Identification of Pollution Sources in Urban Areas Using Reverse Simulation with Reversed Time Marching Method

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Abstract

The present research introduces a technique to determine the location of pollution sources in urban areas through the use of inverse CFD modeling. The technique depends primarily on the solution of the transport equation with time integration in the negative direction. This is called the Reversed Time Marching Method (RTMM). In order to examine the accuracy of RTMM in identifying pollution sources, two examples were given. In the first one, a simple laminar flow was considered and a pollutant was emitted for variable wind conditions. In the second example, the wind flow around a single building was investigated for two different sources. Steady-state numerical simulations were carried out at first in order to estimate flow fields. Then, forward-time simulation was used to calculate pollutant concentrations. In the last stage, the scalar transport equation was solved again but with a reversed flow field and negative diffusion term. By using peak concentration, one could identify the source of the pollution. Results of the study demonstrated that RTMM can identify pollution sources in urban areas with a satisfactory degree of accuracy. However, more work is needed to decrease the wide spread of the concentration field around source location to facilitates the source identification.

Keywords: reverse simulation; air quality; urban areas; CFD

1. Introduction

Nowadays, reverse modeling seems to be a promising topic in terms of environmental research. The importance of reverse modeling arises from the increased numbers of pollution sources due to continuing industrial expansion coupled with population growth, especially in large cities. In addition, terrorist attacks are becoming more frequent and deadlier, such as the sarin gas attacks on the Tokyo subway in 1995, which resulted in 12 deaths and over 6,000 injured (Yokoyama 2007 and Okumura 1996). Moreover, the ability to predict pollution sources, source strength, and release time is required to create a complete picture of the air quality conditions within the release domain. Accordingly, investigations to identify pollution (or release) sources immediately after any release became a matter of urgency in order to ensure the public's safety. Reverse modeling is one efficient and promising tool in this regard.

In recent years, some researchers have studied reverse modeling techniques to identify pollution sources either in the air or in groundwater. Chen et al. (2007) studied contaminant source identification in a 2-D aircraft cabin and in a 3-D office by applying inverse CFD modeling. They used the quasi-reversibility equation instead of the contaminant transport equation since it is numerically stable when time is reversed. According to the study results, they concluded that the inverse CFD model could identify the contaminant's source, but was not very accurate in terms of the contaminant's strength because of the dispersive property of the quasi-reversibility equation. Gomez-Gesteira et al. (1999) used the particle tracking method to investigate contaminant dispersion process in two different sites located along the North West coast of Spain under summer conditions. Bagtzoglou et al. (1992) applied the particle tracking method to identify the sources of contamination in groundwater systems by reversing the velocity field and leaving the diffusion/dispersion unchanged. Wilson et al. (1994) studied the particle tracking method to determine groundwater pollution sources through the solution of stochastic differential equations backwards against time in 1-D and 2-D. Their method results in time- (or space-) dependent probability maps for the water in the study well, which they termed travel time probability maps and location probability maps. Using analytical and graphical techniques, Islam (1999) worked out a method for determining an unknown emission source assuming that the Gaussian plume model describes the dispersion process fully. He developed a graphical method to locate the undeclared emission sources and the results of such method indicated some small zone for the probable location of the sources. However, the errors

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Pollutant concentrations are predicted based on the convection-diffusion equation including convection, transport diffusion, and the relevant emissions source. It can be written as:

$$\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} = \frac{\partial}{\partial x} \left( \frac{K}{\rho} \frac{\partial c}{\partial x} \right) + \frac{S}{\rho} \quad t \rightarrow \infty$$ (1)

where \(c\) denotes the pollutant concentration (kg/kg), \(t\) is the time (s), \(u\) is the Cartesian component of the velocity (m/s), \(x_i\) is the Cartesian coordinate (m), \(\rho\) is the air density (kg/m^3), \(S\) is the pollutant source strength (kg/m^2/s), and \(K\) is the diffusivity coefficient for the concentration (kg/m/s). The Schmidt number (\(Sc = \nu/K\)) was considered here, where \(\nu\) is the kinematic viscosity. Some studies have been done in order to change the Schmidt number in street canyon models to regress the observed data, and it was found that \(Sc < 1\) has better regression, as demonstrated by Tominaga et al. (2007) and Yoshikawa et al. (1997). Accordingly, in this study, a Schmidt number value of \(Sc = 0.9\) was selected and assumed to be constant during calculations.

In order to explain the principles of reverse simulation, Equation (1) can be simply integrated based on one dimensional flow – as shown as in Fig.1. – using an upwind scheme for space:

$$\Delta x_m = \Delta x / 2$$

![Fig.1. Typical Control Volume for 1-D Flow](Image)

To perform the integration with respect to time, the concentration-time relationship is needed. Usually, the following equation is assumed (Patankar, 1980):

$$\int_{t}^{t+\Delta t} \left( \int_{x}^{x+\Delta x} f \cdot c \cdot dt \right) \cdot dx \cdot dt + \int_{x}^{x+\Delta x} \left( \int_{t}^{t+\Delta t} f \cdot c \cdot dt \right) \cdot dx \cdot dt = \frac{\Delta x}{\Delta t} \int_{x}^{x+\Delta x} S \cdot dx \cdot \rho \quad (5)$$

where \(f\) is a weighting factor used to combine the concentration value at the new time step with both the new and old concentration values.

2. Reversed Time Marching Method

The key point of the Reversed Time Marching Method is utilizing the “reverse tracking of flow field over time”. Mathematically, this implies that the solution of the scalar transport equation on the flow field is obtained with time integration in the negative direction. The process of negative time advancing in the transport equation is equivalent to that of positive time advancing with negative convection and diffusion. Reverse time tracing of the flow field thus means that the diffusion field with reversed velocity field and the diffusion was left unchanged.

It is clear from the previous studies that the diffusion term represents a problem when dealing with the reversed transport equation due to the instability caused by such term. Accordingly, the purpose of this paper is to develop and also to verify a method for backward problems that accounts for the diffusion as well as the convection through use of the reversed time marching method (RTMM). The method depends primarily on solution of the scalar transport equation with time integration in the negative direction. This leads to reversing both the velocity field and the diffusion term. In order to overcome the instability problem caused by the diffusion term, this study proposes the use of a filter to deal with negative concentration gradients in order to avoid unrealistic solutions. The method is applied to two simple examples of a laminar flow without obstacles and of a turbulent flow around a single building. Direct CFD simulations were carried out at first to calculate both flow and concentration fields. The reversed time marching method is then conducted to find the pollution source location.

in the measurement of the meteorological parameters as well as pollutant concentration would provide some additional uncertainty in the method.

The reversed time marching method is not a new technique since it has already been used in a number of previous studies, albeit in different applications. Kato et al. (1992) applied the “Reverse Tracking of Flow Field over Time” to obtain the residual lifetime of air at a point. Kato et al. (2001, 2002, 2004) used the same technique to assess local pollution from upwind regions with backward trajectory analysis of the flows in an atmospheric environment. They reversed only the pollutant transport by convection. The method has also been used in groundwater contaminant transport by Bagtzoglou et al. (1992) and Wilson et al. (1994), where convection transport of contaminant is solved with reversed velocity field and the diffusion was left unchanged.

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In order to determine the source within a domain through the use of inverse modeling, concentration distributions are needed. In reality, the concentrations should come from data measured by concentration sensors. Since this paper intends to explain the method of inverse modeling, a direct CFD simulation was conducted at first to solve the flow field and then the calculated flow field is used to estimate the concentration field, which is used as the initial condition when carrying out the inverse modeling.
By applying a fully implicit scheme (i.e. $f = 1$), Equation (4) can be rearranged to the form:

$$c_p(t + \Delta t) = \frac{1}{1 + \frac{u_h \Delta t}{\Delta x}} \times c_p(t) + \frac{K \Delta t}{\rho \Delta x^2} \times c_v(t + \Delta t)$$

Equation (8) shows that a particle location at a time $\Delta t$ in the past can be calculated by simply moving it from the present position under a reversed velocity field and negative diffusion. This means that the time is reversed by reversing the velocity field (advection term) together with the diffusion term. Also, it is evident from Equation (8) that the reversed time marching method is very easy to implement and can be used to evaluate pollution sources. However, there are two important notes arising from this equation. First, neglecting the diffusion can be a problem when convection is weak. The second problem is that, if the transport equation is solved (as shown in Equation (8)), the solution is numerically unstable due to the negative sign of the diffusion term. The reason is that in forward time modeling the pollutant transport is spontaneously transported from high concentration during the current time to low concentration in the following time. However, in inverse modeling to solve pollutant transport in the previous time, the pollutant needs to be transported from low concentration at the current time to high concentration at the previous time, which is impossible.

In order to make the above equation solvable with numerical stability, this study proposes the use of a filter to deal with negative concentration gradients in order to avoid unrealistic solutions. Then, Equation (8) can be rewritten as:

$$\frac{\partial (c \hat{c})}{\partial t} + \frac{\partial (-u_i) \hat{c}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{K}{\rho} \frac{\partial \hat{c}}{\partial x_i} \right) \quad t \to \infty$$

where the symbol " $\hat{c}$ " means that this term is filtered. The filter for the diffusion term is set in such a way that the negative concentration values are changed to the minimum positive value of the concentration within the solution domain. This can be expressed as:

$$\text{if } (c < 0), c = c_{\text{min}}$$

Indeed, the filtration process of the diffusion term in the reversed transport equation affects the solution accuracy and decreases the method's effectiveness in identifying the sources of pollution. This will be investigated in the following examples.

3. Examples of Applying the RTMM in Identifying Source Locations

3.1 Simple laminar flow

A 3-D numerical model for modeling a simple laminar flow is designed as shown in Fig.2. The dimensions of the computational domain are 90 m × 30 m × 30 m ($L \times W \times H$). The minimal mesh size above the ground is set as 0.18 m, and the vertical growing factor for mesh points is 1.05. The total number of cells is 594,000. A pollution source of strength 0.01 kg/m²/s and dimensions 0.5 m × 0.5 m × 0.5 m was considered at a location 12 m from the inlet at a height of 2 m.

3.2 Turbulent flow around a single building

The second example for identifying the source of pollution in urban areas using RTMM is shown in Fig.3, in which wind flows around a single building. The building dimensions are 10 ($x \times 10$) ($y \times 30$) m and the computational domain dimensions are 300 ($x \times 110$ ($y \times 70$) m with a mesh size of 444,800 cells.

Two different locations for the source were considered in order to examine the effect of pollutant source location on the prediction accuracy of the RTMM. Location (I), which is 2.5 m upwind of the building, and location (II), which is 2.5 m downwind of the building. In both cases, the source strength was set at 0.01 kg/m²/s with dimensions of 0.5 m × 0.5 m × 0.6 m.

4. Numerical Simulation

Numerical simulations were carried out using the CFD code Star-CD, based on the finite-volume discretization method. During forward simulation, steady-state analysis was adopted for the flow field and the Monotone Advection and Reconstruction Scheme (MARS) (Bram, 1979) was applied to the spatial difference. The standard k-ε model was used to simulate the turbulence effects and the pressure / velocity linkage is solved via the SIMPLE algorithm (Patankar, 1980).

At the inflow boundary, a constant flux layer was assumed for the turbulent energy $k$, and turbulent intensity was assumed to be 10% of the inflow wind...
velocity at a representative height \( z_o \) of 74.6 m. Free slip condition was applied to the top and side boundaries. The generalized logarithmic law with parameter \( E = 9 \) (m) was applied to building walls and the ground surface as smooth walls.

Tables 1. and 2. summarize the parameters used in the numerical simulations for both examples, together with the applied boundary conditions.

Once the flow field is solved, it is considered steady. In fact, airflow characteristics within outdoor environments are unsteady due to fluctuations in both speed and direction. However, in the present stage of this study, fluctuations in the applied wind are not considered in the analysis. Accordingly, the wind flow is treated as steady. After solving the flow field, the concentration fields in both direct and reverse simulations are solved against time. The wind flow distribution together with the pollutant concentrations of the direct simulation are used as initial conditions for the reverse simulation. A time step of 0.1 s was used with the implicit scheme.

In direct simulation (forward-time simulation), a pollutant source of strength 0.01 kg/m³/s was released in the period from \( t = 0 \) to 30 s. Then, the solution of the transport equation is continued with the absence of the source until \( t = 100 \) s for the case of laminar flow and until \( t = 200 \) s for the case of wind flow around a single building. Fig.4. shows the characteristics of the pollutant release as a function against time.

In reverse simulation, the flow field calculated by direct simulation is reversed at first and the source term is set to zero. Then the transport equation is solved from the moment of \( t = 100 \) s in the reverse time direction. The time at which the reversed simulation is stopped is not known in reality. In other words, starting from the moment of solving the transport equation in the reverse time direction, the time \( t = 0 \) at which the calculations has to be stopped is not known in advance. Since the present examples are introduced just to explain the idea of reverse simulation using RTMM, the end time is assumed.

5. Results and Discussions

5.1 Case of laminar flow

Fig.5. shows the concentration fields for two different constant inflow velocities of 0.01 and 0.5 m/s. In...
subplots (a) and (b), the concentration fields at $t = 1$ s and $100$ s obtained by direct simulation are presented, while the subplot (c) shows the distribution of pollutant concentrations obtained through reverse simulation.

With the steady-state airflow pattern, direct CFD modeling was used to calculate pollutant concentration distribution at $t = 100$ s, where a pollution source was released from $t = 0$ to $30$ s. The distributions of steady-state airflow and transient pollutant concentration at $t = 100$ s were used as initial data for the inverse CFD modeling. The inverse CFD modeling calculated backwards pollutant transport from $t = 100$ s to $0$ s as shown in Fig.5.(c).

In order to determine the pollutant release location, the distribution of pollutant concentration should be in a small region around the release source as shown in Fig.5.(c), and by using the maximum pollutant concentration over all locations at this instance (the peak pollutant concentration), one could identify the pollution source. The peak concentration computed by inverse CFD modeling in Fig.5.(c) clearly shows the position of the pollutant source.

By comparing the two concentration fields of $u = 0.01$ m/s and $0.5$ m/s given in Fig.5.(c), the case where $u = 0.5$ m/s shows a more dispersive concentration field compared with the case of $u = 0.01$ m/s. This can be attributed to the increased plume size with the increase in wind velocity. However, the RTMM appears to effectively identify the release sources in both cases.

5.2 Case of turbulent flow around a single building

Fig.6. shows the computed airflow pattern around a single building under steady state. The subplot (a) shows the flow field calculated by the direct simulation and the subplot (b) shows the reversed flow field which was used to carry out the reverse simulation. In subplot (a), a symmetrical flow field is shown around the building, where two identical circulation regions are formed around the building.

It is expected that the effectiveness of RTMM in identifying the pollution source is affected by its location. So, as mentioned before, two locations for the pollutant source were examined here, namely locations (I) and (II). The first location is upwind of the building and the second location is in the wake region downwind...
5.2.1 Source location (I):

The concentration fields around the building obtained for the source at location (I) are shown in Fig. 7. In subplot (a), at $t = 1$ s, the plume starts to diffuse where the concentration field makes contact with the upwind face of the building. The plume then travels with the wind downwind of the building. The pollutant continues to be released until the moment $t = 30$ s. At that time, the emission source was stopped and the scalar transport equation was solved against time using direct simulation without the source. At $t = 200$ s, two identical regions were formed far from the building. The conditions at such time were used as the initial conditions for the inverse modeling.

Fig. 7.(c) shows the concentration field obtained by the inverse modeling. In such figure, the concentration field area is wider than that of the direct simulation. By detecting the location of the maximum concentration overall in the domain volume, the source location of the building.

Fig.6. Wind Flow Field around a Building; (a) Direct Flow Field, (b) Reversed Flow Field

Fig.7. Concentration Fields when the Source is in Location (I); (a) at $t = 1$ s Obtained by Direct Simulation, (b) at $t = 200$ s Obtained by Direct Simulation, (c) at $t = 1$ s Obtained by Reverse Simulation
is clearly determined. It is located downwind of the building along the domain centerline. However, the figure implies two problems. The first one is that the maximum concentration occupies a wide area in front of the block, which means that estimations for the location of the source will not be 100% accurate. It is thought that the wide spread of the concentration field is attributed to what is called "false diffusion", introduced by the first order approximation of the advection term in the upwind difference scheme (Tsai et al., 1983).

The second problem is that, compared to the peak concentration obtained with the direct CFD modeling as shown in Fig.7.(b), the source strength identified by the inverse CFD modeling of Fig.7.(c) is more dispersive. The reason is that the reversed transport equation is not exactly the same as the governing transport equation due to the presence of a filter. Indeed, these two problems affect the prediction accuracy of the RTMM and this appears clearly in the wide area of the maximum concentration, which gives a wide range of possibilities for the pollution source location. This is not considered to be the ideal distribution when a gas release position is required. At the same time, the dispersive property of the reversed transport equation renders the estimated source strength inaccurate. These two problems will be investigated in detail in Part (II) of this study.

5.2.2 Source location (II):

Fig. 8. shows the concentration fields around the building when the pollutant source is at location (II). The subplot (a) shows the source location, which is 2.5 m downwind of the building's rear wall. As with the case for location (I), the pollutant is emitted in the period from \( t = 0 \) to 30 s, and then the transport equation was solved in the absence of the source term until the moment \( t = 200 \) s. In subplot (b), two high concentration regions are formed behind the building. However, diffusion of the pollutant in this case is limited to a narrow region compared to the case for location (I).

Fig. 8.(c) shows the concentration field obtained using inverse modeling. The figure demonstrates that the concentration increases in the direction of the reversed wind from right to left. Also, the figure shows that the peak concentration region occupies a narrow region compared with the case for location (I). This can be attributed to the presence of the source in the wake region where a lower wind velocity exists and convection is weak. In such case, the location of the pollution source as estimated by the reverse simulation is not clear. In Fig.8.(c), there are two peak concentration regions near the edges of the block. So the location of the source is not accurately identified. This indicates that the prediction accuracy of the RTMM is diminished in cases of weak convection.

6. A Technique for Improving RTMM Prediction Accuracy

From the above examples, it is clear that the RTMM performs to a certain degree of accuracy. However, in all of these examples, wide diffusion fields are shown around the source location. A technique for improving the prediction accuracy of the RTMM is suggested by our group. This technique is to use what is called a "pollution sink" in the reversed transport equation. This may decrease the widespread of the concentration field around the source and render identification of the source more easily. The reversed transport equation is then rewritten as:

\[
\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}[(-u_i)c] = \left[ -\frac{\partial}{\partial x_j}\left( \frac{K}{\rho} \frac{\partial c}{\partial x_j} \right) \right] S, \quad t \to \infty \quad (11)
\]

where the last term on the right-hand side is the sink term.

In order to apply the sink term technique to identify pollution source characteristics, some criteria are needed. Such criteria have to satisfy the following
requirements:
1) Sufficiently general to be applied to any case.
2) It should show where to put the sink within the study domain
3) The criteria should give a reasonable value for the sink strength to carry out the calculations.

In order to identify a pollution source using sink term technique, the following procedure is applied which couples CFD with optimization approach:

1) Setting the sink at any location within the domain with any strength $(S)$. 
2) Carrying out CFD simulation to solve the scalar transport equation with any release time $(T)$. 
3) At time $(T)$, we calculate the whole concentration in the domain, which is:

$$ C = \int_{V} c \, dV $$

4) Then, we use optimization approach to find the minimum value of the concentration $(C)$ within the domain.

5) If the initial guess doesn't give the minimum domain concentration, another trial with new sink location and new values for $S$ and $T$ selected by the optimization technique is used until the minimum concentration within the domain is obtained. 

A flow chart for the above mentioned procedure is illustrated in Fig.9.

It is worth mentioning here that; this technique is applied for the case of a single release source. In case of multiple emission sources, another technique can be applied. This will be explained in detail in Part (II).

### 7. Conclusions

The present research introduces a technique to determine pollution source locations in urban environments – when the pollutant concentration field is known – through use of the reversed time marching method (RTMM). The method depends primarily on solution of the transport equation of the contaminant with time integration in the negative direction. This leads to reversing the velocity field and also the diffusion term. In order to make the reversed transport equation solvable with numerical stability, this study proposes the use of a filter to deal with negative concentration gradients in order to avoid unrealistic solutions. For examining the accuracy of RTMM in identifying pollution sources in urban areas, two examples were given and discussed.

In conclusion, it can be said that the RTMM can be applied to identify pollution source locations in urban areas with acceptable results. However, the study results implied two problems: the wide spread of the concentration field and the dispersive property of the reversed transport equation. These problems reflect the need for more efforts designed to overcome these two problems and to improve the prediction accuracy of the RTMM.

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