Kalman Filtering in the Air Quality Monitoring

Fabrício P. Harter, Haroldo F. de Campos Velho e Marco A. Chamon

ABSTRACT

Data assimilation is a process where an improved prediction is obtained from a weighted combination between experimental measurements and mathematical model data. In the present work this procedure is applied to pollutant atmospheric dispersion by using a Kalman filter (KF). This is interesting approach, because the KF gives an output in which the balance between the data from the diffusion model and the experimental data is done automatically, through the Kalman gain. In addition, the Kalman filter computes the propagation of the error.
1. INTRODUCTION

Natural and anthropogenic pollutant sources have caused great impact on the environment. The natural causes, such as volcanic eruptions, can not be controlled by man, on the contrary of the anthropogenic sources. After the industrial revolution the atmospheric pollution has enhanced, and nowadays it becomes a public health problem in some big cities. From these considerations, the air monitoring is an important feature in the present time (Zannetti, 1990).

Data assimilation techniques are used to improve the prediction of an inaccurate mathematical model associating to it observational data. The Kalman filter (KF) is one of methods used to perform the data assimilation process, which provides an optimal response for linear Gaussian stochastic linear system. Nowosad et al. (2000a, 2000b, 2000c) has used a KF (in its versions linear, extended, and adaptive) for data assimilation in a Hénon and Lorenz systems in chaotic regime, as well as for a Dynamo model, a 1D meteorological simulator based on shallow water formulation. Zhang and Heemink (1997) applied a KF and Kriging approach (optimal interpolation) to the 2D advection-diffusion equation. These authors concluded that the Kriging approach presents good results, when the number of observations is large enough (9 observations points at 41x41 grid points, with observations at each 11 time-steps). The KF is more precise for a less number of observations points (3 observations points at 41x41 grid points, with observations at each 11 time-steps). However, the KF has a computational cost greater than the Kriging approach.

In this paper a linear KF is applied to the advection-diffusion equation. Some numerical experiments are done to test the performance of the filter related to the number of observations. Description of the mathematical diffusion model and Kalman filter are presented in the Sections 2 and 3, respectively. Section 4 presents the numerical experiments and the final comments are addressed in the Section 5.

2. DESCRIPTION OF ADEVECTION-DIFFUSION MODEL

Considering the mean stream bowling in the direction-\(x\), and the advection in this is the predominant mechanism for the
transport, the pollutant diffusion can be described by the following diffusion equation and boundary conditions

\[ U \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} \left( K \frac{\partial c}{\partial z} \right) \]

(1)

\[ K \frac{\partial c}{\partial z} = 0 \quad \text{for} \quad z = 0 \quad \text{and} \quad z = h \]

where \( c \) is the pollutant concentration, \( U \) is the mean wind speed, \( K \) is the vertical turbulent eddy diffusivity for stable boundary layer (Degrazia and Moraes, 1992; Campos Velho, 1992), \( h \) is the boundary layer height. The partial differential equation was solved by using a finite difference approximation: the explicit Euler method for integration in the direction-\( x \) and central difference approximation for diffusion operator (Hoffman, 1993). Defining \( d = \Delta x / U \Delta z^2 \) the Eq. (1) can be expressed in finite differences

\[ c_{n+1} = F_n c_n \]

\[ F_n = \begin{bmatrix}
    1 - d(K_{i+1/2} + K_{i-1/2}) & 2d K_{i+1/2} & \cdots & 2d K_{i-N_z/2} \\
    dK_{i-1/2} & 1 - d(K_{i+1/2} + K_{i-1/2}) & \cdots & dK_{i-N_z/2} \\
    \vdots & \vdots & \ddots & \vdots \\
    2d K_{i-1/2} & \cdots & 1 - d(K_{i+1/2} + K_{i-1/2})
\end{bmatrix} \]

(2)

on the vertical grid \( i = 1, 2, \ldots, N_z \). The index \( n \) refers the position in the direction-\( x \), starting from \( n = 0 \). This finite difference approximation is numerically stable for \( d \leq 0.3 \).

3. KALMAN FILTER

The Kalman filter is frequently used in control and estimation problems. From the first applications on aerospace domain (Jazwinski, 1970), it has been employed in others fields, such as meteorology and oceanography (Daley, 1991; Bennett, 1992). A brief description of the KF is done, following Jazwinski (1970).

Let be the prediction model
\[ c_{n+1} = F_n c_n \]  

(3)

where \( F_n \) is a mathematical description of the system. The observational model is represented by

\[ z_n = H_n c_n + v_n \]  

(4)

being \( v_n \) the noise of the experimental data, and \( H_n \) represents the observational system. The typical assumptions of Gaussianity, zero mean, and orthogonality for the noises are assumed. The concentration \( c_{n+1} \) is estimated through the recursion expression

\[
c^a_{n+1} = (I - G_{n+1} + H_{n+1}) F_n c^a_n + G_{n+1} z_{n+1}
\]

(5)

where \( c^a_{n+1} \) is the estimator of \( c_{n+1} \), \( G_n \) is the gain of KF, chosen to minimize the variance estimation error of \( J_{n+1} \), given by

\[
J_{n+1} = E\left\{ (c^a_{n+1} - c_{n+1})^T (c^a_{n+1} - c_{n+1}) \right\}
\]

(6)

with \( E\{\cdot\} \) the expected value. The algorithm for KF is shown in Figure 1, in which \( Q_n \) is the covariance matrix of the dynamic model noise, \( P_n^f \) is the prediction error covariance, \( R_n \) is the covariance of the noise \( v_n \), and \( P_n^a \) is the covariance of the estimation error. The assimilation is done using the innovation

\[
r(t + \Delta t_n) = r_{n+1} = z_{n+1} - z_{n+1}^f = z_{n+1} - H_n c^f_{n+1}.
\]

(7)

**Fig. 1.** A sketch for linear Kalman filter.
4. NUMERICAL EXPERIMENTS

With the purpose to test the assimilation scheme described previously, the following parameters were used in Eq. (2): \( \Delta x = 6 \, \text{m} \), \( \Delta z = 10 \, \text{m} \), \( U = 0.31 \, \text{m}.\text{s}^{-1} \), \( h = 400 \, \text{m} \). For the observational matrix system \( H_n = I \), and covariance matrices for modeling noise and observation noise, \( Q_n = 0.5I \), \( R_n = 2I \), respectively, being \( I \) the identity matrix of order \( N_z = 41 \). The number of points in the direction-\( x \) is \( N_x = 2000 \). The true concentration value was assumed as being given by Eq. (2) added to a constant small source of pollutants and a stochastic forcing term (with zero mean).

The diffusion problem simulates a pollutant puff released at origin of the coordinate system. This condition is modeled by a delta function:

\[
e(x, z) = Q \delta(z) \quad \text{for } x = 0.
\]  

(8)

Three classes of experiments were performed. Firstly, a high number of sensors were used in the observation grid varying the number of samples for direction-\( x \). Secondly, the number of samples in the direction-\( x \) was fixed with different number of sensors uniformly spaced in the vertical coordinate. Finally, the performance of assimilation process is investigated for several arrangements of the observation grid in the vertical direction; where the number of sensors in the vertical coordinate and in the direction-\( x \) are maintained constants.

In the first case of our experiments, the performance of filter was analyzed with respected to the number of measurement points and with the frequency of the samples. The following experiments were carried out: observations inserted at each \( \Delta x \) (EXP1), at \( 100 \, \Delta x \) (EXP2), at \( 200 \, \Delta x \) (EXP3), at \( 300 \, \Delta x \) (EXP4), at \( 500 \, \Delta x \) (EXP5), at \( 700 \, \Delta x \) (EXP6). The number of measurements (observation grid) was taken equal to the number of vertical grid points \( (N_m = N_z) \). Table 1 shown the errors for each experiment and Figures 2a-2c show respectively EXP3, EXP5, EXP6 for the concentration data for \( z = 150 \, \text{m} \). The labels of figures CP, CO, and CE are respectively the concentration predicted by mathematical model, observed concentration, and the estimated concentration by KF.

The error is computed by
error = \frac{1}{N_x N_z} \sum_{n=1}^{N_x} \sum_{i=0}^{N_z} (c_{i,n}^{\text{exact}} - c_{i,n}^a)^2 . \quad (11)

Clearly, the estimation made by KF is better when the number of samples is increased. However, the computational effort is enhanced for a greater number of samples.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Frequency of observations</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>every $\Delta x$</td>
<td>0.328</td>
</tr>
<tr>
<td>2</td>
<td>at 100 $\Delta x$</td>
<td>7.236</td>
</tr>
<tr>
<td>3</td>
<td>at 200 $\Delta x$</td>
<td>11.880</td>
</tr>
<tr>
<td>4</td>
<td>at 300 $\Delta x$</td>
<td>13.877</td>
</tr>
<tr>
<td>5</td>
<td>at 500 $\Delta x$</td>
<td>21.627</td>
</tr>
<tr>
<td>6</td>
<td>at 700 $\Delta x$</td>
<td>31.779</td>
</tr>
</tbody>
</table>

The assimilation process also was analyzed with relation to the number of measurement points in the vertical coordinate. In this class of experiments, the observations were sampled at 100 $\Delta x$. In the EXP7 was used $N_m = 9$ at the following positions: $z = 0, 50, 100, 150, 200, 250, 300, 350$ and 400 m; for EXP8 was used $N_m = 7$ at the following positions: $z = 0, 100, 150, 200, 250, 300$ and 400 m; in the EXP9 was used $N_m = 5$ at the following positions: $z = 0, 100, 200, 300$ and 400 m. Figures 5a-5c show the results for this experiments.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Number of sensors in direction-z</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>$N_m = 9$</td>
<td>22.377</td>
</tr>
<tr>
<td>8</td>
<td>$N_m = 7$</td>
<td>44.650</td>
</tr>
<tr>
<td>9</td>
<td>$N_m = 5$</td>
<td>77.933</td>
</tr>
</tbody>
</table>
Fig. 2. Effect of the observation frequency in the KF: (a) EXP3; (b) EXP5; (c) EXP6.
From Table 2 and Figure 3, it is seen that the error decreases when the number of observation levels enhance. It is pointed out that the observations are uniformly distributed.

The last case of experiments is focused on the analysis of the filter performance under different arrangements of the observation grid. Five positions ($N_v = 5$) of measurements were used in the vertical, with experimental data inserted at every $\Delta x$. Three different arrangements were considered: Grid-1, uniformly distributed sensors - $\text{EXP}10$; Grid-2 with sensors positioned close to the ground ($z = 0, 20, 40, 60$ and $80$ m) - $\text{EXP}11$; Grid-3 sensor positioned near to the top of boundary layer ($z = 320, 340, 360, 380$ and $400$) – $\text{EXP}12$. Table 3 presents the errors for these different arrangements.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Type of grid</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Grid-1</td>
<td>77.933</td>
</tr>
<tr>
<td>11</td>
<td>Grid-2</td>
<td>355.897</td>
</tr>
<tr>
<td>12</td>
<td>Grid-3</td>
<td>394.200</td>
</tr>
</tbody>
</table>

5. FINAL REMARKS

The Kalman filter was applied for data assimilation for atmospheric pollutant dispersion governed by advection-diffusion equation. Three classes of experiments were performed. The results show that as greater the samples of observation the estimative is improved, in so far as direction-$x$ (experiments of Class-1) as direction-$z$ (experiments of Class-2). The arrangement with uniformly distributed sensor in the vertical direction (Grid-1) presented the best performance for the three different vertical observation grid. However, this is not conclusive statement, more experiments need to be performed.

The assimilation procedure based on Kalman filter is effective for dispersion models, and it can be used for operational air monitoring systems. The neural networks can be an alternative scheme for the data assimilation process in atmospheric dispersion
models, as suggested in recent studies (Nowosad et al., 2000b, 2000c).

Fig. 3. Assimilation with different observation grids: (a) \(N_m = 9\), (b) \(N_m = 7\), (c) \(N_m = 5\).
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