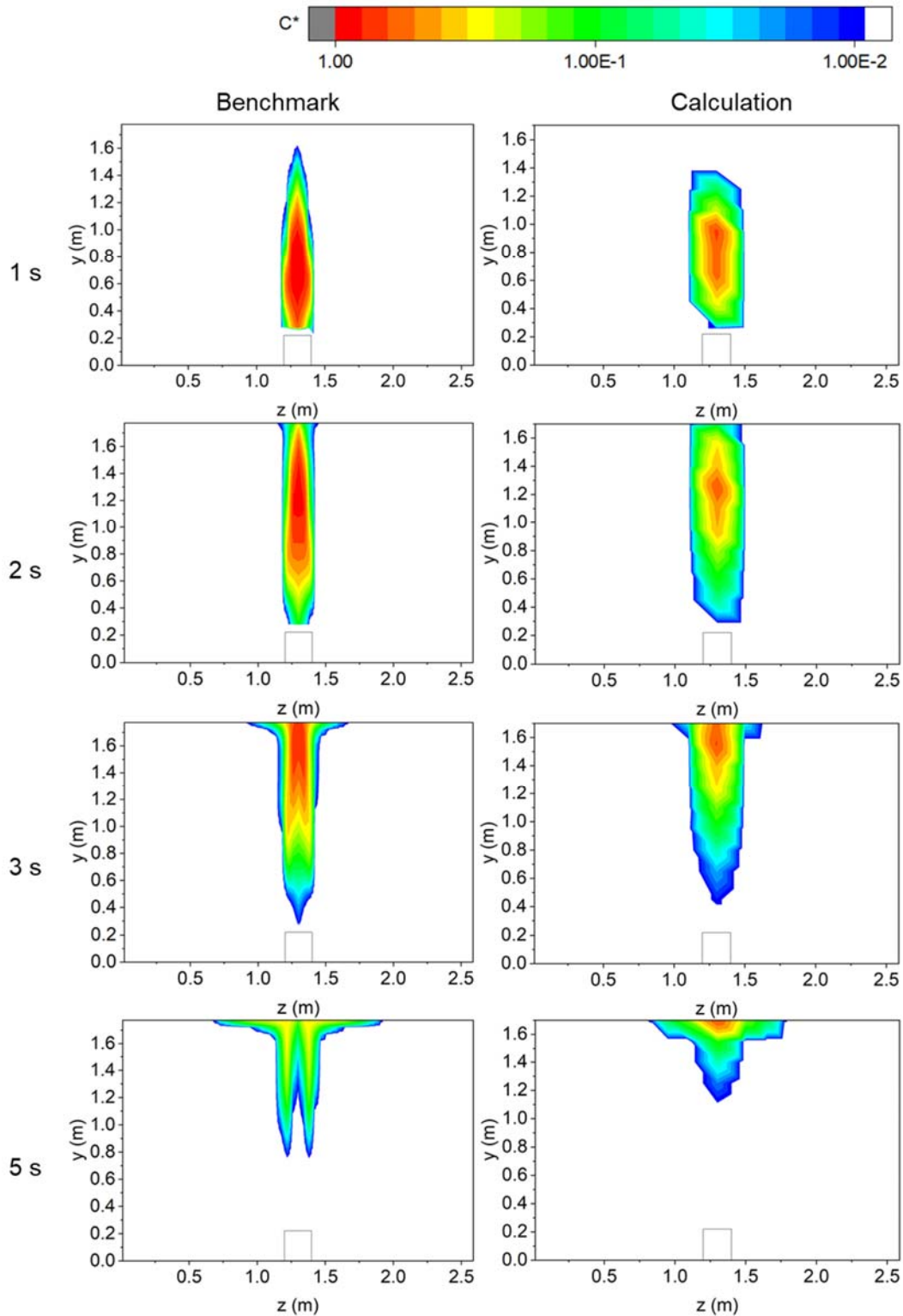
377 Fig. 8. Distribution of the airflow sampling points with a resolution of 0.15 m for Case 2.

378

379 Fig. 9 compares the contaminant transport in the first 5 s at the cross section of the central x-
 380 plane from the benchmark and the stand-alone Markov chain solver. The comparison shows
 381 that the stand-alone Markov chain solver based on the measured airflow field provided a
 382 reasonably good prediction of the upward transport of the contaminants, which was mainly

383 driven by the thermal plume generated by the heat source. However, in the first 3 s, the
384 maximum contaminant concentration calculated from the stand-alone Markov chain solver was
385 lower than that of the benchmark. From the benchmark, the contaminant concentration
386 gradients in the z direction were obvious in the first 3 s. However, the gradients were not
387 reflected due to the relatively large airflow sampling cell with a 0.15 m resolution. Therefore,
388 if the objective is to obtain the general trend of contaminant transport, the stand-alone Markov
389 chain solver based on the measured airflow field can be used. However, if the detailed
390 concentration gradients need to be captured, the proposed method may not be appropriate.

391



392

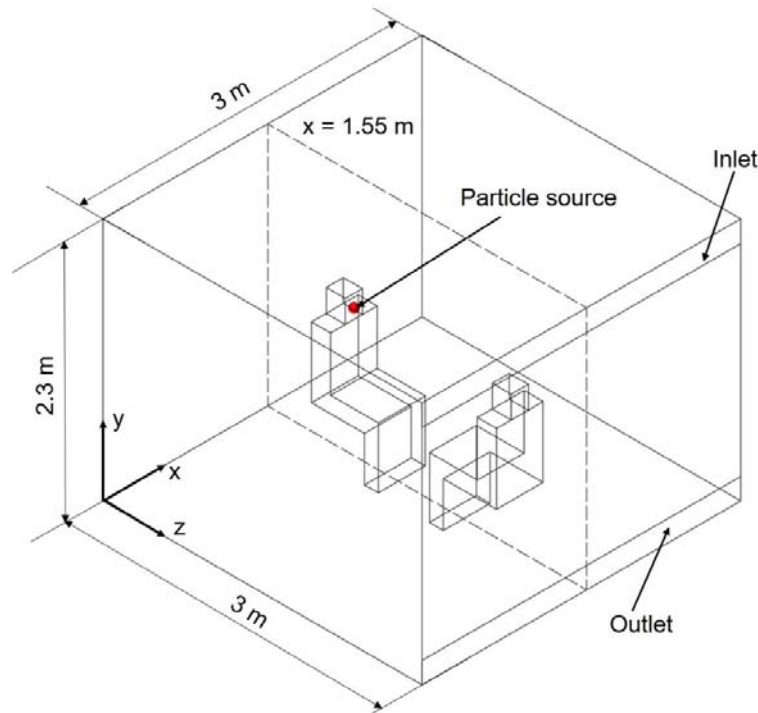
393 Fig. 9. Comparison of the contaminant transport between the benchmark and the results
 394 calculated from the measured airflow field at a 0.15-m resolution using the stand-alone Markov
 395 chain solver for Case 2.

396

397 **4.3 Case 3: Person-to-person contaminant transport in a ventilated chamber**

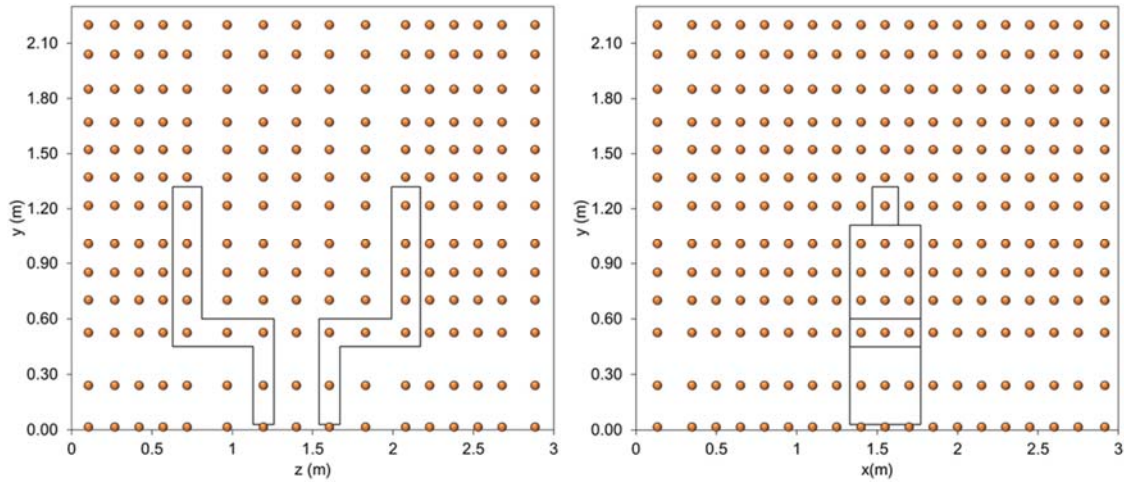
398 The configuration of the ventilated chamber with two occupants seated face to face [36] is
399 shown in Fig. 10. The dimensions of the chamber were 3 m (L) × 3 m (W) × 2.3 m (H). The
400 distance between the occupants was approximately 1 m. The contaminants were released in the
401 breathing zone of one occupant, which was assumed to be a single pulse source within the
402 duration of 0.2 s. It was assumed that the mouth and nose of the occupant were covered with a
403 tissue, and the initial momentum of the exhaled contaminant was neglected [36]. The supply
404 air inlet was installed on the side wall near the ceiling, and the outlet was installed on the same
405 wall but near the floor. The air exchange rate was 3 ACH, and the supply air temperature was
406 21 °C. The surface temperature of the human bodies was 32 °C. The airflow was calculated by
407 CFD with a grid resolution of 1,415,560, which passed the grid independence test. The
408 distribution of the airflow measuring points based on a resolution of 0.15 m is shown in Fig.
409 11. Note that at the locations near boundaries such as walls and occupants, the airflow sampling
410 cells were larger due to the limitation of geometric structure. In total, there were 3,952 airflow
411 sampling points. The Markov chain grid was then constructed with a grid number of 5,712
412 based on the airflow sampling points and sizes of boundary zones. The calculated contaminant
413 concentrations were normalized by the maximum concentration at the source. The time step
414 size was set at 0.2 s for Case 3.

415



416
417 Fig. 10. Configuration of the chamber with two occupants for Case 3 studied by Chen et al.
418 [36].

419



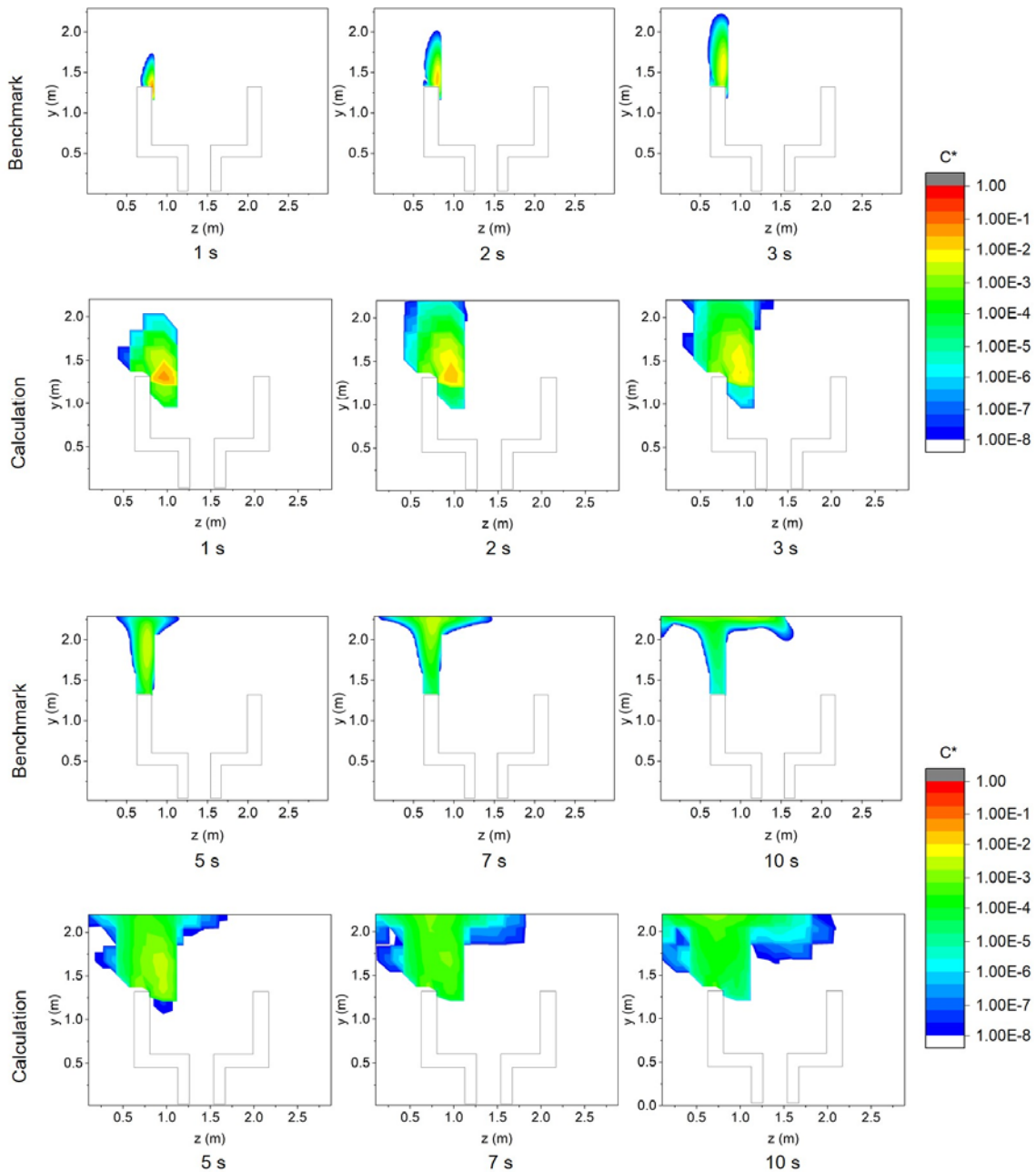
420

421 Fig. 11. Distribution of the airflow sampling points with a 0.15 m resolution for Case 3.

422

423 The results for transient contaminant transport in the first 10 s at the cross-section of plane $x =$
 424 1.55 m are shown in Fig. 12. The stand-alone Markov chain solver based on the measured
 425 airflow field predicted the general trend of contaminant transport reasonably well when
 426 compared with the benchmark. However, the solver calculated more disperse concentration
 427 patterns than did the benchmark. This was because the use of coarse airflow sampling grids led
 428 to failure in predicting the high-gradient concentration regions. Therefore, as in Case 2, if the
 429 aim is to obtain the general contaminant transport trend, the stand-alone Markov chain solver
 430 based on measured airflow field can be used effectively. However, if capturing the detailed
 431 concentration gradients is crucial, the proposed method will not be feasible.

432



433
 434 Fig. 12. Comparison of the contaminant transport between the benchmark and the results
 435 calculated from the measured airflow field at a 0.15-m resolution using the stand-alone Markov
 436 chain solver for Case 3.

437

438 5. Discussion

439 In practical applications, such as hospital wards [6], aircraft cabins [37], and restaurants [38],
 440 where many cross-infections have occurred, it may be challenging to measure the complex
 441 thermo-fluid boundary conditions. Furthermore, the existing turbulence model may be yield
 442 accurate airflow distribution in those complex environments. Consequently, the existing
 443 approach of using commercial CFD software to predict contaminant transport may not be

444 effective. Therefore, this study aimed to preliminarily explore the feasibility of predicting the
445 contaminant transport using a stand-alone Markov chain solver based on the measured airflow
446 field in an enclosed environment. Note that the source location and strength need to be provided
447 in the calculations. According to the computer experiments presented in this study, if the
448 airflow is simple, such as in the isothermal Case 1, the stand-alone Markov chain solver based
449 on the measured airflow field can predict the trend of contaminant transport and peak
450 concentrations reasonably well. However, if the airflow is complex, such as in the non-
451 isothermal Cases 2 and 3, the stand-alone Markov chain solver based on the measured airflow
452 field can reasonably predict only the general trend of contaminant transport. Besides, the
453 developed Markov chain solver in this study aims for the contaminant transport in a steady
454 airflow field. For transient airflow fields, for example, considering natural ventilation, moving
455 occupants, and door and window behaviors, the solver cannot be directly implemented. It
456 should be noted that the capability of the proposed method depends strongly on the resolution
457 of the airflow measurements. This study used a resolution of 0.15 m that was based on the size
458 of the ultrasonic anemometer. In the future, if non-invasive airflow measuring techniques such
459 as volumetric PIV [21] and LIDAR [31] systems have advanced to an affordable and portable
460 level, the applicability of the stand-alone Markov chain solver based on the measured airflow
461 field will be extended. Furthermore, it would be worthwhile to conduct field measurements of
462 whole-space airflow to further demonstrate the feasibility of the proposed approach. Currently,
463 the challenges are the time and effort needed for manual operation of the measurements if
464 ultrasonic anemometers are used. A cable robot-based automated measuring system is under
465 development, which would facilitate on-site measurements in the future.

466

467 **6. Conclusions**

468 This study explored the feasibility of using a Markov chain model to predict contaminant
469 transport from the measured airflow field in an indoor environment. A stand-alone Markov
470 chain solver was developed so that the calculations need not rely on commercial software. The
471 required airflow information, including the three-dimensional velocity components and
472 turbulence kinetic energy, was obtained on the basis of the resolution of ultrasonic
473 anemometers (0.15 m), via virtual airflow measurements simulated by CFD. Three cases were
474 used to investigate the feasibility of the proposed method, and the calculation results were
475 compared with the benchmark calculated by the commercial CFD software. The following
476 conclusions can be drawn:

- 477 (1) When the airflow is simple, such as in the isothermal Case 1, the stand-alone Markov
478 chain solver based on the measured airflow field can predict the trend of contaminant
479 transport and peak concentrations reasonably well.
- 480 (2) When the airflow is complex, such as in the non-isothermal Cases 2 and 3, the stand-
481 alone Markov chain solver based on the measured airflow field can reasonably predict
482 only the general trend of contaminant transport.

483

484

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488

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