

IDENTIFY CONTAMINANT SOURCES IN AIRLINER CABINS BY INVERSE MODELING OF CFD WITH INFORMATION FROM A SENSOR

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ABSTRACT

In case contaminants are found in an aircraft cabin, it is useful to identify the contaminant source location and strength. This can be done through inverse Computational Fluid Dynamics (CFD) modeling. Since inverse CFD equations are ill-posed, this study proposes to solve a quasi-reversibility (QR) equation and a pseudo-reversibility (PR) equation. The QR equation improves the numerical stability by replacing the second-order diffusion term with a fourth-order stabilization term in the governing equation of contaminant transport. The PR equation identifies contaminant sources by reversing airflow. Both methods solve for backward location probability density function (PDF) of contaminant, which can be linked to the contaminant source location. The source strength can be further determined by scaling the nominal contaminant concentration computed by CFD with the concentration measured by a sensor. Our study shows that the two methods can identify the contaminant source location and strength. The QR method performs slightly better than the PR method but with a longer computing time.

KEYWORDS

Inverse modeling, Computational fluid dynamics (CFD), Quasi-reversibility equation, Pseudo-reversibility equation, Backward location probability

INTRODUCTION

Airborne contaminants, such as infectious disease viruses, may exist in an airliner cabin. In severe cases, contaminant sources should be identified as soon as possible so that proper measures can be taken to protect the passengers and crew. During the Severe Acute Respiratory Syndrome (SARS) outbreak in 2003, the SARS viruses possibly released from an infected passenger in the flight from Hong Kong to Beijing (Olsen et al. 2003) have led to the death of four other passengers because the virus sources could not be identified immediately to take corresponding protective actions. Further, without appropriate sensors and contaminant source identification technologies, commercial airliners can be attractive targets for terrorist attacks with chemical/biological warfare agents (NRC 2006). If airborne contaminant

sensors are deployed on airplanes and the sensor information can be used to identify what, when, where and how much contaminant is released, the risk of infectious disease transmission and chemical/biological attacks can be significantly reduced.

Airborne contaminant transport in enclosed spaces, such as an aircraft cabin, depends on airflow pattern (Li et al. 2007). With a known contaminant source location and strength, Computational Fluid Dynamics (CFD) can be used to simulate the contaminant transport in aircraft cabins (Horstman 1988). If we can reverse the contaminant transport, the contaminant source can be identified.

However, the inverse CFD modeling is ill-posed (Tikhonov and Arsenin 1977) since it does not satisfy the solution stability (Alifanov 1994). Both regularization (Tikhonov and Arsenin 1977) and stabilization (Lattes and Lions, 1969) methods can be used to improve the solution stability. Skaggs and Kabala (1995) compared the two methods and concluded that the stabilization method used significantly less computational effort, although the stabilization method might provide little inferior results. So far the regularization method can only be applied in uniform flows (Atmadja and Bagtzoglou 2001).

Our previous study (Zhang and Chen 2007) applied successfully the stabilization method to identify a contaminant source in an aircraft cabin. The study used the quasi-reversibility (QR) method by replacing the second-order diffusion term in the CFD equations with a fourth-order term and solved the contaminant transport inversely. The results show that the contaminant source locations can be correctly identified.

One can also solve inverse contaminant transport with reversed flow distributions. This approach is called the pseudo-reversibility (PR) method. Kato et al. (2001) used the method to assess local pollution from upwind regions via backward trajectory analysis of the flows in atmospheric environment with success.

At present, both the QR and PR methods require accurate airflow and contaminant distributions in the flow domain as the initial conditions. For an aircraft cabin, the airflow pattern is relatively stable even with occasional movements of passengers and crew (Mazumdar and Chen 2007). Thus, the airflow distributions can be obtained by CFD simulations. The contaminant concentration distributions are unknown and should be measured by sensors. However, these sensors are expensive, heavy and bulky so they cannot be deployed in a large quantity.

On the other hand, there are successful studies in identifying contaminant sources with a few sensors together with the optimization or probability methods. The optimization method uses a large amount of forward modeling (Khemka et al. 2006). In groundwater contaminant transport, Neupauer and Wilson (1999, 2001) used backward location probability to illustrate the likely position of a solute particle source, which can be valuable to identify contaminant source locations.

With similarities between the solute particle transport in groundwater and the airborne contaminant transport in an enclosed space, it seems possible to use the QR or PR method together with the backward location probability to identify when, where, and how much the contaminant is being released in an aircraft. This paper presents such effort and results.

RESEARCH APPROACH

This section describes the principle of identifying the contaminant source location by using the QR and PR methods with the information measured by a single sensor.

Identification of contaminant source location based on a single sensor

As reviewed in the previous section, backward location probability can be useful to identify contaminant source location. Before discussing the details on backward location probability, let us introduce first forward location probability.

Forward location probability represents the chance of contaminant appearing at a specified location after it has been released from a source (Dagan 1987, Jury and Roth 1990). Take an example of particle transport in a two-dimensional flow as shown in Figure 1(a). A downstream sensor detects the particle plume with some time delay ($t=t_0$) after the source released at $t=0$. The particle concentration at the sensor location reflects the possibility of particles appearing at the location. The higher the concentration at a location, the more possible the particles appear at the location. Mathematically, the

forward location probability density function (PDF) at time, t , can be expressed as (Neupauer and Wilson 2001),

$$f(\vec{x};t) = \frac{\phi(\vec{x};t)}{\int_{\Omega} \phi(\vec{x};0^+) d\Omega} \quad (1)$$

where $f(\vec{x};t)$ is the forward location PDF at position \vec{x} and time t , $\phi(\vec{x};t)$ is the local contaminant concentration, $\int_{\Omega} \phi(\vec{x};0^+) d\Omega$ is the total

contaminant released. If none of the contaminant has been extracted out of the domain since the release, the integration of Equation (1) in the space should be equal to one. Although Equation 1 was derived from particle contaminant transport, it can also be used for gaseous contaminants.

To calculate forward location PDF, the governing equation of contaminant transport should be solved to obtain local concentration. Although contaminants in enclosed spaces can exist in gaseous, liquid droplet, and solid particle forms, this paper deals with only the gaseous contaminant for simplicity. The governing transport equation for a gaseous contaminant is,

$$\frac{\partial[\phi(t)]}{\partial t} = -\frac{\partial}{\partial x_i} [u_i \phi(t)] + \frac{\partial}{\partial x_i} \left[\frac{\Gamma}{\rho} \frac{\partial \phi(t)}{\partial x_i} \right] + S_{\phi} \quad (2)$$

By combining Equations 1 and 2, forward location PDF can be solved.

Similarly, the backward location probability can also be explained by using the example of particle transport in the two-dimensional flow as shown in Figure 1(a). Once the sensor has detected the particle plume at time, t_0 , one can release a nominal source at the sensor location and solve reversely contaminant transport as shown in Figure 1(b). The chances of contaminant appearing at a location in the previous time ($t < t_0$) can be expressed by the backward location probability as,

$$f'(\vec{x};t) = \frac{\phi(\vec{x};t)}{\int_{\Omega} \phi(\vec{x};t_0^-) d\Omega} \quad (3)$$

where $f'(\vec{x};t)$ is the backward location PDF, $\phi(\vec{x};t)$ is the backward contaminant concentration due to the nominal source, and $\int_{\Omega} \phi(\vec{x};t_0^-) d\Omega$ is the total contaminant released at $t=t_0$ at the sensor

location. Since the higher the PDF, the more possible the contaminant appears at a location, the position with the highest backward PDF at $t=0$ should be the contaminant source location. Thus, the contaminant

source location can be identified with the backward location PDF.

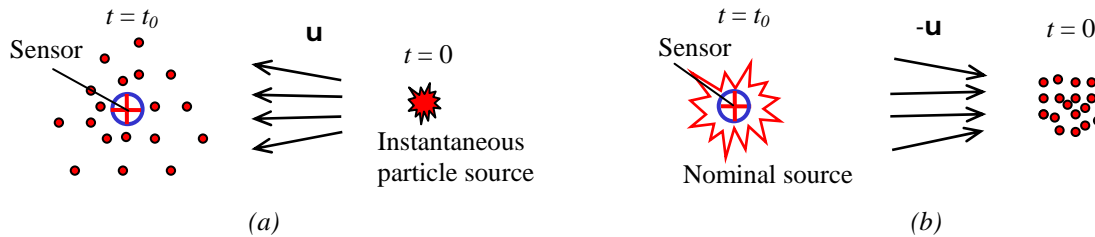


Figure 1 Particle transport in a two-dimensional flow to illustrate location probability (a) forward transport, (b) backward transport

To calculate backward location PDF with Equation 3, the distribution of backward contaminant concentration due to release of the nominal source is required. However Equation 2 cannot be used to solve for the distribution since it is unstable with time reversion. To make inverse contaminant transport solvable, this study proposes to solve the quasi-reversibility (QR) and pseudo-reversibility (PR) equations together with Equation 3.

The quasi-reversibility equation

One method to obtain a stable solution of the backward contaminant concentration due to the nominal source is by replacing the second-order diffusion term in Equation 2 with a fourth-order term. In the meanwhile, the nominal source at the sensor location is also required to be reflected in the QR equation thus yielding,

$$\frac{\partial[\phi(\tau)]}{\partial \tau} = -\frac{\partial}{\partial x_i} [u_i \phi(\tau)] + \varepsilon \frac{\partial^2}{\partial x_i^2} \left[\frac{\partial^2 \phi(\tau)}{\partial x_i^2} \right] + S_\phi \delta(\vec{x} - \vec{x}_0) \delta(\tau - \tau_0) \quad (4)$$

where ε is the stabilization coefficient, \vec{x}_0 is the sensor location, $\tau_0 (=t_0)$ is the time when the peak contaminant concentration is detected at the fixed sensor location. The last term on the right-hand side of Equation 4 is the nominal instantaneous source at the sensor location.

With an appropriate ε , the solution scheme becomes stable (Zhang and Chen 2007). However, Equation 4 is conditionally stable depending on the value of ε . The QR method is still computationally demanding with the discretizing of the fourth-order stabilization term.

The pseudo-reversibility equation

Instead of reversing time as the QR method, the PR method solves the inverse contaminant transport by reversing flows with the following equation,

$$\frac{\partial[\phi(t)]}{\partial t} = -\frac{\partial}{\partial x_i} [u_i' \phi(t)] + S_\phi \delta(\vec{x} - \vec{x}_0) \delta(t - t_0) \quad (5)$$

where t is the time in ascending order ($\Delta t > 0$) but u_i' is a reversed velocity component whose direction is opposite to u_i . The diffusion term in Equation (5) is neglected to decrease the dispersive effect, since the ideally reversed contaminant transport should be without diffusion. Because the time step, Δt , is positive in Equation (5), the discretized equation is stable with the time-implicit scheme as normally used in Equation 2 for forward modeling.

To calculate the backward PDF with Equations 4 or 5 together with Equation 3, the information required from a sensor is its location (\vec{x}_0) and the contaminant transport time (t_0) from the moment the source started to release to the moment that the peak contaminant concentration was detected by the sensor. The measured concentration at the sensor is not needed in identifying the contaminant source location with backward PDF. However, the measured concentration is used to identify the contaminant source strength that will be discussed later in this paper.

RESULTS AND DISCUSSION

The numerical schemes for both the QR and PR equations have been embedded into a commercial CFD program, FLUENT (<http://www.fluent.com/>), as a user defined function. To demonstrate the applications, this study first used a two-dimensional, empty aircraft cabin and then a three-dimensional cabin. The two-dimensional cabin case is simple and

results can be obtained fast, while the three-dimensional case is more realistic.

Contaminant source identification in a two-dimensional aircraft cabin

The environmental control systems for modern commercial airliner cabins create a very strong flow in a cross section and minimize flow along the longitudinal direction. The airflow in an aircraft cabin is close to two dimensional. Thus, our study has tested the QR and PR methods in a two-dimensional, empty aircraft cabin as shown in Figure 2. The aircraft cabin was 4.72 m wide and 2.10 m high. Conditioned air was supplied from the two linear slot inlets at the ceiling, and the air was extracted from the outlets at the side walls near the floor level. A contaminant was released in the cabin from $t=0.0$ s to $t=0.04$ s. Two release locations were considered: one on the left cabin floor and another in the left upper cabin as shown in Figure 2.

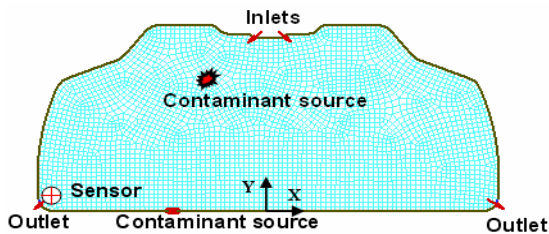


Figure 2 Schematic of inverse modeling in a two-dimensional aircraft cabin

This paper used CFD to obtain the airflow data and the sensor information of contaminant concentration versus time, although in reality the concentration should be measured by a sensor.

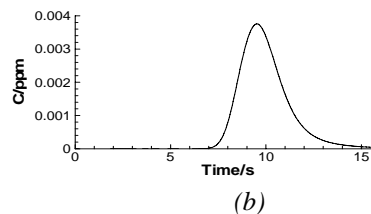
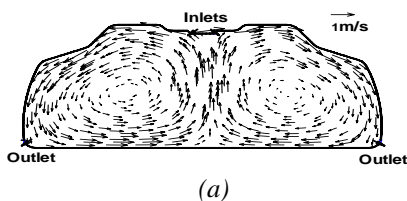


Figure 3 Information needed for the inverse modeling (a) steady-state airflow pattern, (b) unsteady contaminant concentration at the sensor location that shows a peak

With the source location identified, a CFD simulation can be run to obtain the contaminant concentration versus time with another nominal source released at the identified location. Since the contaminant concentration depends linearly on the contaminant strength, the linear scale-up or scale-down of the nominal source strength can be used to determine the actual source strength. To illustrate the application, Figure 5 shows the contaminant concentration versus time when contaminant sources

Figure 3 shows the airflow pattern in the cabin and the concentration over time representing the measured concentration by a sensor near the left outlet. This sensor was deployed for the demonstration of the inverse modeling, which does not mean the sensor must be located at the outlet position in actual operation. According to Mazumdar and Chen (2007), the optimal sensor location should be in the middle of the ceiling in an aircraft with such an air distribution system. The airflow pattern on the left cabin is counter-clockwise as shown in Figure 3(a). It took about 10 s to transport the contaminant from the source to the outlet, so the contaminant concentration reached its peak at the sensor location at about $t=10$ s as shown in Figure 3(b).

With the airflow distribution (Fig. 3a), the inverse simulation started at $t=10$ s with a nominal source released instantaneously at the sensor location. The distribution of backward location PDF at $t=0$ was obtained by using both the QR and PR methods. The simulations were conducted in a personal computer with a Pentium 2.6 GHz processor and 1 Gb of memory. It took about 100 minutes to complete the QR simulation and around 30 minutes for the PR simulation. The QR method used much longer time because of the fourth-order stabilization term. Figure 4 shows the contaminant source location identified by the two methods, with the highest PDF value illustrating the source location. The distribution of backward PDF looks dispersive. The reason is that the fourth-order term in the QR equation cannot completely reverse the diffusion effect. The PR method reversed the flow but not the diffusion. Thus, the dispersion is unavoidable. Nevertheless, both methods can identify the contaminant source location. A closer look at the results shows that the QR method is slightly better than the PR method.

were released with the same strength at the actual source location and the identified locations. The differences among them are negligible. Therefore, the source location and strength can be determined with the QR or PR method. Although not explicitly stated, the time of release is also identified. For this particular case, it was about 10 s earlier than when the sensor measured the peak contaminant concentration.

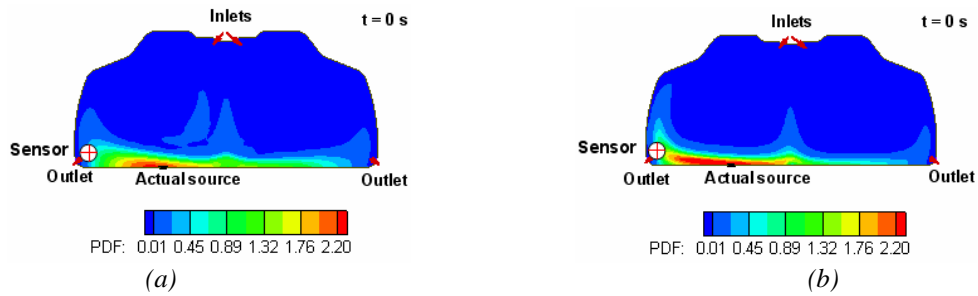


Figure 4 Contaminant source location identified by the highest PDF and its comparison with the actual source location illustrated by the black bar (a) by the QR method and (b) by the PR method

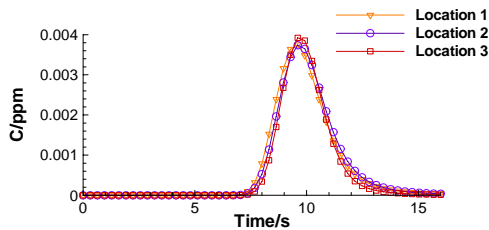


Figure 5 Comparison of contaminant concentration versus time at the sensor, Location 1 for the actual source, Location 2 for the source identified by the QR method, and Location 3 for the source identified by the PR method

The above results show that both the QR and PR methods can identify the contaminant source released on the left cabin floor. With the sensor placed at the

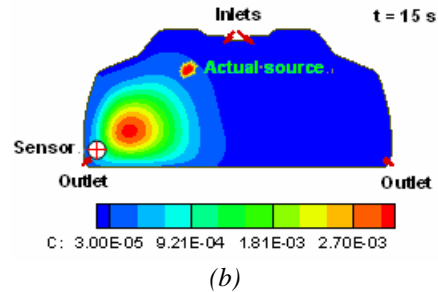
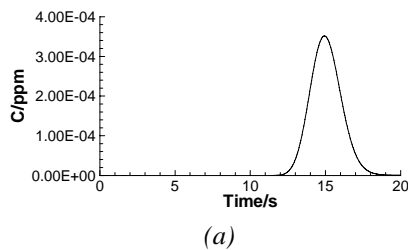


Figure 6 Contaminant concentration for the source released inside the cabin (a) “measured” at the sensor location, (b) distribution at $t=15$ s in the cabin

With the airflow pattern (Figure 3(a)) and the unsteady contaminant concentration at the sensor location (Figure 6(a)), a nominal source was released instantaneously at the sensor location and the distribution of backward PDF was reversely simulated from $t=15$ s to $t=0$ s. Figures 7(a) and 7(b) show the distribution of backward PDF at $t=0$ s obtained by the two methods. The contaminant source location identified by the QR method is in a small region close to the left ceiling, while the PR method identified a much large area in the same location. Clearly, the sensor location in this case is inappropriate so that neither method was able to identify the contaminant source location. However, if the sensor is located in the center of the contaminant plume at $t=15$ s (Sensor 2 in Figures 7(c) and 7(d)), in the right down stream of the contaminant source,

left outlet, would the two methods be able to identify a contaminant source released somewhere else rather than on the cabin floor? To answer this question, another case was studied for a source released inside the left cabin as shown in Figure 2. Similar to the previous case, the measured contaminant concentration at the sensor location should be known in advance. Figure 6(a) shows the unsteady concentration simulated by forward CFD modeling. Figure 6(b) shows the simulated contaminant concentration distribution at $t=15$ s. Clearly the sensor was not able to measure the maximum concentration in the cabin because it was not placed in the right down stream of the contaminant source.

the two methods can identify correctly the contaminant source location as shown in the figures. The results from the PR method are a little more dispersive than those from the QR method.

The above applications indicate that identification of contaminant source location and strength based on a single sensor with the QR or PR methods is possible if the sensor is appropriately placed in the down stream of the contaminant source. Otherwise, multiple sensors are needed

Contaminant source identification in a three-dimensional aircraft cabin

This study has tested further the QR and PR methods in a three-dimensional mockup of a twin-aisle aircraft cabin as shown in Figure 8. The mockup had four-row seats with 50% of occupancy rate. Fourteen heated manikins with box shape were used to simulate the seated passengers. Air was supplied at the ceiling level from linear slot diffusers and exhausted from the outlets at the floor level on the side walls. This investigation has identified a contaminant source from the leg level of a passenger seated next to the window in the first row with a

sensor located in the middle ceiling of the first row. The contaminant source was released from $t=0.0$ to 0.04 s.

The same as those for the two-dimensional aircraft cabin, CFD modeling was used to obtain the airflow data and the transient contaminant concentrations measured by the sensor as shown in Figure 9. The contaminant reached the peak concentration at the sensor location about 17 s later after release.

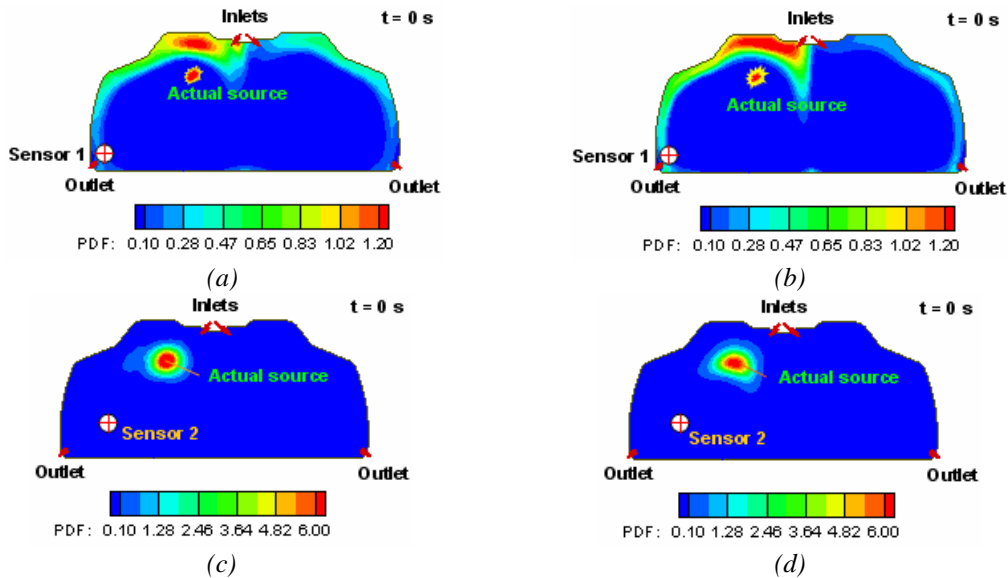


Figure 7 Contaminant source location identified (a) by sensor 1 with the QR method, (b) by sensor 1 with the PR method, (c) by sensor 2 with the QR method, and (d) by sensor 2 with the PR method

The inverse simulation was performed by adding an instantaneous nominal source at the sensor location at $t=17$ s. The computation was conducted on a Linux computer with an AMD 64 processor (1.8 GHz) and 2 GB of memory. It took about 180 hours for the QR method and 51 hours for the PR method to complete the simulations. One reason for such long computation time was that the numerical solution used Gauss-Seidel iteration without implementing multigrid acceleration at the current stage. Figure 10 shows the corresponding distributions of backward PDF at $t=0$ s in two different sections for the two methods. The distribution of backward PDF at $t=0$ s is quite dispersive by the inverse simulations. However, the two methods can still identify the contaminant source is from the passenger seated next to the window in the first row.

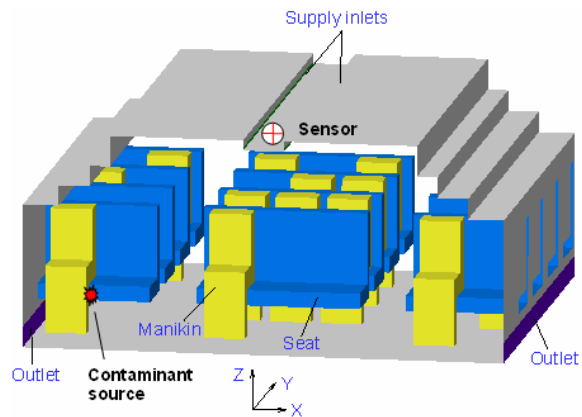


Figure 8 Schematic of inverse modeling for a three-dimensional aircraft cabin

Similar to the cases of the two-dimensional aircraft cabin, the contaminant source strength can also be identified with linear scaling comparison by performing a forward CFD simulation with nominal sources released at the identified locations. The results are not shown due to limited space available in this paper.

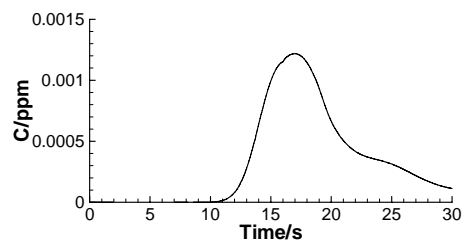
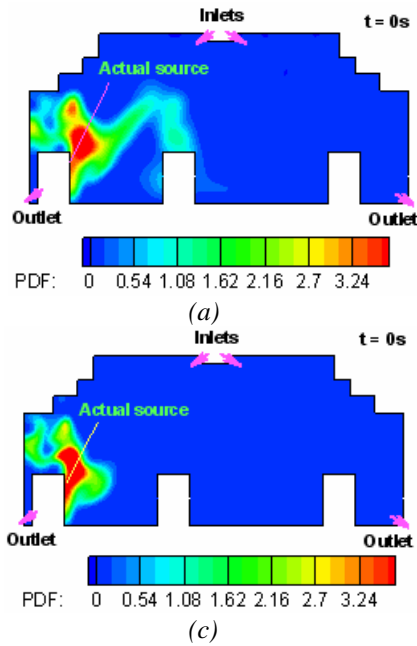


Figure 9 Contaminant concentration at the sensor



location

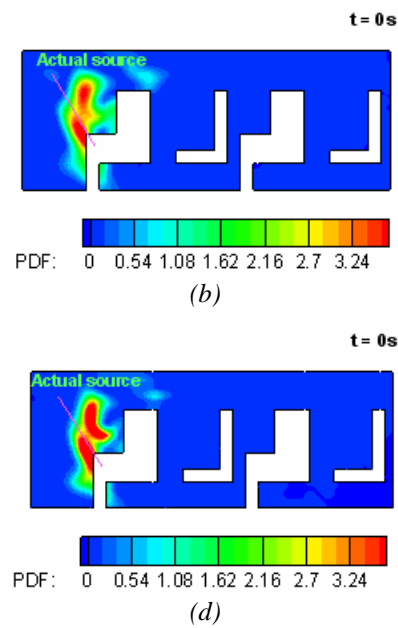


Figure 10 Location of contaminant source identified (a) in the cross section through the first row (across the passengers' knees) by the QR method, (b) in the longitudinal section by the QR method, (c) in the cross section through the first row (across the passengers' knees) by the PR method, and (d) in the longitudinal section by the PR method

CONCLUSION

This study used the quasi-reversibility (QR) and pseudo-reversibility (PR) methods to identify contaminant source locations and strengths in commercial airliner cabins. The methods solved backward probability density function (PDF) of contaminant sources, which can be linked to the source locations. The source strengths were determined by using a CFD simulation and the scaling of the computed contaminant concentration with the measured one. By applying the two methods to a two-dimensional and a three-dimensional aircraft cabin, the following conclusions could be drawn:

1. Both the QR and PR methods can identify the location of a contaminant source with a stable airflow pattern and measured contaminant concentration over time by a single sensor. It is very important that the sensor must be placed in the down stream of the contaminant source.
2. The distribution of backward PDF is dispersive for the two methods because of the approximations used for the diffusion term of the governing contaminant transport equation. The longer the simulation time, the more dispersive the results.
3. The QR method is slightly better than the PR method. However, the QR method needs longer computing time because the solution of the fourth-

order stabilization term is computationally demanding.

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SYMBOLS

$f(\vec{x};t)$	Forward probability density function of location
$f'(\vec{x};t)$	Backward probability density function of location
S_ϕ	Source term
t	Time, in ascending order
u_i	Velocity component in direction i
u'_i	Velocity component in direction i that is opposite to u_i
\vec{x}	Position vector
x_i	Coordinate in direction i
<i>Greek symbols</i>	
δ	Dirac delta function
Γ	Diffusion coefficient of gaseous contaminant scalar
ε	Stabilization constant
ϕ	Gaseous contaminant scalar
ρ	Air density
τ	Time, in descending order
Ω	Domain
<i>Subscripts</i>	
i	Coordinate direction index