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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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ABSTRACT

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

1. Introduction

According to a survey conducted in 2015 by the French Ministry of Ecological Transition, air pollution is the second environmental concern of French people, just after climate change. As people spend approximately 80% of their time in indoor environments, increasing attention has been focused on indoor air quality (IAQ). Volatile organic compounds (VOCs) are characteristic chemical species present in indoor environments. Several studies have shown that the concentration of VOCs can be higher in indoor locations, such as early childhood education facilities [1], schools [2], universities [3], office buildings [4] and homes [5], compared to the concentrations outside. As reported in [6], VOCs in indoor environments can come from the outdoor air via ventilation and from indoor sources. There are a wide range of indoor sources, *e.g.* combustion, smoking, building materials, office machines, furnishings, paints, termiticides and cleaning products. As permanent and occasional exposure, even at low VOC levels, has an impact on human health [7], it is important to monitor indoor air quality and to precisely localize sources to propose an appropriate action plan to improve air quality. The monitoring of air quality is facilitated by the improvement in sensor technologies, notably nanotechnologies. Hence, the gas sensors become cheaper, smaller, more sensitive, less energy-consuming, etc … To get more details on low-cost sensors for air quality purposes, the reader can refer to the review article [8]. The localization of VOC sources can also be useful for the preservation of cultural heritage, notably artwork, and for structural health monitoring purposes. In most regions of France, the presence of woodborers, such as termites, has harmful effects on the safety of structures. The VOC chemical signature of termites can be used for their early detection and localization, which will provide the ability to limit the use of termiticides and to preserve the structure.

To efficiently monitor air quality, the number of sensors and their positioning are crucial. In most measurement campaigns, the gas sensors are placed in an empirical way. For example, in a room, an air quality sensor is usually positioned at the breathing zone height or approximately $0.5m$ from the ceiling in the middle of the room. Unfortunately, this placement does not take into account the characteristics of the room, *i.e.* the geometry and the ventilation. As a consequence, bad sensor placement may lead to the nondetection of some sources. To well-position gas sensors, we can take advantage of

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numerical simulations derived from physical models. In indoor air quality applications, the gas concentration can be predicted using multizone [9–12] and CFD [9,13,14] models. Multizone techniques, which provide the time evolution of the averaged concentration in each zone as output, are easy to use and run on a standard laptop. Nevertheless, they consider strong hypotheses, such as a well-mixed concentration. With the ongoing improvement of computers and numerical methods, CFD approaches appear to be promising for the prediction of indoor air quality and for optimal sensor placement. In fact, CFD provides a fine description of the spatial concentration in the indoor environment, but the computations are time consuming. A good compromise to study the indoor air quality of an entire building would be to couple multizone and CFD models, as proposed in [15]. To the best of the authors' knowledge, few publications have addressed the optimal placement of gas sensors for IAQ applications. The design of an optimal sensor network, *i.e.* the number and positioning of sensors, has been studied in greater depth in terms of chemical and biological warfare (CBW) and transmission of infectious diseases (TID). The sensor positions are chosen to early detect and localize indoor contamination. Different methods aim to maximize the coverage area of sensors and to minimize the response time for various sets of release scenarios. In [16], the sensor coverage area is evaluated using CFD and an adjoint advection-diffusion equation, whereas physical model-free approaches based on a dynamical systems approach are preferred in [17]. Note that the adjoint framework is a useful numerical tool for various applications. First, it provides, at a low computational cost, the functional gradient and the Hessian matrix involved in inverse calculations to update the parameters of fluid mechanics models [18,19] and to reconstruct the concentration fields [20–22]. Additionally, it is used in sensitivity analyses to study the influence of physical model parameters on a quantity of interest [23,24]. The adjoint framework is also considered for estimating the modeling or discretization error on a quantity of interest [25–27].

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 of the source emissions on different surfaces of the environment (furniture, wall, floor, door, etc.) can be planned using innovative sensors, such as fibers placed in a specific device for on-site emission control [9,28]. This method enables accurate in situ quantification of the source emissions for building materials and furniture, but it requires a large number of sensor devices. Another data-driven method to evaluate source emissions is indirect measurements. In contrast to the previous methods, the air quality sensors are placed in the room volume and not directly on a surface. Databases of the chemical signatures of sources and *a priori* information of the studied environment collected via questionnaire, including the type and the age of the building materials, renovations, cleaning products and ventilation, are commonly considered in these methods. Finally, the sensor outputs associated with various chemical compounds are analyzed via statistical tools, such as proper component analysis and linear regression, to identify the source emissions [4,5,29,30]. In practice, the chemical compounds emitted by some items in the studied environment may not be referenced in a database. Consequently, these methods may only approximately identify the sources. Physical model-based approaches via inverse modeling techniques can also be valuable for the localization and the quantification of source emissions. In general, inverse problems that couple model and sensor outputs are not well-posed in the sense of Hadamard, *i.e* the existence, uniqueness and non-high sensitivity of the solution to the sensor outputs. To address this issue, a sufficient number of well-positioned sensors is required, and regularization must be considered in the mathematical formulation of the inverse problem. In deterministic settings, Tikhonov regularization is commonly considered and consists of adding penalization terms to the data misfit functional, as discussed in [15,31] for convective-diffusive transport source inversion. In probabilistic inversion formalism, notably Bayesian model updating, which was applied in [32] for CO2 regional source estimations, the model parameter probability distributions are interesting on two counts. They ensure the problem regularization and provide a confidence interval on the identified source emissions. Nevertheless, probabilistic inversions can be much more time consuming than deterministic ones. Finally, the adjoint framework, previously mentioned for the optimal placement of sensors, can also be used for source localization, as shown in [15,33].

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

2. Materials & methods

2.1. Simulation of pollutant propagation - direct problem

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

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",

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

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 normal vector to the surface.

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