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An algorithm for fast prediction of the transient effect of an arbitrary initial condition of contaminant

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ABSTRACT

Fast predicting the transient effect of an initial condition is crucial for determining effective room ventilation strategies. However, traditional CFD methods conduct time-consuming iterative calculations. In previous studies based on superposition theory, the similarity condition, i.e., the proportional relationships of concentrations among different positions are the same between actual initial condition and initial condition adopted in calculating index AIC (accessibility of initial condition) or TAIC (transient accessibility of initial condition), is required, which is difficult to meet. In this paper, an algebraic expression is established for transient effect of an arbitrary initial condition. To establish the expression, the room is divided into a certain number of zones, and the initial concentration in each zone is assumed to be uniform, whereas the concentration outside the zone is zero (the so-called sub-initial condition). By calculating TAIC of each sub-initial condition in advance, the transient effect of initial condition can be obtained by superposition theory. From an analysis of cases with different initial conditions, the following conclusions can be made: (1) the expression has the same accuracy as a CFD simulation for the condition that initial contaminant distribution in each zone is uniform; (2) a longer predicting time, larger number of zones and more uniform initial distribution in each zone help to improve accuracy; (3) between 12 and 140 zones are suggested for the study in consideration of both accuracy and computing costs. The proposed method may be useful in cases where fast prediction is required, such as emergency ventilation and on-line control.

1. Introduction

Indoor air quality (IAQ) plays an important role in human health and safety [1]. In recent decades, multiple events, such as the SARS and H1N1 influenza outbreaks and toxic gas leakages, remind us to take active measures to decrease indoor air pollution and provide a healthy indoor environment [2–7]. Once hazardous substances are released in a room, an initial distribution of contaminant occurs immediately [8,9]. Fast predicting the transient effect of the initial condition for the following time period will help to make correct on-line decisions to decrease the pollution [10,11].

The computational fluid dynamics (CFD) technique is a popular method used to predict contaminant distribution [12–16]. When boundary and initial conditions are given, the detailed spatial and temporal distribution of the contaminant caused by the initial condition can be predicted with an acceptable accuracy. CFD has been widely used in the research and design of ventilation systems [17–24]. However, the time consumption of the iterative computational routine makes it difficult to be adopted in cases where fast calculations are required, such as emergency ventilation and online parameter control. The nodal models, such as multizone models and zonal models can perform fast prediction by assuming the concentration in an enclose space to be uniform; however, they cannot predict detailed information of non-uniform parameter distribution [25–28]. Some fast CFD models were built so as to fill the gap between nodal models and traditional CFD models. Zuo and Chen [10,29] and Zuo and Jin [30] proposed the fast fluid dynamic (FFD) method to reduce the computing cost by using simple and low order schemes. The results showed that FFD can offer more detailed flow information than nodal models and is much faster than CFD; however, the accuracy is lower than CFD. Wang et al. [31] utilized numerical viscosity from coarse grid CFD to conduct fast prediction. The results showed that the method can reasonably predict general airflow patterns in typical indoor environments.

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Wang and Malkawi [32] further considered improving the computing speed of the annual hourly CFD simulation by reusing previous simulated results to generate new results. All of the above fast methods try to find a compromise between the computing speed and accuracy.

Other attempts have been made for the fast prediction of contaminant distribution based on the superposition theory for a steady flow field. Murakami [33] and Kato et al. [34] defined the scale for ventilation efficiency (SVE) indices for contaminants to quantify the steady effect of different boundary conditions. Once the SVE indices are obtained, the steady concentration distribution can be predicted almost without time consumption. To further predict the transient effect of different boundary and initial conditions, Li and Zhao [35] and Li and Chen [36] defined the accessibility of supply air (ASA), accessibility of contaminant source (ACS) and accessibility of initial condition (AIC) indices to reveal the time-averaged effects of the supply air, contaminant source and initial condition, respectively. Based on the accessibility indices, Yang et al. [37] and Li and Chen [36] established simplified expressions for the time-averaged contaminant concentration at an arbitrary position with uniform initial condition and non-uniform initial condition, respectively. To evaluate the transient effects of different boundary conditions instead of the time-averaged effects, Ma et al. [38] defined the transient accessibility of supply air (TASA), transient accessibility of contaminant source (TACS) and transient accessibility of initial condition (TAIC) indices to quantify the contributions of the supply air, contaminant source and initial condition to the transient concentration. Based on the transient accessibility indices, Ma et al. [38] established an expression for the transient concentration of contaminant at an arbitrary position. All of these indices and expressions avoid repeated iterative computations and can therefore be used in the fast strategy decision.

However, the expressions by Li and Chen [36] and Ma et al. [38] have a limitation in predicting the transient effect of the initial condition. In the expressions, the index AIC or TAIC is calculated based on a specific initial distribution of contaminant. The expressions cannot make an accurate prediction until the proportional relationship of the concentrations among different positions is the same between the actual initial condition and the specific initial condition adopted in the AIC or TAIC calculation (called the similarity condition). However, the concentration distribution is affected by multiple variable factors, such as the contaminant release's location, rate and time duration, so that the resulting initial conditions are various. It is difficult to ensure that the actual initial condition is similar to that used in the AIC or TAIC calculation. As a result, the prediction deviation is caused when the similarity condition cannot be met.

If the room space is artificially divided into a certain number of zones, the whole initial condition will be correspondingly divided into the same number of virtual initial conditions (called sub-initial conditions). For each sub-initial condition, the contaminant distribution in the target zone is the same as the initial condition and the concentrations in the other zones are zero. If the transient concentration caused by the initial condition can be transformed into the summation of the transient concentrations caused by each sub-initial condition, the similarity condition for the whole initial condition will be replaced by the similarity conditions for the sub-initial conditions. The latter is much easier to be approximately met; therefore, the adaptability of the expressions to various initial conditions may be improved. Furthermore, when the fast prediction is based on the divided zones or sub-initial conditions, the uniform contaminant distribution in each divided zone is always assumed for the AIC or TAIC calculation, which may also cause a prediction deviation compared with the direct CFD prediction.

In this paper, a fast prediction method adaptable to various initial conditions is proposed. The prediction accuracy of the method is investigated by a series of numerical cases.

2. Theoretical method for the transient effect of an arbitrary initial condition

In Section 2, the transient expression by Ma et al. [38] is first introduced. Based on the expression, a prediction method for the transient effect of an arbitrary initial condition is proposed.

2.1. Expression for the transient concentration of contaminant

(1) Index of transient accessibility of supply air (TASA) and contribution from supply air

For a steady flow field, assume that the initial contaminant concentration is 0, the emission rates from all of the contaminant sources are 0, and the contaminant concentration in the supply air from the n_Sth inlet is $C_S^{n_S}$ whereas those of the other inlets are 0. Then, the TASA at an arbitrary point p from the n_Sth inlet is defined as [38]:

$$a_{S,p}^{n_S}(\tau) = \frac{C_p(\tau)}{C_S^{n_S}} \tag{1}$$

where $a_{S,p}^{n_S}(\tau)$ is the TASA from the n_Sth inlet to point p at moment τ; $C_p(\tau)$ is the contaminant concentration of point p at moment τ (kg/m^3);$C_S^{n_S}$ is the contaminant concentration in the supply air from the n_Sth inlet (kg/m^3); τ is the predicted moment (s).

For a room with N_S supply air inlets, the contribution from all of the supply air inlets to the formation of the transient concentration at an arbitrary point p is expressed as:

$$C_{p,sa}(\tau) = \sum_{n_S=1}^{N_S}\left[C_S^{n_S} a_{S,p}^{n_S}(\tau)\right] \tag{2}$$

where $C_{p,sa}(\tau)$ is the contaminant concentration of point p at moment τ resulted from concentrations in the supply air from all of the inlets (kg/m^3); N_S is the number of the supply air inlets.

(2) Index of transient accessibility of contaminant source (TACS) and contribution from contaminant source

For a steady flow field, assume that the initial contaminant concentration is 0, the contaminant concentrations in the supply air from all of the inlets are 0, and the emission rate from the n_Cth contaminant source is J^{n_C}, whereas rates from the other sources are 0. Then, the TACS at an arbitrary point p from the n_Cth contaminant source is defined as [38]:

$$a_{C,p}^{n_C}(\tau) = \frac{C_p(\tau)}{\overline{C}_E^{n_C}} \tag{3}$$

where $a_{C,p}^{n_C}(\tau)$ is the TACS from the n_Cth contaminant source to point p at moment τ; $\overline{C}_E^{n_C}$ is the average concentration from all of the outlets caused by the n_Cth contaminant source (kg/m^3), $\overline{C}_E^{n_C} = J^{n_C}/Q$, J^{n_C} is the emission rate from the n_Cth contaminant source (kg/s), and Q is the ventilation rate of the room (m^3/s).

For a room with N_C contaminant sources, the contribution from all of the sources to the formation of the transient concentration at an arbitrary point p is expressed as: