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Computer-aided placement of air quality sensors using adjoint framework and sensor features to localize indoor source emission

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7 Abstract

5

With the improvement in sensor technologies, air quality is increasingly be-8 ing monitored. Two major factors in obtaining relevant information are 9 the optimal placement and the number of air quality sensors. Moreover, 10 in cases of poor air quality, the information of the pollution level given by 11 the deployed sensors is not sufficient. An advanced understanding of the 12 data is required to precisely identify the source pollution and thus propose 13 effective solutions. In this article, a virtual testing strategy based on com-14 putational fluid dynamics (CFD) is presented for the optimal placement of 15 indoor air quality sensors. We determine the placement of sensors in view 16 of localizing the maximum of sources emitting on the indoor environment 17 surfaces. Therefore, an adjoint framework is used to obtain the observable 18 region associated with a given sensor position. The proposed method takes 19 into account technical sensor features, such as the limit of detection (LOD). 20 Two applications are studied: a simple 2D case and a real 3D room. In 21 these examples, we first show that reducing the LOD of the sensors by one 22 order of magnitude can increase the observable area by more than 50%. 23

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Then, we note that one-fourth of the potential sensor placements observe almost nothing and that 80% of the potential sensor placements have an observable area two times smaller than the optimal sensor position determined by the proposed CFD-based strategy.

24 Keywords: sensor placement, computational fluid dynamics, adjoint

²⁵ problem, source emission, sensor detection limit, indoor air quality

26 1. Introduction

According to a survey conducted in 2015 by the French Ministry of 27 Ecological Transition, air pollution is the second environmental concern of 28 French people, just after climate change. As people spend approximately 29 80% of their time in indoor environments, increasing attention has been 30 focused on indoor air quality (IAQ). Volatile organic compounds (VOCs) 31 are characteristic chemical species present in indoor environments. Several 32 studies have shown that the concentration of VOCs can be higher in indoor 33 locations, such as early childhood education facilities [1], schools [2], univer-34 sities [3], office buildings [4] and homes [5], compared to the concentrations 35 outside. As reported in [6], VOCs in indoor environments can come from 36 the outdoor air via ventilation and from indoor sources. There are a wide 37 range of indoor sources, e.q. combustion, smoking, building materials, of-38 fice machines, furnishings, paints, termiticides and cleaning products. As 39 permanent and occasional exposure, even at low VOC levels, has an impact 40 on human health [7], it is important to monitor indoor air quality and to 41 precisely localize sources to propose an appropriate action plan to improve 42 air quality. The monitoring of air quality is facilitated by the improvement 43 in sensor technologies, notably nanotechnologies. Hence, the gas sensors 44 become cheaper, smaller, more sensitive, less energy-consuming, etc... To 45

get more details on low-cost sensors for air quality purposes, the reader can 46 refer to the review article [8]. The localization of VOC sources can also 47 be useful for the preservation of cultural heritage, notably artwork, and for 48 structural health monitoring purposes. In most regions of France, the pres-49 ence of woodborers, such as termites, has harmful effects on the safety of 50 structures. The VOC chemical signature of termites can be used for their 51 early detection and localization, which will provide the ability to limit the 52 use of termiticides and to preserve the structure. 53

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To efficiently monitor air quality, the number of sensors and their po-55 sitioning are crucial. In most measurement campaigns, the gas sensors are 56 placed in an empirical way. For example, in a room, an air quality sensor is 57 usually positioned at the breathing zone height or approximately 0.5m from 58 the ceiling in the middle of the room. Unfortunately, this placement does 59 not take into account the characteristics of the room, *i.e.* the geometry and 60 the ventilation. As a consequence, bad sensor placement may lead to the 61 nondetection of some sources. To well-position gas sensors, we can take ad-62 vantage of numerical simulations derived from physical models. In indoor air 63 quality applications, the gas concentration can be predicted using multizone 64 [9; 10; 11; 12] and CFD [9; 13; 14] models. Multizone techniques, which pro-65 vide the time evolution of the averaged concentration in each zone as output, 66 are easy to use and run on a standard laptop. Nevertheless, they consider 67 strong hypotheses, such as a well-mixed concentration. With the ongoing 68 improvement of computers and numerical methods, CFD approaches ap-69 pear to be promising for the prediction of indoor air quality and for optimal 70 sensor placement. In fact, CFD provides a fine description of the spatial 71 concentration in the indoor environment, but the computations are time 72

consuming. A good compromise to study the indoor air quality of an entire 73 building would be to couple multizone and CFD models, as proposed in [15]. 74 To the best of the authors' knowledge, few publications have addressed the 75 optimal placement of gas sensors for IAQ applications. The design of an op-76 timal sensor network, *i.e.* the number and positioning of sensors, has been 77 studied in greater depth in terms of chemical and biological warfare (CBW) 78 and transmission of infectious diseases (TID). The sensor positions are cho-79 sen to early detect and localize indoor contamination. Different methods 80 aim to maximize the coverage area of sensors and to minimize the response 81 time for various sets of release scenarios. In [16], the sensor coverage area is 82 evaluated using CFD and an adjoint advection-diffusion equation, whereas 83 physical model-free approaches based on a dynamical systems approach are 84 preferred in [17]. Note that the adjoint framework is a useful numerical tool 85 for various applications. First, it provides, at a low computational cost, 86 the functional gradient and the Hessian matrix involved in inverse calcula-87 tions to update the parameters of fluid mechanics models [18; 19] and to 88 reconstruct the concentration fields [20; 21; 22]. Additionally, it is used in 89 sensitivity analyses to study the influence of physical model parameters on 90 a quantity of interest [23; 24]. The adjoint framework is also considered 91 for estimating the modeling or discretization error on a quantity of interest 92 [25; 26; 27].93

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Once the positions of the sensors are fixed, knowledge of the concentration given by the deployed sensors is not sufficient for proposing efficient solutions for indoor air quality improvement or for localizing woodborers. One needs to localize and to quantify the source emissions. To achieve this purpose, two families of methods can be found in the literature, *i.e.* data-

driven methods and physical model-based methods. Direct measurements 100 of the source emissions on different surfaces of the environment (furniture, 101 wall, floor, door, etc.) can be planned using innovative sensors, such as fibers 102 placed in a specific device for on-site emission control [28; 9]. This method 103 enables accurate in situ quantification of the source emissions for building 104 materials and furniture, but it requires a large number of sensor devices. 105 Another data-driven method to evaluate source emissions is indirect mea-106 surements. In contrast to the previous methods, the air quality sensors are 107 placed in the room volume and not directly on a surface. Databases of the 108 chemical signatures of sources and *a priori* information of the studied envi-109 ronment collected via questionnaire, including the type and the age of the 110 building materials, renovations, cleaning products and ventilation, are com-111 monly considered in these methods. Finally, the sensor outputs associated 112 with various chemical compounds are analyzed via statistical tools, such 113 as proper component analysis and linear regression, to identify the source 114 emissions [4; 5; 29; 30]. In practice, the chemical compounds emitted by 115 some items in the studied environment may not be referenced in a database. 116 Consequently, these methods may only approximately identify the sources. 117 Physical model-based approaches via inverse modeling techniques can also 118 be valuable for the localization and the quantification of source emissions. 119 In general, inverse problems that couple model and sensor outputs are not 120 well-posed in the sense of Hadamard, *i.e* the existence, uniqueness and non-121 high sensitivity of the solution to the sensor outputs. To address this issue, 122 a sufficient number of well-positioned sensors is required, and regularization 123 must be considered in the mathematical formulation of the inverse problem. 124 In deterministic settings, Tikhonov regularization is commonly considered 125 and consists of adding penalization terms to the data misfit functional, as 126

discussed in [15; 31] for convective-diffusive transport source inversion. In 127 probabilistic inversion formalism, notably Bayesian model updating, which 128 was applied in [32] for CO2 regional source estimations, the model parame-129 ter probability distributions are interesting on two counts. They ensure the 130 problem regularization and provide a confidence interval on the identified 131 source emissions. Nevertheless, probabilistic inversions can be much more 132 time consuming than deterministic ones. Finally, the adjoint framework, 133 previously mentioned for the optimal placement of sensors, can also be used 134 for source localization, as shown in [33; 15]. 135

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In the present article, we propose a virtual testing strategy, taking into 137 account the specificities of the indoor environment (geometry and venti-138 lation) via CFD and gas sensor features (limit of detection), to efficiently 139 select the number and positions of sensors to localize indoor sources. We de-140 fine the "optimal sensor placement" as the combination of gas sensors that 141 maximizes the coverage area. The authors showed in previous works [21] 142 that the sensor observable area can be computed at a reasonable cost using 143 the adjoint framework. Herein, we emphasize that the coverage area can be 144 increased not only by adding sensors but also by using sensors with a lower 145 limit of detection. The rest of this article is organized as follows. In Section 146 2.1, a physical direct model to predict the gas dispersion is presented. Then, 147 we define the adjoint equations in Section 2.2 and introduce a new adjoint-148 based criterion integrating sensor features to evaluate the observable area of 149 potential sensor positions in Section 2.3. An overview of the optimal sensor 150 placement strategy is given in Section 2.4, and it is applied to a 2D case and 151 a real 3D room in the last section. 152

153 2. Materials & Methods

154 2.1. Simulation of pollutant propagation - Direct problem

To predict the dispersion of gas, advection-diffusion-reaction models are 155 commonly used [9; 13; 14]. As a first step, we consider non-reactive gases, 156 *i.e.* reaction phenomena are not modeled. Hence, the cartography of the 157 gas concentration in a two- or three-dimensional space domain Ω is obtained 158 from the advection-diffusion model. Four types of boundaries can be dis-159 tinguished. A boundary presenting a known prescribed concentration C_p 160 is denoted $\partial_p \Omega$. Potential pollution emissions, to be precisely located by 161 the optimal placement of gas sensors, are on the boundary $\partial_{\mu}\Omega$, whereas a 162 boundary that does not present source emission is $\partial_n \Omega$. Lastly, $\partial_o \Omega$ denotes 163 the outgoing flow boundary. 164

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The pollutant concentration $C(\mathbf{x}, t)$ in the domain $\Omega \subset \mathbb{R}^n$, $n \in \{2, 3\}$ can be obtained by solving the unsteady advection-diffusion model, which is also called the "direct problem",

$$\begin{cases} \frac{\partial C}{\partial t}(\mathbf{x},t) + \mathbf{v}(\mathbf{x},t) \cdot \nabla C(\mathbf{x},t) - \nu(\mathbf{x},t) \Delta C(\mathbf{x},t) = 0 & \text{in } \Omega \times [0,T] \\ C(\mathbf{x},t) = C_p(\mathbf{x},t) & \text{on } \partial_p \Omega \times [0,T] \\ C(\mathbf{x},t) = C_u(\mathbf{x},t) & \text{on } \partial_u \Omega \times [0,T] \\ \nabla C(\mathbf{x},t) \cdot \mathbf{n} = 0 & \text{on } \partial_n \Omega \times [0,T] \\ \nabla C(\mathbf{x},t) \cdot \mathbf{n} = 0 & \text{on } \partial_o \Omega \times [0,T] \\ C(\mathbf{x},t = 0) = C_0(\mathbf{x}) & \text{in } \Omega \end{cases}$$
(1)

In Eq. (1), \mathbf{v} is the flow velocity, ν denotes the diffusion parameter, which is the sum of the molecular and turbulent diffusion, and \mathbf{n} denotes the outside ¹⁷¹ normal vector to the surface.

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When the flow and the source emission can be considered stationary with respect to the monitoring time, the concentration field $C(\mathbf{x})$ can be obtained at a lower computation cost using a steady advection-diffusion model

$$\begin{cases} \mathbf{v}(\mathbf{x}) \cdot \nabla C(\mathbf{x}) - \nu(\mathbf{x})\Delta C(\mathbf{x}) = 0 & \text{in } \Omega \\ C(\mathbf{x}) = C_p(\mathbf{x}) & \text{on } \partial_p \Omega \\ C(\mathbf{x}) = C_u(\mathbf{x}) & \text{on } \partial_u \Omega \\ \nabla C(\mathbf{x}) \cdot \mathbf{n} = 0 & \text{on } \partial_n \Omega \\ \nabla C(\mathbf{x}) \cdot \mathbf{n} = 0 & \text{on } \partial_o \Omega. \end{cases}$$
(2)

For example, Eq. (2) can be used to model the dispersion of moisture or woodborers emissions during a measurement campaign under mastered air flow conditions, *e.g.* when the indoor occupants have left. In the following, we limit our study to stationary cases.

180 2.2. Sensitivity area of a gas sensor - Adjoint problem

Physically, the solution of the adjoint problem corresponds to a sensitivity function in terms of a quantity of interest. Hence, to obtain the sensor observable area, we choose the gas concentration at the sensor location \mathbf{x}_{s} as the quantity of interest. It is given by

$$J = \int_{\Omega} f_s(\mathbf{x} - \mathbf{x}_s) C(\mathbf{x}) d\Omega$$
(3)

where f_s is a space function to extract the gas concentration at the sensor location \mathbf{x}_s . In practice, we can take:

$$f_s(\mathbf{x} - \mathbf{x}_s) = \begin{cases} 1/|\Omega_s| \text{ for } \mathbf{x} \in \Omega_s \\ 0 \text{ elsewhere.} \end{cases}$$
(4)

The domain Ω_s is a sphere of radius R_s centered at the sensor location $\mathbf{x_s}$.

From the quantity of interest, we introduce the adjoint problem (5) and compute its numerical solution \tilde{C} .

$$\begin{cases} -\mathbf{v}(\mathbf{x}) \cdot \nabla \tilde{C}(\mathbf{x}) - \nu(\mathbf{x}) \Delta \tilde{C}(\mathbf{x}) = f_s(\mathbf{x} - \mathbf{x}_s) & \text{in } \Omega \\ \tilde{C}(\mathbf{x}) = 0 & \text{on } \partial_p \Omega \\ \tilde{C}(\mathbf{x}) = 0 & \text{on } \partial_u \Omega \\ \nabla \tilde{C}(\mathbf{x}) \cdot \mathbf{n} = 0 & \text{on } \partial_n \Omega \\ \nu \nabla \tilde{C}(\mathbf{x}) \cdot \mathbf{n} + \mathbf{v}(\mathbf{x}) \cdot \mathbf{n} \ \tilde{C}(\mathbf{x}) = 0 & \text{on } \partial_o \Omega \end{cases}$$
(5)

Note that the adjoint problem (5) is a backward-advection-diffusion problem with a source emission located at the sensor position. This adjoint problem can be solved with the same CFD software as that used for the direct problem. For greater detail on the derivation of the adjoint problem, the reader can refer to [21].

2.3. Computation of sensor observable area - A new adjoint-based criterion
After defining the adjoint problem, we propose an adjoint-based criterion
(6) that takes into account the sensor features, *i.e.*, the LOD of the gas
sensor, in view of obtaining the sensor observable area.

$$|\nabla J| \frac{A_s S}{dI_m} > 1 \tag{6}$$

200 where:

• J (resp., ∇J) is the functional (resp., functional gradient) associated with the gas concentration at the sensor location $\mathbf{x_s}$ defined in Eq. (3)

• A_s is the minimum source area expected to be localized

• S is the order of magnitude of the source emission

•
$$dI_m$$
 is the limit of detection of the gas

The sensitivity of the gas concentration at the sensor location \mathbf{x}_{s} to the surface source emissions, which corresponds to the functional gradient ∇J , can be evaluated using the adjoint framework. Following the method in [21], we can show that:

$$\nabla J(\mathbf{x}) = \nu(\mathbf{x}) \nabla \tilde{C}(\mathbf{x}) \cdot \mathbf{n}$$
(7)

sensor

 $_{210}$ where **n** denotes the unit outer normal vector along the surface.

211

20

In summary, the observable area of a gas sensor located at a given position \mathbf{x}_{s} can be numerically predicted by

$$\mathbf{x} \in \partial_u \Omega$$
 such that $|\nu(\mathbf{x}) \nabla \tilde{C}(\mathbf{x}) \cdot \mathbf{n}| \frac{A_s S}{dI_m} > 1.$ (8)

Let us physically interpret the different terms in the proposed criterion (8). The first part $|\nabla J(\mathbf{x})|$ takes into account the sensor position $\mathbf{x}_{\mathbf{s}}$ and gives the sensitivity map of the gas sensor output to the surface source emission. It is numerically obtained from the solution \tilde{C} of the adjoint problem defined in Eqs. (5). In [21], we proved that a null value of $|\nu(\mathbf{x})\nabla \tilde{C}(\mathbf{x}) \cdot \mathbf{n}|$ on a boundary $\partial_b \Omega \subset \partial_u \Omega$ implies that potential source emissions on $\partial_b \Omega$ cannot be detected by a sensor at the position $\mathbf{x}_{\mathbf{s}}$.

The new contribution in this article concerns the next two terms. The second term $A_s \times S$ relies on *a priori* information of the source emissions that are expected to be detected. If we are interested in emissions on large surfaces, such as painted walls, A_s should be approximately a few tens of square meters. By contrast, if we are interested in emissions on small surfaces, such as furniture, A_s should be approximately one square meter. A small value of A_s , *i.e.* less than one square meter, can also be useful for the early detection of termites. The order of magnitude of potential emissions is taken into account with the parameter S. For formaldehyde furniture emission it can be higher than 1ppm [34] whereas it is a hundred times lower for VOCs emitted by molds [35]. In the proposed criterion (8), the observable area for a given positioned sensor depends on the product $A_s \times S$. Hence, the higher this product is, the larger the observable area.

Lastly, the sensor detection limit, depending on technology features, corresponds to the third term in the proposed criterion (8). In the Results Section, we show how the observable area increases as the limit of detection of the sensors decreases.

238 2.4. Outline of the virtual testing strategy for the optimal placement of air
 239 quality sensors

This section aims to present the steps in computer-aided sensor placement. The process is summarized in Figure 1.



Figure 1: Architecture of the computer-aided method for the optimal placement of air quality sensors

The proposed strategy necessitates a mock-up of the studied environment 242 and a fine description of the air flow. The air flow map can be obtained from 243 experiments, empirical models or computational fluid dynamics. Let us em-244 phasize that [22] previously pointed out that a rough approximation of the 245 real flow can lead to a non-representative concentration simulation. Thus, 246 special attention must be given to obtaining the air flow map; otherwise, 247 the proposed placement of gas sensors can be incorrect. After defining a 248 list of n_t potential sensor positions, we solve the adjoint problem (5) asso-249 ciated with each sensor position. All the n_t adjoint solutions are stored in 250 a database. Note that this step is fully parallelizable and is performed only 251 once in a off-line stage. 252

In the proposed virtual testing strategy, the observable area is computed for 253 the n_t sensor positions. As shown in the previous section, the observable 254 area is obtained from the adjoint-based observable criterion (8). In addition 255 to the adjoint solution, a priori information of the sensor technology is also 256 required, *i.e.* the limit of detection dI_m of the sensor and the source to be 257 localized, *i.e.* the orders of magnitude of area A_s and level S of the source 258 emissions. Lastly, the optimal placement corresponds to the one with the 259 largest observable area. When the number n_m of desired sensors is strictly 260 greater than one, the optimal placement is performed in a hierarchical man-261 ner. We start by optimally placing the first sensor and fix its position; then, 262 we seek the optimal placement of the second sensor and fix its position, 263 and so on. As practical outputs for the users, the computer-aided method 264 provides, as a visualization on the numerical mock-up, the observable area 265 of each selected sensor position and the coverage area in square meters for 266 each sensor and for the combination of all n_m sensors. 267

268 3. Results

269 3.1. Application 1 - 2D simple problem

To gain a better understanding, let us first consider a 2D academic prob-270 lem (see Figure 2). The 2D domain Ω is a square with 10 m sides, and the 271 flow \mathbf{V} is uniform. The velocity amplitude (resp. the velocity orientation 272 angle) is 1m/s (resp., 27^{o}), and the diffusion parameter ν is $2.2 \times 10^{-2} m^{2}/s$ 273 which corresponds to the order of magnitude of the turbulent diffusion. As 274 introduced in Section 2.1, $\partial_o \Omega$ denotes the outgoing flow boundary. In this 275 example, we aim to optimally place gas sensors to localize and quantify 276 sources coming from the boundary $\partial_u \Omega$. We focus on the detection of a 277 source emitting on an area greater than 1m on $\partial_u \Omega$ and whose order of 278 magnitude of the amplitude is approximately 100ppm. From this informa-279 tion, we take $A_s = 1m$ and S = 100ppm in the observable criterion (8). 280 Moreover, in the domain Ω , gas sensors can be placed at a limited number 281 of positions. The sixteen potential sensor positions are shown in Figure 2. 282



Figure 2: Geometry of the 2D problem (left) and potential positions of the gas sensor (right)

283

In the followings, firstly the influence of the LOD of the gas sensor on

the observable area is studied for a unique given sensor. Then, the virtual testing strategy is illustrated to optimally place several sensors.

3.1.1. Influence of the LOD on the observable area for a given sensor posi tion

In this section, we consider a given sensor position, that is, Sensor #3288 (see Figure 2). The objective is to evaluate its observable area for different 289 LODs of the gas sensor. We use the proposed adjoint-based criterion (8). 290 First, one needs to solve the adjoint problem defined in Eq. (5), which 291 corresponds to a backpropagation of a pollutant emitted at Sensor location 292 #3 (see Figure 3). Then, from the adjoint solution \tilde{C} and the LOD dI_m , we 293 compute the criterion (8) and deduce the observable area associated with 294 the considered sensor. In Figure 3, we present the adjoint field \tilde{C} and the 295 observable area of Sensor #3 for two different LODs: 10ppm and 0.1ppm. 296 For the considered flow, source emissions on the bottom edge cannot be 297 detected by Sensor #3. The observable area is located around the middle 298 of the left edge. Its precise position along the left edge is $4.9m \pm 1.1m$ for 299 an LOD of 10ppm and $4.9m \pm 2.2m$ for an LOD of 0.1ppm. 300

The evolution of the observable area for a wide range of LODs is pre-301 sented in Figure 4. As expected, a reduction in the LOD leads to an increase 302 in the observable area. The observable area for Sensor #3 is one and a half 303 times larger (resp. two times larger) when using a gas sensor with a 1ppm304 LOD (resp., 0.1ppm LOD) than one with a 10ppm LOD. In summary, this 305 study shows that the LOD of the gas sensor has a strong impact on the ob-306 servable area for detecting source emissions. Consequently, the LOD must 307 be considered in the optimal placement strategies of air quality sensors. 308

309



Figure 3: Adjoint problem solution \tilde{C} associated with Sensor #3 and its observable area for an LOD of 10 ppm and 0.1 ppm - Definition of Source Areas A, B, C for numerical validation of the observable criterion



Figure 4: Observable Area of Sensor 3 as a function of the LOD - The observable area for an LOD of 0.1ppm is 100% larger than that with an LOD of 10ppm

On the basis of the adjoint-based criterion (8), we were able to evaluate the observable area associated with a given sensor position. Let us numerically validate this observable criterion. Sensor position #3 is still considered, and three source locations are defined on the left edge of the 2D

domain (see Figure 3). The different sources are 1 meter in length, and their 314 amplitude is 100ppm. As predicted by the proposed virtual testing strategy, 315 a source in Area A can be detected by the sensor with both LODs (0.1ppm)316 and 10ppm), a source emitted in Area B can be detected only by the sensor 317 with an LOD of 0.1ppm, and neither the 0.1ppm LOD sensor nor the 10ppm 318 LOD sensor can detect a source in Area C. For each source, we simulate 319 the associated gas dispersion by solving the direct advection-diffusion equa-320 tions (2) and obtain the gas concentration at Sensor position #3. From this 321 concentration, we can verify whether the source is detected by the sensors 322 with an LOD of 0.1ppm or 10ppm. In Table 1, the results show that the 323 sensor observable area is well predicted by the adjoint-based criterion (8). 324 A 100ppm source emitted in Area B leads to a gas concentration of 3.27ppm 325 at Sensor position #3. This concentration can be detected by the 0.1ppm326 LOD sensor but not by the 10ppm LOD sensor. This result is in agreement 327 with the predicted observable area shown in Figure 3. 328

		Source detected by the sensor ?	
Source location	Concentration	(Y: Yes, N: No)	
	at sensor position $#3$	0.1ppm LOD	10ppm LOD
Area A $(4.9m\pm0.5m)$	56.06 ppm	Y	Y
Area B $(3.3m \pm 0.5m)$	3.27 ppm	Y	Ν
Area C $(2.2m \pm 0.5m)$	0.04 ppm	N	N

Table 1: Numerical validation of the adjoint-based observable criterion - Concentration at Sensor position #3 simulated for different source locations and verification of the source detection for a 0.1ppm LOD sensor and a 10ppm LOD sensor

329 3.1.2. Optimal placement of gas sensors considering a fixed LOD

The optimal placement of the gas sensors is achieved using the virtual 330 testing strategy presented in Section 2.4. First, we determine the optimal 331 placement of the first sensor. Hence, for each sensor position, the associated 332 adjoint problem is solved and saved in a database. The use of the adjoint 333 solutions and the LOD in criterion (8) enable the evaluation of the observable 334 area of each sensor. Herein, the LOD is fixed to 10ppm. The sensor position 335 with the largest observable area is selected as the "optimal placement". 336 The observable area associated with each sensor is summarized in Figure 5. 337 Note that the sum of the observable areas on the bottom and left edges 338 corresponds to the total observable area on the boundary $\partial_u \Omega$. We observe 339 that Sensors #1 to #11 can detect a source emission only on the left edge, 340 whereas Sensors #12 and #14 are able to detect a source emission located 341 in the lower-left corner of the domain involving the left and bottom edges. 342 Among the 16 potential positions, 13 positions have a total observable area 343 between 1 and 2.5m, and only 3 positions give an observable area larger 344 than 3m. Sensor #12, which has a total observable area slightly larger than 345 those of Sensor #15 and Sensor #16, is selected as the optimal placement. 346 As mentioned in Figure 1, the placement of several air quality sensors 347 is performed in a hierarchical manner. After finding the optimal placement 348 of the first sensor, we fix this sensor and determine the optimal placement 349 of the second sensor, and so on. Previously, Sensor #12 was determined 350 as the optimal placement for the first sensor. To determine the optimal 351 placement of several sensors, we evaluate the observable areas (see Figure 352 5) and select the sensor combination with the highest total observable area. 353 The combination of Sensors #12 and #16 gives the highest total observable 354



Figure 5: Optimal placement (red rectangles) in the 2D domain of several sensors of with an LOD of 10ppm - Observable Areas - Isovalues of the total observable area are represented as solid lines

area, that is, 6.5*m*. We can see that adding Sensor #16 improves the observable area on only the bottom edge, increasing from 2m to 5.5m. The observable area on the left edge is increased by the optimal placement of three sensors, *i.e.*, Sensors #12, #16 and #4. We note that the the total observable area is three times larger for the optimal placement of four sensors (#12, #16, #4, #2) than for the optimal placement of a single sensor #12.

³⁶² 3.1.3. Optimal placement of several sensors considering different LOD

In Section 3.1.1, we showed that the LOD has a significant influence on the observable area for detecting source emissions. As a consequence, two factors can be investigated to improve the observable area: the number of gas sensors and the LOD. In this section, we study the optimal placement

of several sensors in the 2D domain when considering sensors with an LOD 367 of either 10ppm or 1ppm. The results are summarized in Figure 6. We ob-368 serve that the optimal positions of gas sensors may differ according to the 369 LOD. At a 10ppm LOD, Sensor #12 is selected as optimal, whereas Sensor 370 #16 is optimal at a 1ppm LOD. Note that Sensor #16 with a 1ppm LOD 371 has a total observable area that is approximately twice the size of that of 372 Sensor #12 with a 10ppm LOD. To reach a total observable area of 9m, we 373 can either use two Sensors (#16, #14) with a 1ppm LOD or three Sensors 374 (#12, #16, #4) with a 10ppm LOD. 375





Figure 6: Evolution of the observable area as a function of the number of sensors and the LOD (10ppm and 1ppm)

In Figure 7, we present the observable area associated with the optimal placement of four gas sensors with LODs of either 10ppm or 1ppm. The coverage is disparate on $\partial_u \Omega$ for a 10ppm LOD while it is widespread for a 1ppm LOD. Nevertheless, for both cases, source emissions cannot be detected in the upper part of the left edge and the right part of the bottom edge due to the considered flow V and the distribution of the sixteen potential sensor positions. Lastly, for the optimal placement with 1ppm LOD gas sensors, the observable area of some sensors overlaps, notably Sensors #12 and #16. Thus, a source emitted in the overlapped region would be detected by both Sensors #12 and #16.



Figure 7: Map of the observable area for the optimal placement of 4 sensors with LODs of 10 ppm (left) and of 1 ppm (right)

387 3.2. Application 2 - 3D laboratory room

In this section, we illustrate the computer-aided method for the optimal placement of gas sensors in a real 3D laboratory room, including furniture and ventilation systems, located at the IFSTTAR research institute. The dimensions of the room are $5.9m \times 6.2m \times 4.2m$, which correspond to a volume of $150m^3$. As mentioned in Figure 1, we first need a numerical mockup and indoor air flow map (see Figure 8). For that, the incoming flows from the heating duct, the two ventilation grids and the door were measured using

a 1D hot wire anemometer, and the values are reported in Figure 8. Note 395 that the flow exits only from the extractor hood. From this information 396 and the numerical mock-up, we simulate the stationary turbulent flow using 397 the $k - \omega$ SST Reynolds Average Navier-Stokes (RANS) model in the CFD 398 software "Code_Saturne" [36]. In Figure 8, we can see that the airflow 399 entering from the contour of the door is highly turbulent in the vicinity 400 of the door and that a portion of it goes straight in the direction of the 401 extractor hood. In terms of the incoming flow from the second ventilation 402 grid, the main portion circulates close to the ground between the wall and 403 the furniture. Lastly, the velocity flow from the heating duct oriented in 404 the z-direction impacts the top of the furniture immediately below, which 405 generates flow recirculation. From the RANS turbulent flow simulation, 406 let us note that we also evaluate the turbulent diffusion involved in the 407 diffusion parameter ν . A practical rule of thumb consists to compute the 408 turbulent diffusion ν_t from the turbulent viscosity μ_t and the density ρ by 409 $\nu_t = (1/Sc_t)\mu_t/\rho$ where the turbulent Schmidt number Sc_t is taken to 0.7. 410



Figure 8: Numerical mock-up of the laboratory room and measured incoming flows (left) - Flow simulated by CFD software (right)

In the laboratory room, the potential sensor positions presented in Fig-

ure 10 are equally distributed every 50cm at three heights above the ground, 412 namely, 0.5m, 1m and 1.5m. There are 121 sensor positions per height, for 413 a total of 363 potential sensor positions. The potential sensor positions are 414 shown in Figure 10. Herein, we aim to select the sensor positions that pro-415 duce the maximum observable on all the lateral surfaces (door face, furniture 416 face, extractor hood face, back face). To evaluate the observable area, we 417 compute the adjoint concentration \tilde{C} associated with each sensor position 418 and store the values in a database. In practice, the adjoint problems (5) are 419 solved using the Streamline Upwind Petrov-Galerkin (SUPG) formulation 420 [37] in the finite element code "FreeFem++" [38]. In Figure 9, we present 421 the adjoint solution associated with Sensor position #86, which is located 422 close to the furniture wall 0.5 m above the floor. The adjoint field C being 423 a sensitivity function of the concentration at the sensor position to source 424 emissions, Figure 9 shows that a gas sensor at position #86 is sensitive to 425 sources on a part of the furniture face and of the back face. Thus, a single 426 sensor at position #86 may not be able to detect source emissions on the 427 extractor hood and door faces. 428



Figure 9: Simulation of the adjoint concentration \tilde{C} associated with the optimal sensor position #86

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To quantify the observable on each lateral face, we use the observable

criterion (8), taking into account the sensor features. Herein, we consider 430 that the source emission to be detected has an amplitude of approximately 431 10ppm on a surface of approximately $0.25m^2$ and that the limit of detection 432 of the sensor is 0.01ppm, *i.e.* $A_s = 0.25m^2$, S = 10ppm and $dI_m = 0.01ppm$ 433 in Eq. (8). The observable criterion (8) involving the ratio $A_s S/dI_m$, the ob-434 servability results presented in the next paragraphs will be the same for other 435 combinations of A_s , S and dI_m , as long as $A_sS/dI_m = 250$. For each poten-436 tial sensor position, we compute the observable criterion and determine the 437 observability on the four lateral walls. The highest observable area, which 438 is approximately $7m^2$, is obtained for Sensor position #86. Consequently, 439 Sensor #86 is considered to be the optimal placement of the first sensor. 440 In Figure 10, we use sectors to represent the sensor positions with "accept-441 able observability", i.e. more than half of the maximum $7m^2$ observability. 442 Note that 15% (64 positions) of all the potential sensor positions satisfy this 443 criterion. These results highlight the fact that haphazard placement of gas 444 sensors may make it impossible to detect source emissions. 445

Figure 10 shows that most of the sensors are sensitive to source emissions on the furniture and back faces. Only 6 sensor positions (resp. 8 sensor positions) can cover a part of the extractor hood face (resp. the door face). We can see that the observable areas differ depending on the height of the sensor because the air flow is highly three-dimensional in an indoor environment.

After fixing Sensor #86 as the first optimal sensor position, the proposed numerical strategy selects Sensors #9, #235 and #268 as the optimal positions of four sensors to maximize the observable area on the wall faces. The optimal positions are represented by red circles in Figure 10, and the associated observability maps are shown in Figure 11. Sensors #86 and #9 are selected to cover both the furniture face and the back face. Neverthe-

less, Sensor #86 is sensitive to source emissions on the upper part of the 457 furniture face, whereas Sensor #9 can detect sources on the lower part. The 458 sensitivity of the gas concentration at Sensor position #9 to sources emit-459 ted from the lower part between the furniture and the wall is due to the air 460 flow. Indeed, the air flow from the second ventilation grid passes under the 461 furniture and licks the lower part of the furniture wall (see Figure 8). Then, 462 the main part of the flow goes out from the corner of the furniture and the 463 door faces, where Sensor #9 is located. Sensor #235 provides information 464 for the extractor hood face and covers additional areas on the back face. 465 Finally, the observability on the door face is provided by the fourth sensor, 466 that is, Sensor #268. 467

Let us consider Sensor positions #86, #9, #235 and #268 and study the 468 influence of the LOD on the observability of the sources. The parameters A_s 469 and S are kept at $0.25m^2$ and 10ppm. In Figure 11, we show the observable 470 area associated with each sensor for a 10 ppb LOD and for a 2 ppb LOD. 471 As expected, a lower sensor LOD increases the observable area. At a 10 472 ppb LOD, Sensor #86 can detect sources on a portion of the furniture and 473 back faces. When the LOD is decreased to 2 ppb, sources can be detected 474 on a larger surface of the furniture and back faces and on the door and 475 extractor hood faces, which were not observable at a 10 ppb LOD. Similar 476 results are obtained for Sensor #235. Reducing the LOD to 2 ppb enables 477 the observation of new surfaces, such as the door face. Nevertheless, we can 478 see an exception for Sensor #9. In this case, as the flow is confined between 479 the wall and the furniture, the observable area is slightly increased for a 480 2 ppb LOD compared to that for a 10 ppb LOD. Finally, we observe that 481 some wall areas are covered by multiple sensors when the LOD is 2 ppb. 482

483 In the last paragraph, we propose numerical validation of the observable

criterion (8) in the 3D laboratory room. A 10 ppm source positioned on 484 the door face, as shown in Figure 11, is injected on a surface of $0.25m^2$. 485 From a direct simulation, we predict the gas dispersion in the laboratory 486 room and obtain the concentrations at the different sensor positions. The 487 results are given in Table 2. The concentration is higher than 10ppb only at 488 Sensor position #268. Hence, at a 10ppb LOD, the source can be detected 489 by only Sensor #86. In Figure 11, we can see that this result was correctly 490 predicted by the proposed observable criterion when considering a 10ppb491 LOD. At a 2ppb LOD, the observable criterion indicates that the source 492 represented in Figure 11 can be detected by all the optimal sensor positions 493 except Sensor #9. The predicted result is validated by the gas concentration 494 from the direct simulation reported in Table 2, showing that only the gas 495 concentration at Sensor #9 is below the 2ppb LOD. Therefore, Sensor #9 is 496 not able to detect the source, completing the validation study. 497

		Source detected by the sensor ?	
Sensor position number	Concentration	(Y : Yes, N : No)	
	at sensor position	2ppb LOD	10ppb LOD
#86	3ppb	Y	Ν
#9	< 1 ppb	Ν	Ν
#235	3ppb	Y	Ν
#268	49ppb	Y	Y

Table 2: Numerical validation of the adjoint-based observable criterion in the 3D laboratory room - Concentration at sensor positions #86, #9, #235 and #268 simulated for the source location defined in Figure 11 and verification of the source detection for 2ppb LOD sensors and 10ppb LOD sensors

498 4. Conclusions & Prospects

We proposed a CFD-based virtual testing strategy for the optimal place-499 ment of gas sensors to efficiently localize surface source emissions in indoor 500 air quality assessment. This strategy relies on a criterion that integrates the 501 adjoint framework and sensor features, such as the limit of detection, to eval-502 uate, at a reasonable computation cost, the coverage area associated with 503 different sensor positions. We considered the "optimal sensor placement" 504 to be the combination of sensors that maximizes the coverage area. In the 505 two studied applications, we showed that many potential sensor positions 506 observe almost nothing and thus are unable to localize sources, which high-507 lights the importance of using such sensor placement strategies. Then, we 508 emphasized that the coverage area can be increased not only by adding sen-509 sors but also by using sensors with a lower limit of detection. Hence, when 510 positioning indoor air quality devices, we have to consider both the limit 511 of detection and the number of sensors. Finally, this work can be extended 512 to the localization of sources emitted inside a defined volume, especially for 513 outdoor air quality purposes. 514

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Figure 10: Potential positions of gas sensors at three levels h = 0.5m, h = 1m and h = 1.5m and observability representation by wall surface for sensors with an observable area more than half of the highest observability achieved by Sensor #86 - Optimal sensor positions are shown as white circles



Figure 11: Map of the observable areas associated with gas sensors #86, #9, #235 and #268 at two different LODs (10 ppb and 2 ppb). The total observable areas are indicated in parentheses - Definition of a $0.5m \times 0.5m$ source (white square) for the numerical validation of the observability criterion