The role of simulation in preventing indoor air pollution: a foregone conclusion?

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Abstract. Indoor air pollution has become a broad problem due to various indoor or outdoor pollutant sources and limited ventilation. A performance-based approach, which is built upon accurate modelling and simulation of indoor air pollutant characteristics, has obvious advantages over the prescription-based method to achieve better indoor environment. Moreover, the simulation could play a key role in actively preventing indoor air pollution from happening in the first place. In this study, a mechanistic air quality simulation tool was introduced. To verify the reliability of simulation results, two actual field cases with different levels of complexity and time duration were discussed. One was performed in a full-scale experimental room with a single formaldehyde source of a medium density board, in which indoor formaldehyde concentrations varied naturally. Long-term (more than three years) comparison between the simulation results and measurement were conducted. Another occurred during the decoration process in an actual apartment. The formaldehyde concentration levels were well predicted at the design stage and later verified by the field data. Nevertheless, a lot more efforts are required to make indoor air quality (IAQ) simulation tools readily useful in actual engineering applications.

1. Introduction
Modern built environments are filled with various natural or man-made air contaminants, leading to the increasing sensitivity of the public to indoor air quality (IAQ). Investigations on IAQ have demonstrated that pollutant concentrations such as volatile organic compounds (VOCs), particulate matter (PM), and semi-volatile organic compound (SVOC) inside buildings may reach a high level [1-4]. Recently, the performance-based approach has been adopted to design indoor environment and select control strategies [5]. Similar to building energy systems, the detailed IAQ outcomes (i.e., indoor pollutant levels) need to be simulated by first principles models. However, mass transfer of pollutants is an extremely complex process, influenced by emission sources, adsorption sinks, ventilation, and air cleaning simultaneously [6-9]. In addition, indoor pollutant concentrations could be influenced by environmental conditions, such as temperature and humidity. The above key factors should be well considered by the performance-based approach.

Compared with the traditional “prescription-based” method which is largely empirical in nature, the performance-based approach is built upon accurate modelling and simulation of indoor air pollutant characteristics. If properly used, it could prevent indoor air pollution in a time- and cost-effective way. The key to this approach is predicting the indoor pollutant levels precisely, during the design and material-selection stage, by considering the key factors influencing the indoor air concentrations. This ensures that early preventive actions can be considered before an air-pollution problem actually occurs. However, such a competitive method has not received enough attention in the IAQ world. Many doubt whether accurate modeling of complex IAQ problem is possible, and yet convincing verification and actual engineering application cases are rare in the open literature.
This study attempts to address the above issues by discussing the feasibility to use a performance-based simulation tool to actively prevent indoor air pollution from happening. A long-term verification case and a real-world application case are used to demonstrate the credibility and key challenges of this process.

2. Methods

In general, indoor contaminant levels could be influenced by many factors, including the emission sources, adsorption sinks, ventilation, and possible uses of the air cleaners. However, the influencing mechanism of these factors may be different, depending on pollutant types and their origin. For example, natural ventilation is beneficial for indoor VOC elimination but may bring more PM into buildings especially under outdoor air pollution conditions. To achieve better IAQ, the effects of multiple factors on different pollutant types should be considered. Among the main indoor contaminants, the mass transfer process of VOCs is the most complicated, and thus taken as an example next.

The VOCs emission from their sources, such as building materials, to indoor air is a dynamic process, involving mass transfer inside the material, at the material-air interface, and in the bulk air. The processes are likely to be affected by environmental conditions, such as temperature, humidity, and velocity of air flow, leading to more challenges in an accurate description of pollutant emissions. Meanwhile, some porous building materials can act as sinks of pollutants. Therefore, VOCs emitted from one material can be adsorbed by other materials and then gradually released into the air under suitable conditions, affecting the indoor concentrations in the long term. The airflow exchange between a building and outdoors plays a key role in diluting the indoor-generated pollutants. In the case of multi-zone situations, the internal airflows determine the pollutant inter-exchange between zones. Both external and internal airflows vary with outdoor meteorological and indoor environment conditions. The possible uses of air cleaning devices, such as portable air cleaners have the ability to reduce indoor pollutant load to some extent, including the adsorption process of VOC molecules from the air to inside of the activated carbon filter.

To prevent indoor air pollution from happening, all the above influencing factors, as well as various pollutants, need to be simultaneously considered prior to the actual activities, and this is achieved by using reliable simulation tools along with supporting databases. A simulation tool containing several input-output modules is illustrated in Fig 1. It should be mentioned that each input module was described by the first-principle model, which clarified the pollutant-transport mechanisms. In addition, realistic influencing factors affecting indoor concentrations, such as the combined effect of temperature, humidity and time duration were considered [10]. To make such a tool workable in practice, databases containing supporting information of various pollutant sources, sinks, ventilation, and air cleaning devices are also needed.

![Figure 1. Illustration of the framework of an IAQ simulation tool](image-url)
By applying such a tool at the design stage, a prescient result can be projected using a computer, as shown in Fig 2. At first, the pollutant-concentration goal, i.e., the level that must not exceed at a certain time, should be set. Some may choose “meeting the minimum indoor air-quality standard requirement two weeks after the indoor decoration is complete” as their goal, while others may select a higher standard (lower concentration levels). With the simulated “future” scenarios, in case a problem is foreseen, it will suggest necessary correctional actions before the plan is actually implemented. For example, if the simulation finds that a design cannot meet the goal, optimization will be performed such as selecting low-emission sources or enhancing ventilation. This process should become a norm in future IAQ design and operation providing reliable simulation tool together with supporting databases become available.

3. Case description
To verify the feasibility of the above-mentioned approach, cases involving different contaminants have been tried. Among these, simulation verification of VOCs has suffered more challenges, because of their complicated mass transfer mechanisms and relatively recent appearances. Therefore, two actual field cases regarding formaldehyde, a major gaseous pollutant indoors, with different levels of complexity and time duration are discussed next.

The first case intended to verify the long-term performance of the simulation model proposed. A full-scale experimental room with a single formaldehyde source of medium density board was built. Interior temperature and humidity, as well as the air change rate between outdoor and indoor, were allowed to vary naturally with the ambient environment. Long-term (more than three years) of dynamic indoor formaldehyde concentrations were measured using the 3-methyl-2-benzothiazolinone hydrazine (MBTH) method, and the results were compared with that of simulations.

The second case intended to test the feasibility of the simulation tool in predicting potential IAQ problems in an actual apartment. A piece of blockboard was planned for permanent use during interior decoration. The time-varying indoor formaldehyde concentrations were predicted to exceed the allowable limit. Nevertheless, the material was still introduced into the apartment. The indoor concentrations were measured and verified the accuracy of the simulation results. Later, the blockboard had to be removed from the apartment. The comparison between simulation and measurement were conducted again.

4. Results and discussion
The comparison of formaldehyde concentrations between measurement and simulation in the full-scale experimental room is shown in Fig 3. Indoor environmental monitoring data indicated that the temperature varied from -10.9 °C to 31.4 °C, while that of relative humidity fell into a range between 46.5% to 83.6%, almost covering the range of indoor environmental parameters commonly observed in buildings. In such a complex environment, time-varying indoor formaldehyde was simulated, and
the results indicated the concentrations varied seasonally with peak values decreasing with years. Meanwhile, frequent field sampling (ranging from a few days to four weeks) of actual indoor formaldehyde concentration was conducted from October 2012 to February 2015, and simulation results agreed well with the measurement data. Such a long-term model verification, especially in an actual room with environmental conditions changing sharply, gives a certain level of credibility to the simulation model.

**Figure 3.** Comparison of formaldehyde concentrations between measurement and simulation during a three-year time, in the full-scale experimental room

The comparison of formaldehyde concentrations between measurement and simulation in the second case is shown in Fig 4. The tool successfully predicted the unacceptable level of formaldehyde due to the use of the blockboard indoor. Although not shown in the figure, the simulation results also indicated that such a high level of formaldehyde concentration would last years before decreasing to an acceptable level. Hence, the best solution would be to replace this blockboard by a different, low-emitting material. Unfortunately, this suggestion was not adopted by the owner and the blockboard was still introduced into the apartment. Despite the lesson learned from such a mistake, an unexpected “benefit” was that this situation provided an opportunity to verify the reliability of the simulation results. The measured concentration verified the initial suggestions. After recognizing the aforementioned problem, the owner was still hesitant to dismantle the installed blockboard hoping that the problem would not last long. Hence, the board remained inside for approximately 40 days. Another field measurement was conducted at 984 h, and the formaldehyde concentration was still as high as 0.439 mg/m³ under all windows closed condition. A decision was finally made to remove the blockboard. The concentration reduced immediately afterwards, and the simulation result was verified for the second time. By applying such a real case, the simulation prevention method during the design stage was proved to hold back indoor air pollution from happening.
Figure 4. Comparison of formaldehyde concentrations between measurement and simulation in the actual apartment. The first part (0–72 h) represents the introduction of the blockboard indoors. The middle part (72–984 h) is the duration between the material introduction and removal. The third part (984–1056 h) represents the time after the blockboard was removed.

The above model verification cases were both based on real-world instead of laboratory settings. Many factors in the laboratory could be well-controlled, but situations in actual buildings are much more complex, making the simulation prediction more difficult. Long-term data verification is another challenge. More case studies with multiple pollutant types, sources, and interactions are yet to be conducted in the future to further test the methodology.

5. Future perspectives
One benefit of this study is to transfer the model verification from laboratory to real rooms, which are closer to the actual conditions of the buildings. However, a lot more efforts are required to make IAQ simulation tools readily useful in actual engineering applications, including:

(1) Health effect. Since different pollutant may have various effects on health even if they have the same concentration levels, and a health index of individual compounds and their interactions should be considered.

(2) Occupant behavior. Humans can be considered as an important part of the buildings. On the one hand, occupant behaviors can determine IAQ. On the other hand, the IAQ could have an influence on occupant behaviors. The interrelation between occupant behaviors and IAQ need to be considered.

(3) Smart sensors and big data. On-line air pollutant monitoring technology shall be considered, which provides an extended “eye” to reach out remote sites at a larger scale and collecting “big data”. Advanced simulation technologies combining these on-line monitors provide an effective tool to predict the indoor contaminant levels and optimize the control strategies.

(4) Various control strategies. In terms of the new building, source control may be the most effective way to prevent air pollution. However, this strategy may face limitations in the existing building. In such cases, holistic control strategies combining source control, ventilation, and air cleaning may be considered depending on different scenarios

6. Conclusion
This study introduced a performance-based approach, which is built upon accurate modelling and simulation of indoor air pollution characteristics to achieve a better indoor environment. Two typical cases occurred in an actual environment under different levels of complexity and time duration were
presented to verify its feasibility. It was demonstrated that the simulation prevention method could play an active role to prevent indoor air pollution from happening. Nevertheless, a lot more efforts are required to make IAQ simulation tools readily useful in actual engineering applications.

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