Experimental verification of tracking algorithm for dynamically-releasing single indoor contaminant

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Abstract
Identifying contaminant sources in a precise and rapid manner is critical to indoor air quality (IAQ) management as disclosed source information can facilitate proper and effective IAQ controls in environments with airborne infection, fire smoke and chemical pollutant release etc. Probability-based inverse modeling method was shown feasible for locating single instantaneous source in IAQ events. To tackle more realistic sources of continuous release, this paper advances the method to identify continuously releasing single contaminant source. The study formulates a suite of inverse modeling algorithms that can promptly locate dynamic source with known release time for IAQ events. Two field experiments are employed to verify the prediction: one in a multi-room apartment and the other in a hospital ward which was involved in a SARS outbreak in Hong Kong in 2003. The developed algorithms promptly and accurately identify the source locations in both cases.

Keywords
indoor air quality, source identification, inverse modeling, experiment validation, SARS

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1 Introduction

Recent world health report indicates that indoor air pollution is responsible for more than 1.6 million annual deaths and 2.7% of the global burden of disease, which makes it one of the top two environmental risks to ill health (WHO 2010). It was estimated that poor indoor air environment can cost the U.S. alone tens of billions of dollars each year in lost productivity and medical care (Fisk 2000). In addition, building environmental safety is always an important and critical concern to building occupants. Various indoor environmental accidents (e.g., fire smoke and airborne chemical and biological agents) can cause a large number of casualties in a short period of time (Karter 2003; Liu and Zhai 2007).

Poor indoor air quality (IAQ) primarily results from the dispersion of microbiological and chemical contaminants, such as, CO₂, NOₓ, dust, pollen, tobacco smoke, and volatile organic compounds (VOC) from various sources (Wikipedia 2011). In practice, contaminant source control, ventilation, and air purification are typically used to achieve a good indoor air quality. Supplying fresh air and cleaning dirty air are effective IAQ management methods if the contaminant source(s) or contaminated zone(s) can be determined. Without contaminant source conditions (location, release time and strength), current building mechanical systems could even facilitate contaminant propagation, serving as a natural pollutant carrier; and air cleaning devices (e.g., filter and ultraviolet system) might suffer from inefficiency if not placed at proper contaminant transport paths. Disclosing contaminant source conditions is thus critical to IAQ control.

To develop a quick and reliable approach to identifying indoor contaminant sources, Liu and Zhai (2007) performed a comprehensive literature review on various contaminant tracking methods and concluded that the adjoint probability...
method originally developed by Neupauer and Wilson (1999, 2001) for groundwater pollutant source tracking may be appropriate for IAQ study. Upon this adjoint probability concept, Liu and Zhai (2008, 2009) developed a series of theories and methods that identify the location of a single instantaneous contaminant source with given release time in various indoor environments. The developed method has undergone a number of numerical experiments, verifying the effectiveness of the algorithm. However, the method still needs validation using realistic field experiments that may incorporate many operational uncertainties. In addition, most IAQ incidents may experience a continuous contaminant release with either constant or dynamic release intensity. Such examples may include chemicals being released from building materials, furnishings, and household products like air fresheners; particulate matter (PM) from instance smoking and furnace combustion; and virus from continuous (or intermittent) coughing and sneezing. Compared to instantaneous sources, these continuously or intermittently releasing sources are referred as dynamic sources. Developing proper algorithms for tracking dynamic sources and verifying the inverse tracking methods using physical experiments are the two main focuses of this paper.

2 Previous research: Locate an instantaneous source

The probability-based dynamic source tracking method developed here is based on the algorithm for tracking the location of an instantaneous source in indoor environment (Liu and Zhai 2007, 2008, 2009). The key concept of this method is the forward location probability density function that describes the probability of a contaminant parcel originated from a source location to reach a sensor (observation) location in the spatial domain after a certain time period. If the spatial domain is divided into many (assume N) cells (zones), contaminants detected at one observation cell may originate from N potential source cells. A conventional method to find the probable connection between the detector and source locations is to release some contaminants at each potential source location, perform a forward contaminant dispersion test, and find the amount of contaminant mass trapped at the sensor cell. The ratio of the trapped mass at the sensor location to the total released mass is defined as the forward location probability of the contaminant from the source to the sensor location. The source location with the maximum probability among the N potential sources is the most possible source location. This conventional method would thus require N forward pollutant transport experiments to locate the source. The method developed by Liu and Zhai (2008, 2009) is able to derive N probabilities in one calculation so that the computational burden is greatly alleviated. The method follows the general procedure as described below to track the location of an instantaneous source in indoor environment.
(1) Determine the flow domain of the IAQ event to be studied, for instance, a gymnasium, a theater, or an office building.
(2) Collect essential information about the flow domain that may impact the airflow and contaminant transport. Typical domain characteristics include, but are not limited to, geometries, obstacles, flow and thermal conditions of air inlet(s) and outlet(s), surface temperatures, surface materials that may affect the contaminant concentrations, etc.
(3) Collect sensor information, including sensor number, resolution, accuracy, locations, and recorded concentration data (if available).
(4) Divide the flow domain into small cells or zones depending on the spatial resolution requirement of source identification. Build an airflow model for the flow domain and perform an airflow simulation to obtain the airflow field in the domain.
(5) Calculate the standard adjoint location probability (SALP), based on an alarm sensor output (on/off), by solving the adjoint contaminant transport equation. The adjoint equation for computational fluid dynamics (CFD) modeling takes the following form:

\[
\frac{\partial \psi^*}{\partial \tau} - \frac{\partial \nabla \psi^*}{\partial X_j} = \frac{\partial}{\partial X_j} \left[ \nu_{C,j} \frac{\partial \psi^*}{\partial X_j} \right] + \delta (\bar{x} - \bar{x}_o) \cdot \delta (\tau)
\]

\[
\psi^*(\bar{x},0) = 0 \quad \psi^*(\bar{x},\tau) = 0 \quad \Gamma_1
\]

\[
\left[ \nu_{C,j} \frac{\partial \psi^*}{\partial X_j} + V_j \psi^* \right] n_i = 0 \quad \Gamma_2
\]

\[
\left[ \nu_{C,j} \frac{\partial \psi^*}{\partial X_j} \right] n_i = 0 \quad \Gamma_3
\]

\[
\psi^* \text{ is the adjoint location probability, } \nu_{C,j} \text{ is the effective turbulent diffusion coefficient at } X_j \text{ direction, and } \Gamma_i, \Gamma_2, \Gamma_3 \text{ are the domain boundaries for the 1st, 2nd and 3rd type boundary conditions of the forward CFD contaminant transport equation (Liu and Zhai 2008). In the forward CFD contaminant transport equation, the 1st type boundary condition is of fixed concentration, the 2nd type boundary condition is fixed flux, and the 3rd boundary condition is a linear combination of the previous two and is rarely used in indoor environment modeling. Note that the initial and boundary conditions constrain the adjoint probabilities at the initial time and on the boundaries.}

(6) Improve the accuracy of the prediction by combining multiple sensor outputs and/or incorporating concentration readings into the calculation. This will produce a set of conditioned adjoint location probability (CALP) for single instantaneous source, using Eq. (2) if multiple alarm signals are detected and used, or Eq. (3) if multiple concentrations are recorded and used.

\[
f_x(x; \tau_0, \tau_1, \ldots, \tau_N) = \prod_{k=0}^{N} f_x(x; \tau_0, \tau_k) + \int_{\xi_{-\infty}}^{\xi_{\infty}} \prod_{k=1}^{N} f_x(x; \tau_0, \tau_k) dx
\]

\[
f_x(x; \hat{C}_1, \ldots, \hat{C}_N; \tau_0, \tau_1, \tau_N)
\]

\[
= \frac{\int_{\xi_{-\infty}}^{\xi_{\infty}} \int_{\xi_{-\infty}}^{\xi_{\infty}} \prod_{k=1}^{N} P(\hat{C}_k; M_0, \hat{x}, \tau_0, \tau_k) \cdot f_x(x; \tau_0, \tau_k) d\xi}{\int_{\xi_{-\infty}}^{\xi_{\infty}} \int_{\xi_{-\infty}}^{\xi_{\infty}} \prod_{k=1}^{N} P(\hat{C}_k; M_0, \hat{x}, \tau_0, \tau_k) d\xi dM_0}
\]

Where \( f_x(x; \tau_0, \tau_k) \) is the SALP for the \( i \)th observation.

(7) Pinpoint the source location to be the cell or zone with the largest CALP value.

3 New development: Locate a dynamic source

Equations (1) – (3) relate the resulted contaminant concentration with initially released pollutant mass from an instantaneous source at certain time ago. When the source is dynamic (with continuous release), the final detected concentration is an accumulation of concentrations resulted from the pollutant mass released at every time point before the measurement time. In the same manner of defining and deriving SALP in Eq. (1), this research develops another SALP for dynamic sources, named SALP-D, which is defined as the ratio between the resulted concentration due to single dynamic source and the initially released mass.

Figure 1 illustrates an example of a dynamic source, which releases contaminants for at least eight seconds. It can be...
deemed as the sum of several single instantaneous sources at different time points. For example, the dynamic source shown in Fig. 1 can be obtained by adding the following discrete sources together: a source releasing 1.5 mg contaminants in the 1st second, a source releasing 2.25 mg contaminants in the 2nd second, a source releasing 2.75 mg contaminants in the 3rd second, …, and a source releasing 2.45 mg contaminants in the 7th second, and so on.

Mathematically, the mass discharging rate of the source follows this equation

\[
\frac{dM(t)}{dt} = M_0 \cdot h(t)
\]  

(5)

where \(M_0\) is the initially released contaminant mass from the source, \(h(t)\) is the change rate of the ratio between dynamically released mass and the initial released mass. The curve in Fig. 1 shows an example of function \(h(t)\) with \(M_0 = 1\) mg. If \(h(t)\) is constant over a time period, the source has constant releasing strength, a special type of dynamic source.

In Fig. 1, assume a measurement is made at the 4th second. Among all discrete sources that compose the dynamic source, those releasing contaminants before the time of 4 s (i.e., four discrete sources at \(t = 1\) s, 2 s and 3 s in this example) contribute to the measured concentration. More specifically, the added source at \(t = 1\) s, \(dM(t = 1)\), spreads for 3 seconds and produces a concentration contribution of \(dM(t = 1) \cdot f_s(\bar{x}_1;t = 3, \bar{x}_1)\) to the measured value; similarly, the added source at \(t = 3\) s, \(dM(t = 3)\), spreads for 1 second and results in a concentration increase of \(dM(t = 3) \cdot f_s(\bar{x}_3;t = 1, \bar{x}_3)\).

Figure 2 illustrates the contribution of discrete source in each second to the measured concentration at \(t = 4\) s. The contributed concentration from each discrete source can be calculated via

\[
dC(\bar{x}_n,t = T) = dM(t) \cdot f_s(\bar{x}_n; T - t, \bar{x}_n)
\]  

(6)

By substituting Eq. (5) into Eq. (6) and integrating both sides, the measured concentration is obtained as

\[
C(\bar{x}_n,t = T) = \int_0^T dC(\bar{x}_n,t = T)
= \int_0^T M_0 \cdot h(t) \cdot f_s(\bar{x}_n; T - t, \bar{x}_n) \cdot dt
\]  

(7)

According to the definition of SALP (i.e., ratio between resulted concentration and contaminant mass released at the first time step), a revised SALP for dynamic source, SALP-D, can be expressed as below:

\[
\text{SALP-D} = \sum_{k=1}^N f_s(\bar{x}_n; t, \bar{x}_n) \int_0^T h(t) \cdot f_s(\bar{x}_n; T - t, \bar{x}_n) \cdot dt
\]  

(8)

SALP-D quantifies the probability of a dynamic source at certain location in the domain. To calculate SALP-D with Eq. (8), \(h(t)\) function and SALP \(f_s(\bar{x}_n; T - t, \bar{x}_n)\) at different time steps shall be given or calculated in advance. Similar to the identification of single instantaneous contaminant source, more sensor outputs (either alarm signals or concentration readings) can improve the prediction accuracy of the algorithm by using the following equations. For cases with multiple alarm signals,

\[
f_{\bar{x}}(\bar{x}, \tau_0, \bar{x}_1, \bar{x}_2, ... , \bar{x}_N, \tau_1, \tau_2, ..., \tau_N) = \prod_{k=1}^N f_s(\bar{x}_n; \tau_k, \bar{x}_k, \tau_k)
\]  

(9)

And for cases with multiple measured concentration values,
\[ fd_x(\bar{x} | \hat{C}_{i_1}, \ldots, \hat{C}_{i_N}, \tau_{i_1}, \ldots, \tau_{i_M}) = \frac{\int_{M_0} \prod_{i=1}^{N} P(\hat{C}_i | M_0, \bar{x}; \tau_{i_1}, \tau_{i_2}, \ldots) \cdot fd_x(\bar{x}; \tau_{i_1}, \tau_{i_2}, \ldots) \, dM_0}{\int_{M_0} \prod_{i=1}^{N} P(\hat{C}_i | M_0, \bar{x}; \tau_{i_1}, \tau_{i_2}, \ldots) \cdot d\bar{x} \, dM_0} \]  

(10)

The improved adjoint location probabilities defined in Eqs. (9) and (10) are named as conditioned adjoint location probabilities for single dynamic source (CALP-D). Figure 3 summarizes the general procedure for identifying the location of a dynamic source. Comparing to the procedure for locating an instantaneous source, the dynamic source identification uses SALP-D, instead of SALP.

4 Experimental verifications

To test the effectiveness of the improved adjoint probability method in identifying single dynamic contaminant source, two physical experiments were performed in China, with one in an apartment unit in Tianjin and the other one in a hospital in Hong Kong. This section documents the experiment processes and how the sources in these two cases were identified with both multi-zone airflow model and CFD based inverse models.

4.1 Apartment experiment

The tested apartment, located on the third floor of a middle-rise apartment building in Tianjin, China, consists of two bedrooms, one living room, one bathroom, one kitchen, one storage room, and two enclosed balconies. Figure 4 shows the floor plan of the apartment, whose floor to floor height is 2.6 meters. Multiple windows exist in balconies 1, 2, living room, bedroom 2, and the bathroom. All windows were closed during the experiment except the ones in balcony 1 (W1) and bedroom 2 (W4). A floor fan of 52 watts was placed very close to the window in bedroom 2, and operating at its full speed to induce airflow into the apartment through the window W4. The airflow was supposed to exit the apartment through the window W1. An airflow velocity measurement...
on the floor fan determined the total volume flow rate of the fan was about 1250 m³/h. The apartment was vacant during the test and there was no other heat source or sink inside the space. In addition, the monitored indoor and outdoor temperatures were almost identical during the testing season. Hence, temperature influence was not considered for the airflow and contaminant transport. During the experiment, a CO₂ source placed at the center of bedroom 2 (height of the source = 0.8 m) was releasing CO₂ at a constant rate of 5 L/min from 16:35 on the test day. Two CO₂ sensors were placed at the center of the bedroom 1 and the living room, respectively, at the height of 0.4 m and 0.3 m, which recorded the CO₂ concentration every one minute. One was a PPMonitor Stand Alone System (SAS), and the other one was a HWF-1 infrared CO₂ monitor. Both were calibrated before the test. The accuracy of the sensors provided in the manual is ±40 ppm + 3% of reading. The measured CO₂ concentration in ambient environment was 404 ppm. Figure 5 plots the CO₂ concentration readings from two sensors in 25 minutes. The concentrations were used by the inverse modeling algorithm as inputs to predict the source location.

4.1.2 Multi-zone inverse modeling for the apartment

The multi-zone inverse modeling can quickly locate the room containing the contaminant. To perform a multi-zone inverse modeling, a multi-zone model of the apartment was built first. In the model, all the windows and interior doors were represented by typical openings, whose leakage data were assumed according to the ASHRAE residential database (ASHRAE 2009). Areas of open doors and windows were specified based on the measurements. Concentration readings from two sensors were treated as the average CO₂ concentration of the two rooms where the two sensors were located.

The multi-zone inverse modeling requires the input of airflow field in the apartment. This airflow field could be obtained through either measurement or simulation. The required flow field should represent the main characteristic of airflow under the real conditions, rather than being precisely accurate. This study performed a forward multi-zone airflow simulation to predict the airflow field in the apartment. All leakage areas were modeled as one way large openings with the orifice model. The one way model was used because the net airflow rate through these areas is the major input for the later probability calculation, and the simulation assumed uniform properties for indoor and outdoor environment. The simulated airflow field was calibrated using the measured CO₂ concentration profiles, by adjusting the main assumed input parameters to the multi-zone model (i.e., the leakage area of each window to the outside for this case). The calibrated model was then used to simulate various flow conditions under dynamic weather and operating scenarios. In reality, this calibration process for a specific building can be accomplished before any inverse modeling will be carried out to respond an IAQ incident.

For this apartment case, with the initial leakage area for each window, the multi-zone model predicted the CO₂ concentrations that agree reasonably well with those obtained from the experiment, as illustrated in Fig. 6. As a result, no parameter was adjusted during the calibration. This indicates that a reasonable “guess” (based on the building type and age—so regulations) would be appropriate for a quick airflow simulation for source tracking purpose. The accuracy of the CO₂ sensors used is ±40 ppm + 3% of reading, which leads to the reading uncertainty of about 60 ppm. The fluctuation of indoor CO₂ concentration may also reveal the unsteady characteristics of some local airflow as typically encountered in low-speed indoor environment. This transient nature of local airflow, however, has less impact on the major indoor flow pattern and thus will not influence the source tracking using the developed algorithm.

The predicted airflow field in the house was directly used in the inverse modeling to identify the room with the CO₂ source.

Figure 7 shows the simulated flow field in the apartment, where the green lines represent the volume flow rates along...
Fig. 7 Predicted airflow field in the apartment by the multi-zone airflow model (purple line: pressure magnitude; green line: flow magnitude)

the airflow paths between rooms, and between the rooms and the ambient.

To verify the capability of the developed tracking algorithm, the study tested three different sensing scenarios that may occur in real IAQ monitoring events:

- Scenario 1: 1 concentration reading from sensor 1 (bedroom 1) at \( t = 10 \) min;
- Scenario 2: 2 concentration readings from sensor 2 (living room) at \( t = 10 \), and 20 min;
- Scenario 3: 2 readings, one from sensor 1 and the other from sensor 2 at \( t = 10 \) min;

The measurement error was determined to be between \(-58\) ppm and \(58\) ppm (±40 ppm ± 3% of reading with an averaged reading of 600 ppm for each sensor at \( t = 10 \) min) according to the instrument manual. Figure 8 shows the predicted source location probabilities with the three sensing scenarios. The predictions with different sensor outputs all point out the right source zone—bedroom 2.

4.1.3 CFD inverse modeling for the apartment

In order to further identify the exact source location in bedroom 2, a CFD based inverse modeling was performed. A CFD model of the apartment was built as illustrated in Fig. 9, in which two open windows were represented by two equally sized openings while other closed windows were assumed to have small leakages. The window in front of which the floor fan stands was assumed to have a constant incoming airflow. All objects in the model had the same temperature, indicating no presence of buoyancy effect. Figure 9 shows the predicted airflow field by CFD. To ensure a proper representation of the indoor airflow characteristics during the test, a similar airflow calibration process using \(\text{CO}_2\) concentration was carried out, which adjusted the primary unknown input of CFD—the leakage area of each closed window. Because the experiment used a mechanical fan at the front of a window to simulate constant and strong natural ventilation, this air driving force is much more dominant to the indoor environment than the influence of the infiltration. As a result, a less accurate leakage model will have less impact on the source prediction. For a space that is dominated by infiltration, a much serious calibration or validation on infiltration or indoor airflow will be needed.

Fig. 8 Predicted source location probabilities (%) in the apartment under three different sensing scenarios
With two rounds of adjustment and calibration, the concentrations from the CFD model reach an acceptable agreement with those from the experiment, as revealed by Fig. 10. Note that a precisely accurate airflow field is not necessary for the inverse tracking method to correctly locate the contaminant source. As a result, a coarse CFD grid (about 260,000) with a typical turbulence model for indoor environment modeling (e.g., KERNG model used in this study) is adequate for this contaminant source identification task. The coarse grid CFD reached 0.1% convergence within 1200 iterations (due to the iso-thermal nature of the case).

The calibrated airflow model can then be used to track the source location. This study used one concentration reading at $t = 3$ min from sensor 1 (bedroom 1), which had the same measurement error as above. Figure 11 presents the predicted source location probabilities, where the black triangle represents the actual source location. The results show that the source location was predicted with acceptable accuracy.

4.2 Hospital ward experiment

4.2.1 Descriptions of the ward experiment

The hospital experiment was conducted by Li et al. (2004) in Ward 8A at the Prince of Wales Hospital in Hong Kong, in an attempt to assist the epidemiological studies of a severe acute respiratory syndrome (SARS) outbreak in this ward in 2003.

The tested hospital ward had four main cubicles, separated by a corridor and a nurse-station, a store, and a store/cleaning room. The ward had an overall dimension of 24 m (length) by 18 m (wide) by 2.7 m (high). The four cubicles were semi-enclosed and each was about $7.5 \times 6 \times 2.7$ m. There were normally eight beds in each cubicle, but at the time of the outbreak 10 beds were located in each cubicle. The ward was centrally air-conditioned. The supply air was delivered into the cubicles/nurse-station via a number of four-way air...
supply diffusers (0.6 m × 0.6 m) mounted on the suspended ceiling at the center of the cubicle and over the nurse-station. Return grilles (0.3 m × 0.6 m) were located at the suspended ceiling in the corridor outside each cubicle and the nurse-station. Excess air escaped through two exhaust fans inside the patients’ bathrooms and two fans in the store/cleaning room, as well as through the ward entrance. Figure 12 illustrates the ward floor plan and the CFD-predicted indoor airflow pattern by Li et al. (2004). Detailed experimental data and CFD analysis of the airflow patterns were shown in Li et al. (2004).

To explore the SARS transmission characteristics in the ward, the post-SARS experiment placed an aerosol generator in a bed next to the index patient’s bed on the central line of Bed S (1.1 m above the floor and 1.2 m away from the wall perpendicular to the bed) to mimic the virus exhalation of the original SARS patient. After sufficient long time release of aerosols, the particle concentration was measured at all the beds as indicated in Fig. 13. During the experiment, the supply and exhaust airflow rates in the ward were also measured. The mean supply air temperature was measured to be 14.3°C. A total heat gain of 11.64 kW was identified in the ward, including 2.232 kW from lighting, 2.964 kW from 39 patients (76 W each), and 6.444 kW from others.

4.2.2 CFD inverse modeling for the hospital ward

Using the brief descriptions of the ward, a new CFD model was built for the ward. To calibrate the airflow model, a forward contaminant transport simulation was performed with the CFD model. The predicted concentration distribution pattern was then compared with the experiment results, which shows a reasonable agreement. CO₂ was used as an indicator for the fine aerosols and this method was shown to be feasible in Li et al. (2004). As a result, no adjustment was made in the CFD model.

With the predicted airflow in the ward, an inverse modeling was conducted with the real concentration readings from the sensors at beds 1, 9, and 13 (shown in Fig. 13). Figure 14 illustrates the predicted source location, which is very close to where the aerosol source was. The relatively accurate prediction of the source patient location shows that the developed inverse method is capable of predicting the location of the source patient in an airborne infection outbreak.
5 Conclusions

This paper extends the previous study of inverse tracking method for single instantaneous source by developing theories and algorithms that can locate continuously-releasing contaminant source with given release time. With the new concept of dynamic standard adjoint location probability (SALP-D), the previously developed adjoint probability method can be used to identify single dynamic pollutant source with known releasing time and strength profile. Two physical experiments using constant CO₂ sources have been conducted to verify the effectiveness of the improved algorithm, with one in a multi-room apartment and the other in a hospital ward. Both multi-zone and CFD based inverse modeling have been performed in the apartment case to locate the room with source as well as the exact location of CO₂ source in the room, while CFD based inverse modeling was used for the hospital ward due to the open floor feature of the large space. During the simulation, approximate airflow fields in both cases were acquired through a concentration-based calibration process. The calibrated close-to-reality airflow field was then used with the actual sensor outputs to predict the source location in the spaces. The study results verify that the inverse modeling algorithm developed can successfully track the source location with good accuracy and speed. Although both test cases had a constant source releasing rate, the method developed works for any dynamic source with varying releasing rates, should the source releasing profile is provided. The current inverse tracking algorithm can only handle a single contaminant source with known release time under steady state indoor airflow conditions. The advance of the method for detecting more complex contamination conditions (e.g., multiple-sources, unknown release time, and unsteady flow) will be reported in the near future.

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