Assimilation of Stratospheric Chemical Tracer Observations Using a Kalman Filter. Part II: $\chi^2$-Validated Results and Analysis of Variance and Correlation Dynamics

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ABSTRACT

A Kalman filter system designed for the assimilation of limb-sounding observations of stratospheric chemical tracers, which has four tunable covariance parameters, was developed in Part I of this two-part paper. The assimilation results of CH$_4$ observations from the Cryogenic Limb Array Etalon Sounder instrument (CLAES) and the Halogen Observation Experiment instrument (HALOE) on board the Upper Atmosphere Research Satellite are described in this paper.

A robust $\chi^2$ criterion, which provides a statistical validation of the forecast and observational error covariances, was used to estimate the tunable variance parameters of the system. In particular, an estimate of the model error variance was obtained. The effect of model error on the forecast error variance became critical after only 3 days of assimilation of CLAES observations, although it took 14 days of forecast to double the initial error variance. Further, it was found that the model error due to numerical discretization, as arising in the standard Kalman filter algorithm, is comparable in size to the physical model error due to wind and transport modeling errors together. Separate assimilations of CLAES and HALOE observations were compared to validate the state estimate away from the observed locations. A wave breaking event that took place several thousands of kilometers away from the HALOE observation locations was well captured by the Kalman filter due to highly anisotropic forecast error correlations. The forecast error correlation in the assimilation of the CLAES observations was found to have a structure similar to that in pure forecast mode except for smaller length scales. Finally, an analysis of the variance and correlation dynamics was conducted to determine their relative importance in chemical tracer assimilation problems. Results show that the optimality of a tracer assimilation system depends, for the most part, on having flow-dependent error correlation rather than on evolving the error variance.

1. Introduction

In Ménard et al. (2000, hereafter referred to as Part I) we introduced the formulation of a Kalman filter system specifically designed for the assimilation of chemical tracer observations from limb-sounding instruments. The assimilation system is based on a two-dimensional approximation on isentropic surfaces and has been implemented on distributed-memory parallel computers by Lyster et al. (1997). The Kalman filter requires as input the initial tracer mixing ratio $\mu_0$, the initial error covariance $P_0$, the model error covariance $Q_k$, and the observational error covariance $R_k$ at each time step $k$. The observational error covariance was decomposed into a measurement error covariance $R_k^m$ provided by the instrument team and a representativeness error covariance $R_k^r$ to be estimated on the basis of the observed-minus-forecast (OmF) residuals. The input error covariances $P_0$, $Q_k$, and $R_k^r$ were modeled on the principles that data shock should be minimized and that the analysis increments should have a $-2$ spectral slope, typical of stratospheric tracer fields (Ngan and Shepherd 1997). It was shown, in Part I, that data shocks can be minimized when the error standard deviation is made proportional to the current state estimate and when the initial state estimate is a spunup mixing ratio field resulting from a long-term tracer transport simulation. The requirement on the spectrum of the analysis increments has been accommodated by using a first-order autoregressive (FOAR) correlation model for $P_0$ and $Q_k$. For simplicity, it has been assumed that the observational error is uncorrelated and that the correlation length scales for $P_0$ and $Q_k$ are identical. The Kalman filter system thus has one tunable correlation length-scale parameter, $L$, and three tunable relative error standard deviation (std dev) parameters: $\beta$ for the representativeness error, $\delta$ for the model error, and $\gamma$ for the initial
error. The discrete propagation of the forecast error covariance was made to obey tracer conservative properties of the error covariance field that were established by Cohn (1993). The standard computation \( \mathbf{M} \) of the Kalman filter was found not to obey the conservative properties but to exhibit strong numerical diffusion on the variance and on the correlation length scales.

In this paper, the Kalman filter system developed in Part I is used to assimilate \( \text{CH}_4 \) observations from the Cryogenic Limb Array Etalon Spectrometer (CLAES) instrument and the Halogen Occultation Experiment (HALOE) instrument on board the Upper Atmosphere Research Satellite (UARS). The CLAES instrument is a thermal emission sounder that provides extensive horizontal coverage: from 80°S to 34°N in south limb viewing or from 34°S to 80°N in north limb viewing (Roche et al. 1993). The two viewing configurations alternate each 36 days as the satellite yaws 180° in its orbit to minimize solar exposure of the thermal infrared instruments. The HALOE instrument uses the solar occultation technique and provides daily measurements on two narrow latitude bands, one at the satellite sunrise and the other at the satellite sunset (Russell et al. 1993). The assimilation of HALOE \( \text{CH}_4 \) observations can be validated against the assimilation of CLAES \( \text{CH}_4 \) observations used as the control, especially in regions that are some distance away from the HALOE observation locations.

All experiments we have conducted in this paper are statistically validated using the robust \( \chi^2 \) diagnostic introduced in section 2b of Part I. This diagnostic defined in observation space compares the sample covariance of the OmF residuals with the innovation covariance matrix obtained from the Kalman filter algorithm. Since the latter matrix uses both the computed forecast error covariance and the observational error covariance specified in the assimilation algorithm, the \( \chi^2 \) diagnostic can be used to validate these error covariances. In fact, we will show in section 2 that by monitoring the evolution of \( \chi^2 \), an estimate of all three tunable variance parameters of the system can be made. There are two advantages in using the \( \chi^2 \) diagnostic for parameter tuning. One lies in the fact that it neither assumes nor requires knowledge of the probability distribution of the OmF residuals. The other is that the assimilation results automatically verifies the \( \chi^2 \) diagnostic [Eq. (2.22) of Part I] – a necessary condition for statistical validation. The \( \chi^2 \) tuning procedure is, however, limited in the number and type of parameters it can estimate. The correlation length-scale parameter, \( L \), will be shown to be almost insensitive to the \( \chi^2 \) value and has been estimated using, instead, the maximum-likelihood method (Dee and daSilva 1999).

An analysis of the relative importance of evolving the error variance vis-à-vis the error correlation for chemical tracer assimilation problems was also conducted by varying the Kalman filter algorithm in three different ways: 1) by prescribing the forecast error covariance (variance and correlation fields), which is a form of statistical interpolation widely used in data assimilation; 2) by allowing only the error variance to evolve in the Kalman filter algorithm with an error correlation identical to that of the statistical interpolation scheme; and 3) by allowing only the error correlation to evolve in a Kalman filter algorithm, with the error variance prescribed in a way similar to that of the statistical interpolation scheme. Since all these schemes have covariance parameters of their own, and in order to provide meaningful intercomparisons of the results, \( \chi^2 \) tuning and the maximum-likelihood method were used to estimate the free covariance parameters. Furthermore, these experiments were conducted using HALOE and CLAES observations separately to assess which of the two components, the error variance or the error correlation, contributes more effectively in reconstructing the field far away from the observation locations.

The Kalman filter formulation that we have used is unique in several aspects. The input error covariances use a relative error formulation with an FOAR correlation model, and the evolution of the error covariance was modified to enforce tracer properties of the covariance field. In this paper, the above computational and modeling features will also be challenged in the context of the full assimilation system. By replacing these features by standard ones, and by conducting \( \chi^2 \)-validated assimilation experiments, the forecast error variance was used to assess our specific filter formulation.

The organization of this paper is as follows. In section 2 we discuss the covariance parameter tuning, and in particular the effect of incorrect specification of the error standard deviation parameters on the value of \( \chi^2 \). In section 3 the result of \( \chi^2 \)-validated assimilation experiments are presented using separately CLAES and HALOE observations. An analysis of the variance and the correlation dynamics in assimilation is presented in section 4 where the results of simplified filtering schemes are compared against the result of the Kalman filter. An assessment of the unique computational and modeling features of the Kalman filter system is presented in section 5. The results are summarized in section 6.

2. Covariance parameter tuning

In principle, when the innovation covariance matrix, \( \mathbf{S}_i = \mathbf{H}_i \mathbf{P}_x \mathbf{H}_i^T + \mathbf{R}_i \), is representative of the sample covariance of the innovations \( \mathbf{v}_i = \mathbf{m}_i - \mathbf{H}_i \mathbf{x}_i \), the conditional expectation of \( \chi^2_i = \mathbf{v}_i^T \mathbf{S}_i^{-1} \mathbf{v}_i \) is equal to the number of observations \( m_i \) at time \( t_i \), that is

\[
\left\langle \chi^2_i \mid \mathbf{m}_i \right\rangle = m_i, \tag{2.1}
\]

(see section 2a of Part I). Here \( \mathbf{H}_i \) denotes the forward observation operator, \( \mathbf{P}_x \) is the forecast error covariance matrix, and \( \mathbf{R}_i \) is the observational error covariance ma-
The state variable is the tracer mixing ratio. We denote the observation vector of mixing ratio by $m^o_k$ and the forecast state estimate by $m^f_k$. The conditional expectation $E(m^o_k | m^f_{k-1})$ is made with respect to a given set of all the observation vectors up to time $t_{k-1}$.

In practice, we take a running (time) average of $\chi^2_k$, divide by the total number of observations $M$, used in the time average, and verify that the result is approximately equal to one, that is,

$$\chi^2_k = \frac{1}{M_k} \sum_{i=k-\Delta k/2}^{k+\Delta k/2} \nu_i^T S_i^{-1} \nu_i = 1,$$

(2.2)

where

$$M_k = \sum_{i=k-\Delta k/2}^{k+\Delta k/2} m_i.$$

(2.3)

The running mean time window, $\Delta k$, is expressed in number of analysis steps. Because the OmF are the results of the assimilation, the forecast state depends on the previous realization of the observations. Consequently, the time average of the assimilation residuals in (2.2) is a statistic of the conditional mean.

The running mean $\chi^2_k$ has an inherent statistical variability that depends on the total number of observations, $M_k$, in the time window $\Delta k$. For arbitrary probability distribution of the innovations $\nu$, $\chi^2_k = \nu^T S_k^{-1} \nu$ is asymptotically normal distributed with mean $m$, and variance $2m$, for large innovation dimension (e.g., Lupton 1993). Since an analysis is performed at each time step and that there are typically 13–14 CLAES observations per time step, the size of the observation vector is too small to invoke asymptotic arguments. However, in the running mean (2.2) the sum of $\chi^2_k$’s embraces a large number of observations. With a time window $\Delta k = 96$ used in our experiments, the sum of $\chi^2$’s contains about 1300 CLAES observations. So one can argue that the variance of $\Sigma_k \chi^2_k$ is $2M_k$, and consequently the statistic $\chi^2_k$ has a variance equal to $2/M_k$, which, in turn, gives a standard deviation of about 0.04 for $M_k \approx 1300$.

Applying the running mean $\chi^2_k$ to the variance parameter tuning, we found that incorrect specifications of the relative representativeness error std dev $\beta$, the relative model error std dev $\delta$, and the relative initial error std dev $\gamma$, produce different evolution patterns in the $\chi^2_k$ time series. In Fig. 1 we present $\chi^2_k$ with $\Delta k = 96$ for several CLAES assimilation experiments using different values for $\beta$, $\delta$, and $\gamma$. The assimilations were conducted on the 1100-K isentrope from 6 to 14 September 1992. Each panel in Fig. 1 represents the result of perturbing one of the three parameters about $\beta = 0.10$, $\delta = 0.003$ and $\gamma = 0.11$ used as the control case. In Fig. 1a four different values of $\beta$ were used. The dashed curve (top curve) for $\beta = 0$ corresponds to the case where only measurement error accounts for observational error. The dashed–dotted curve is for $\beta = 0.05$, the solid curve is for $\beta = 0.10$, and the dotted curve (bottom curve) for $\beta = 0.15$. The best fit of $\chi^2_k$ to unity was found using $\beta = 0.10$. Since the relative measurement error std dev in this case study is about 0.073 (Roche et al. 1996), the representativeness error variance in the case study is twice as large as the measurement error variance. In Fig. 1b we present the $\chi^2_k$ time series for three values of the relative model error std dev $\delta$. The dashed curve is for no model error, $\delta = 0$, the solid line is for $\delta = 0.003$, and the dotted line is for $\delta = 0.01$. We note that a misspecification of $\beta$ produces a trend in $\chi^2_k$. The value $\beta = 0.003$ produces no trend in the $\chi^2_k$ time series. In Fig. 1c the $\chi^2_k$ time series for three values of $\gamma$ is displayed. The dashed curve is for $\gamma = 0.05$, the solid curve for $\gamma = 0.11$, and the dotted curve for $\gamma = 0.15$. The case where $\gamma = 0.11$ shows the least transience in $\chi^2_k$. Overall, the $\chi^2_k$ statistic is most sensitive to the observational error parameter $\beta$ and least sensitive to the initial error parameter $\gamma$.

In practice, there is apparently no way to use the $\chi^2$ validation diagnostic [(2.1) or (2.2)] to estimate the correlation length scale $L$ in addition to the relative error std dev parameters. In fact, we found that $\chi^2_k$ displays very little sensitivity to the correlation length-scale parameter $L$. We can thus estimate the relative error std dev parameters based on the $\chi^2$ validation diagnostic, and use other parametric estimation procedures such as the maximum-likelihood method to estimate the correlation length-scale parameter $L$. With this approach we retain robustness to our variance parameter estimates and guarantee a $\chi^2$-validated assimilation experiment.

To estimate the correlation length-scale parameter, $L$, an off-line maximum-likelihood estimation of the initial forecast error correlation length scale is used. To begin with, we use the transport model (with no assimilation) to generate the forecast state. Then, the forecast state is interpolated at the observation locations, and using CLAES observations we obtain the off-line OmF residuals. Only the residuals on the first day of the assimilation were used in this estimation procedure. This time period is chosen to help minimize the distortion of the initial condition while retaining sufficient data to provide a reliable statistical estimate. Fixing the relative initial error std dev to $\gamma = 0.11$ and using a relative representativeness error of $\beta = 0.10$, a correlation length scale $L = 3600$ km with an FOAR correlation model was obtained with the maximum-likelihood method. The $\chi^2$-validation procedure was also with these offline OmF residuals data and an estimate of $\gamma = 0.11$ was obtained, which is identical to the value obtained previously with the CLAES assimilation residuals. The estimated correlation length scale $L$ was used for both the initial error correlation and the model error correlation models.

The model error and the initial error parameter values were assumed to be the same for the HALOE assimilation experiments. Only parameters related to the observational error, that is, $\beta$, need to be estimated. This was actually carried out in section 5b of Part I where
a value of $\beta \approx 8.6\%$ was obtained on the basis of $\chi^2$. Table 1 summarizes the estimated covariance parameter values.

### 3. Kalman filtering experiments

We have conducted two assimilation experiments, one using just the CLAES observations, and the other using only the HALOE observations. The experiments were conducted for the time period of 6 to 14 September 1992 at the 1100-K isentropic level, when an intense planetary wave breaking led significant mixing of tropical stratospheric air into the southern midlatitudes (Randel et al. 1993), which we will refer to as our “case study.” During this period, the CLAES instrument was south limb viewing, providing coverage of the wave breaking event. By contrast, the HALOE instrument did not provide coverage of the event; half the observations were near 70°N, and the other half near 14°N on 6 September and moving rapidly southward to reach 37°S on 14 September (see Fig. 4 of Part I for observation locations on 8 September). Comparison of the separate assimilation results of HALOE and CLAES observations will serve to reveal the performance of our assimilation system in regions not covered by the HALOE instrument. The covariance parameters obtained in the previous section (see Table 1) were used in these assimilation experiments. The HALOE initial state estimate $\mu_0$ was derived from the CLAES initial state estimate by multiplying it by a factor of 1.4 to account for the systematic difference in the CH$_4$ observations of CLAES and HALOE.

Figure 2 shows the analysis on day 2 (8 September 1992), day 4, day 6, and day 8 for the CLAES assimilation. We observe a developing “tongue” of tropical air that breaks out on 10 September to form a separate “blob” of tropical air in the southern midlatitudes.

### Table 1. Covariance parameter values used in the Kalman filtering experiments.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>$\beta$</th>
<th>$\delta$</th>
<th>$\gamma$</th>
<th>L (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CLAES</td>
<td>0.1</td>
<td>0.003</td>
<td>0.11</td>
<td>3600</td>
</tr>
<tr>
<td>HALOE</td>
<td>0.086</td>
<td>0.003</td>
<td>0.11</td>
<td>3600</td>
</tr>
</tbody>
</table>

Fig. 1. Time series of $\chi^2$ from CLAES CH$_4$ assimilation for perturbed values of representativeness error $\beta$, model error $\delta$, and initial error $\gamma$, about the control case $\beta = 0.1$, $\delta = 0.003$, and $\gamma = 0.11$. 
it continues its advection eastward, the blob of tropical air slowly mixes with its environment as indicated by a gradual decrease of the central value of the blob. On day 8, the tropical blob of air then interacts with a secondary vortex initially located near (40°S, 170°E).

A running mean of the CLAES forecast error variance interpolated at the observation locations and normalized by the observational error variance, hereafter called the error variance ratio, is depicted in Fig. 3. This running mean uses 76 data points to smooth out the time series, which corresponds roughly to the average number of CLAES observations per orbit (on a single level). The thin line (top curve) is the error variance ratio due to transport only. This ratio was obtained from the covariance evolution [Eq. (2.19) of Part I] using the model error covariance $Q_k$ with the estimated parameter values obtained in the previous section. The slow rise with time is consistent with a gradual loss of the predictive skill, and we note that an integration of 14 days is needed to double its initial value. We observe also that the initial error variance is about the same size as the observational error, corresponding to a ratio of unity. The thick line is the error variance ratio for the Kalman filter assimilation. A significant decrease of the error variance ratio to a value of about 0.08 is obtained where it apparently reaches saturation. The dashed line (bottom curve) represents the normalized error variance in a Kalman filter experiment where the model error covariance was neglected; that is, $Q_k$ was set to zero. Although this result does not support the $\chi^2$ condition (2.2), it shows that the computed forecast error variance keeps on decreasing with time and eventually results in rejecting observations; a problem known as “filter divergence” (e.g., Jazwinski 1970, section 8.8). The error variance ratio of the perfect model run (bottom curve), that is, with $Q_k = 0$, reaches half that of the Kalman filter (thick line) in only three days. This is much earlier than the time needed to double the initial error variance in the pure forecast mode, and thus accounting for the model error covariance is more critical in data assimilation than in pure forecast mode.

The forecast error correlation in the CLAES assim-
Fig. 3. Running mean of the forecast error variance interpolated at the observation locations of CLAES CH₄, normalized by the observational error variance. (top) The thin curve represents the forecast error variance when no assimilation is performed. The thick solid line represents the result of the Kalman filter assimilation. (bottom) The dashed line represents the error variance of a Kalman filter running with a model error covariance set to zero.

Fig. 4. Forecast error correlation in the Kalman filter assimilation of CLAES CH₄ data. (top) The correlation between a material particle initially located at (32°S, 90°W) and all the grid points of the domain. Figure 4a depicts the forecast error correlation after one day of assimilation, but with respect to a reference point that has been advected as a material particle for a day starting from the initial location (32°S, 90°W). Comparing Fig. 4 with Fig. 2 of Part I where no assimilation is performed, we note that the correlation patterns are similar but the correlation length scales are smaller in the assimilation case. This result, also observed at other reference points, suggests that the assimilation of uniformly distributed observations does not significantly alter the shape of the error correlation pattern; it retains its flow-dependent signature.

The mixing ratio result of the HALOE assimilation is presented in Fig. 5, where the analysis on days 2, 4, 6, and 8 is depicted. By comparing it with the CLAES assimilation, Fig. 2, and in light of the result of the "naive" covariance modeling discussed in section 4 of Part I, we note that the evolution of the state estimate is smooth, dynamically consistent, and that the wave breaking event is well captured. The low mixing ratios in the polar vortex seen in the CLAES assimilation are, however, not captured by the HALOE assimilation, for this region is too far away from the observation locations.

The effect of observations on the error variance can be depicted by dividing at each grid point the assimilation forecast error variance by the error variance obtained in pure forecast mode. This ratio for the HALOE assimilation is presented in Fig. 6. We note that the effect of observations that is depicted by a small ratio moves southward with the observation locations and intensifies with time (i.e., the minimum ratio value decreases with time). The displacement southward can be explained by the effect of model error, which increases the error variance after the observations have moved away from a location. The effect of observations also propagates into the developing tongue but apparently fails to penetrate the polar vortex.

The forecast error correlation with respect to a few selected observation locations is displayed in Fig. 7. The quantity plotted is the normalized analysis incre-
ment, \( \frac{\mu_i^s - \mu_i^s}{\max|\mu_i^s - \mu_i^s|} \), since there is at most one HALOE observation per time step. The analysis increments of tropical observations depicted in Figs. 7a and 7b are nearly isotropic. Highly anisotropic increments are obtained for subtropical observations, where the wind shear may contribute to creating highly anisotropic forecast error correlation structures. Figure 7c shows that the effect of an observation can, in effect, intensify the wave breaking structure. Figure 7d shows that some observations actually reinforce the mixing ratio gradient between the southern midlatitudes and polar vortex regions.

4. Analysis of variance and correlation dynamics

In this section we investigate which component of the forecast error covariance, the error variance or the error correlation, is more important to evolve in order to maximize the filter performance. To conduct this study, we have compared the results of a statistical interpolation scheme (Daley 1991), a variance evolving scheme (Daley 1992; Todling and Cohn 1994), and a scheme that evolves only the error correlation, against the results of the Kalman filter. These schemes were obtained by modifying the Kalman filter system, but they have covariance parameters of their own. Individual variance parameters were tuned by using the \( \chi^2 \) procedure, and the maximum-likelihood method was used to determine the proper correlation length-scale parameter.

Our statistical interpolation scheme uses a forecast error covariance model identical to that of the Kalman filter initial condition described in section 5a of Part I. The Kalman gain is computed explicitly and no simplification or approximation is made in its computation. The forecast error covariance is thus of the form

\[
P^s(i,j) = \gamma^s \mu^s(i) \mu^s(j) \mathbf{C}(i,j),
\]

(4.1)

where \( \mathbf{C} \) is an isotropic FOAR correlation model. Here, the relative forecast error std dev \( \gamma \), and the correlation length scale \( L \), are tunable parameters. The superscript \( s \) denotes the statistical interpolation scheme.
FIG. 6. Normalized forecast error variance in the Kalman filter assimilation of HALOE CH₄ observations. The contours are the ratio of the forecast error variance during assimilation divided on each grid point by the forecast error variance when no assimilation is performed.

terminate those parameters we used the innovations of a 16-day assimilation of the CLAES observations. After the first four days when the assimilation underwent an initial adjustment, the running mean $\overline{X}_k$ was used to estimate the relative forecast error $\gamma$. A relative forecast error std dev $\gamma = 0.05$ was thus obtained. The maximum-likelihood procedure was used to estimate the correlation length scale in a way similar to the procedure used in section 2. A correlation length scale $L = 1600$ km was obtained.

The variance evolving scheme consists in evolving the error variance according to the transport model with model error variance,

$$V'_k = M_{k-1} V'_{k-1} + V'_k$$

and

$$V'_k(i) = [\delta \mu_k(i)]^2,$$

where $\delta$ is the relative model error standard deviation. The analysis error covariance equation [Eq. (2.16) of Part I] is used to obtain the analysis error variance $V_k$. The forecast error covariance is then computed from

$$P'_{ij}(i, j) = \sqrt{V'_k(i)V'_j(j)C(i,j)},$$

where $C$ is an isotropic FOAR correlation model. The correlation length scale is the same as for the statistical interpolation, that is, $L = 1600$ km. Using the running mean $\overline{X}_k$ on an 8-day CLAES assimilation, an estimate of $\delta = 0.006$ was obtained. That is a relative error twice as large as the $\delta$ value of the Kalman filter; thus, the model error variance is four times that of the Kalman filter. The initial relative error std dev was chosen to be identical to that of the Kalman filter run.

The correlation evolving scheme consists of using the Kalman filter algorithm to compute the forecast error correlation. Also, the variance is similar to the one used for statistical interpolation. Thus the forecast error covariance is given as

$$P_{ij}(i, j) = \gamma^2 \mu_k(i) \mu_j(j) C(i,j).$$
where $\gamma$ is a relative error std dev. Here,

$$C_{k}^{KF}(i, j) = \frac{P_{i}(i, j)}{\sqrt{P_{i}(i, i)P_{i}(j, j)}}$$

(4.6)

is the Kalman filter error correlation obtained using the Kalman filter algorithm with the model error covariance parameters $\delta = 0.003$ and $L = 3600$ km. A relative forecast error std dev $\gamma = 0.04$ was thus obtained by tuning only after the first four days of the assimilation during which the system underwent an initial adjustment. The results of tuning for the simplified assimilation schemes are summarized in Table 2.

Let us first consider the assimilation results of CLAES observations. In Fig. 8 (similar to Fig. 3), the forecast error variance at the observation locations has been normalized by the observational error variance and smoothed using a running mean with 76 observations. We choose to plot the normalized error variance after the first four days since that part of the innovation data was not used in the tuning procedure. The result of statistical interpolation is depicted with the thin solid line (top curve). The result of the variance evolving scheme is plotted with the thick solid line, and that of the correlation evolving scheme plotted with the dashed line (bottom curve). This variance ratio is about 0.2 for

![Figure 7](image-url)  
**Fig. 7.** Forecast error correlation at selected observation locations in a HALOE CH$_4$ Kalman filter assimilation experiment. The black triangle depicts the position of the observation. Panels (a) and (b) are associated with tropical observations, and panels (c) and (d) are associated with subtropical and midlatitude observations, respectively.

### Table 2. Covariance parameter values used in the simplified filtering assimilation experiments.

<table>
<thead>
<tr>
<th></th>
<th>$\beta$</th>
<th>$\delta$</th>
<th>$\gamma$</th>
<th>$L$ (km)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CLAES</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stat. interp.</td>
<td>0.1</td>
<td>—</td>
<td>0.05</td>
<td>1600</td>
</tr>
<tr>
<td>Var. evol.</td>
<td>0.1</td>
<td>0.006</td>
<td>0.11</td>
<td>1600</td>
</tr>
<tr>
<td>Corr. evol.</td>
<td>0.1</td>
<td>0.003</td>
<td>0.04</td>
<td>3600</td>
</tr>
<tr>
<td><strong>HALOE</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stat. interp.</td>
<td>0.086</td>
<td>—</td>
<td>0.05</td>
<td>1600</td>
</tr>
<tr>
<td>Var. evol.</td>
<td>0.086</td>
<td>0.006</td>
<td>0.11</td>
<td>1600</td>
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<tr>
<td>Corr. evol.</td>
<td>0.086</td>
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<td>0.04</td>
<td>3600</td>
</tr>
</tbody>
</table>
Fig. 8. Running mean of the forecast error variance of the simplified assimilation schemes. The forecast error variances of a CLAES CH4 assimilation run are interpolated at the observation locations and normalized by the observational error variance (cf. Fig. 3). (top) The thin curve represents the forecast error variance for statistical interpolation. The thick solid line represents the result of the variance evolving scheme. (bottom) The dashed line represents the result of the correlation evolving scheme.

the statistical interpolation scheme, indicating that the forecast error variance is five times smaller than the observational error (or the forecast error variance in nonassimilating mode). The variance ratio for the variance evolving scheme is about 0.16 indicating a slight improvement in the forecast error variance compared with statistical interpolation. The variance ratio for the correlation evolving scheme is about 0.09, a factor of 2 smaller than the statistical interpolation result. The variance ratio for the correlation evolving scheme is actually close to the Kalman filter variance ratio, which is near 0.07 (see Fig. 3).

Although we found significant differences in the estimation error between the simplified assimilation schemes and the Kalman filter, they do not translate into large differences in the state estimate. Figure 9 depicts the mixing ratio analysis on day 4 for all three simplified schemes and the Kalman filter. We only find minor differences between the four panels. We explain this result by the fact that there is little amplification of errors with tracer dynamics, and because the CLAES observation pattern is dense, offering numerous observations to reduce the error variance. As a result, all schemes produce analysis error variances that are at least five times smaller than the observational error variance, and thus there are only minor differences between the state estimate produced by the different schemes.

In contrast to the CLAES assimilation results, significant differences between the state estimates given by various schemes are found in the HALOE assimilation. The analysis on day 4 is presented in Fig. 10. Figs. 10a–d depict, respectively, the results of the statistical interpolation scheme, the variance evolving scheme, the correlation evolving scheme, and the Kalman filter. We observe that for the statistical interpolation scheme and the variance evolving scheme, the impact of observations is limited to the area observed by the instrument. We note in particular that the tropical values have increased as a result of assimilation, but the developing tongue of tropical air retains its small mixing ratio values like in the pure forecast case. Only when the error correlation is dynamically evolved, as shown in Figs. 10c and 10d, do observations effectively influence the state estimate at large distances from the observation locations. In this case, a more intense wave breaking is obtained, which compares favorably with the CLAES assimilation.

The effect of dynamically evolving the error correlation can be understood as follows. In the absence of observations or for regions that are far away from the observations, the error correlation develops highly anisotropic structures over large distances as a result of advection dynamics. When an observation enters such a region of high anisotropy, the effect of the observation extends immediately far away from the observation location. By contrast, the effect of an observation on the error variance field propagates according to the advection dynamics, which is the same mechanism for propagating the state itself. It thus appears in the tracer problem that little is gained by dynamically evolving the error variance. Rather, the most effective mechanism to reduce the analysis error variance, both in sparse and in dense observation networks, is through the use of dynamically evolving error correlations.

5. Assessment of the covariance modeling and computation

The covariance modeling of the initial, observational, and model errors was established, in Part I, on the basis of assimilation principles and simple numerical experiments. We have not yet shown whether this particular modeling of the input error covariances improves the performance of the assimilation (i.e., reduces the forecast error variance) over assimilations using more standard covariance modeling assumptions. Similarly, our computational covariance prediction algorithm, which is built upon the continuum covariance evolution problem, has not yet been shown to yield improved assimilations. The purpose of the section is to perform those assessments. In each experiment that follows, CLAES observations were used and the free variance parameters were tuned using the $\chi^2$ procedure, and the correlation length scale was estimated using the maximum-likelihood method.

To assess the effect of numerical discretization error
on the evolution of the error covariance, we will compare the result of the Kalman filter using our covariance evolution algorithm [Eqs. (3.6)–(3.9) and (3.12)–(3.13) of Part I] against the results of the Kalman filter using the standard covariance evolution equation [Eq. (2.19) of Part I]. Employing CLAES observations and the standard Kalman filter, we conducted an experiment for our case study and adjusted the model error std dev $\delta$ to meet the $\chi^2$ criterion (2.2). A value $\delta = 0.005$ was found that is nearly twice as large as the $\delta$ value obtained with our Kalman filter formulation. The error variance ratio for the standard Kalman filter is depicted as a thin solid line in Fig. 11. The thick solid line in Fig. 11 shows the result of our Kalman filter formulation [Eqs. (3.6)–(3.9) and (3.12)–(3.13) of Part I] presented here for comparison. The increase of model error variance incurred with the standard Kalman filter algorithm is a compensation of the variance loss that occurs with the $\mathbf{M}(\mathbf{M}^T\mathbf{P})^{-1}$ computation. The variance ratio for the standard Kalman filter reaches a value near 0.011, a ratio comparable to that of the correlation-evolving scheme and somewhat smaller than for the variance evolving scheme.

The choice of a relative error formulation in the covariance models for $\mathbf{P}_0$, $\mathbf{R}_k$, and $\mathbf{Q}_k$ was also reexamined by comparing the results of a $\chi^2$-validated system that used an absolute error formulation for the input error covariances. In the absolute error formulation, the error std dev is made proportional to a typical global mean mixing ratio $\mathbf{\mu}$ that does not change throughout the course of the experiment. Such a model was used for the representativeness error in an experiment using HALOE observations in section 5b Part I. Here we have conducted an assimilation of CLAES observations and established the three absolute error parameters using the $\chi^2$ tuning procedure. We found that the error variance ratio is larger than that for the relative error system. However, the relative representativeness error std dev

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**Fig. 9.** Comparison of CLAES CH$_4$ assimilation on the 1100-K isentropic surface, valid 10 Sep 1992. (a) The result of the statistical interpolation, (b) the result of the variance evolving scheme, (c) the result of the correlation evolving scheme, and (d) the result of the Kalman filter.
in the absolute error formulation; that is, $\alpha$ [see Eq. (5.3) of Part I] was estimated to be 0.05, a value smaller than the relative representativeness error std dev in the relative error formulation, $\beta$. Figure 12 depicts the result of the absolute error system with the thin line and that of the relative error system is depicted with the thick solid line. The forecast error variance behaves differently in those two experiments, and the result may be difficult to compare. Nevertheless, the error variance ratio is a measure of the effective use of the observations in an assimilation system, and these results indicate that the relative error system makes a more effective use of the data than with the absolute error system. Also, a comparison of the forecast error variance at the observation locations between the two systems indicates a better performance with the relative error system than with the absolute error system.

Finally, we have also considered a second-order autoregressive (SOAR) correlation model for the initial and model error covariances instead of the FOAR model used so far. After tuning $\gamma$, $\delta$, and $L$, we found only a small and nonsignificant increase of the error variance ratio with the SOAR model. We conclude that the choice of a correlation model cannot be based on the forecast error variance.

6. Conclusions

We have conducted an assimilation study of chemical tracer observations using a Kalman filter system specifically designed for the assimilation of limb-sounding measurements of stratospheric trace gases. The description of the system, the requirements, and the covariance modeling that followed from these requirements were given in detail in Part I. We recall that our Kalman filter assimilation system is based on a two-dimensional approximation on isentropic surfaces, and both the model error and the representativeness error were accounted for in it. The initial, model, and representativeness errors were modeled on the principles of minimizing data shocks and on creating analysis corrections that has a spectrum similar to that of the true field. These require-
ments have dictated the use of the FOAR model for spatial correlations, and on modeling the error std dev to be proportional to the current state estimate. In addition, modifications to the Kalman filter algorithm were made to accommodate tracer properties in the evolution of the error covariance (Cohn 1993). All accounted for, the Kalman filter assimilation system has three tunable variance parameters and one tunable correlation length scale parameter. In this paper this system has been applied to the assimilation of CH₄ observations from the CLAES and HALOE instruments on board UARS. The tunable parameters have been estimated, the assimilation results have been validated, and an analysis of the performance of the Kalman filter has been conducted.

The estimation of the variance parameters was made by monitoring a running time mean $\chi^2$ diagnostic. It was found that a misspecification of the model error std dev introduces a growth of the $\chi^2$ diagnostic with time. A misspecification of the initial error std dev is only felt initially on the $\chi^2$ diagnostic, and a misspecification of the relative representativeness (or observational) error introduces a translation of the whole time mean. For our case study, for 6–14 September 1992 on the 1100-K isentrope, the relative initial error std dev was estimated to be equal to 0.11, the relative representativeness error std dev equal to 0.10 for CLAES and 0.086 for HALOE CH₄ observations, and the relative model error std dev was estimated as 0.003 per time step of 15 min. In terms of variances, these results indicate that the representativeness error is larger than the instrument error, by a factor of 2 for the CLAES instrument and by two orders of magnitude for the HALOE instrument. The representativeness error variance values are comparable in size with the data repeatability measure obtained in the evaluation of UARS data (Roche et al. 1996; Park et al. 1996).

Despite the use of a simplified two-dimensional transport model with no chemical sources and sinks, the size of the model error variance is such that it takes 14 days of forecast to double the initial error variance, or to increase the variance by a size comparable to the observational error variance. However, in the CLAES assimilation, the effect of model error becomes critical much earlier. After three days of assimilation using a perfect model assumption, $\bar{Q} = 0$, the forecast error variance is half the forecast error variance obtained with model error covariance. It thus appears that accounting for model error covariance is more important and critical in assimilations than in pure forecasts.

The assimilation of CLAES CH₄ reveals an analysis field that has much stronger mixing ratio gradients than with the gradients obtained from transport only, particularly along the subtropical edge and the polar vortex edge. The forecast error variance at the observation locations reduces in time and reaches a nearly stationary value about an order of magnitude smaller than the initial error variance or the observational error variance, which are of comparable size. The saturation in variance is a result of including the model error covariance in the Kalman filter. The forecast error correlation in the observed region displays very similar patterns to that of the error correlation in pure forecast mode, except that the correlation length scales are smaller in the assimilation mode.
The assimilation of HALOE observations, which involves much fewer observations than CLAES’s, was compared to the assimilation of CLAES observations used as the control. The ability to accurately reconstruct the mixing ratio field in the region not observed by HALOE depends not only on having a covariance evolving assimilation scheme but also on using the appropriate covariance models and tuned parameter values for the initial, model, and observational errors. The analysis corrections due to subtropical observations were found to be highly anisotropic and for those observations in the surf zone yielding corrections throughout the whole middle latitudes. In most instances, the analysis corrections contribute to reinforcing the mixing ratio gradients. However, due to the model error covariance, the effect of the observations on the forecast error variance remains centered around the most recent observations, although excursions over large distances are noticed.

An assessment of separately evolving the error variance and the error correlation for chemical tracer problems was conducted by varying the Kalman filter algorithm in three different ways: 1) prescribing both the error variance and the error correlation, as in the statistical interpolation scheme; 2) prescribing only the error correlation and evolving the error variance, known as the variance evolving scheme; and 3) prescribing the error variance and evolving the error correlation, similar to a statistical interpolation scheme with flow-dependent error correlations. These schemes have tunable parameters of their own, and after tuning we found with an assimilation of CLAES observations that the statistical interpolation scheme can only reduce the error variance to 1/5 of the initial value or of the observational error variance. The variance evolving scheme produced a similar reduction of variance. Enhanced performance was obtained with the correlation evolving scheme where the error variance became close to that of the Kalman filter. Similar experiments were conducted with HALOE observations and showed that only schemes that evolve the error correlation had some success in capturing the wave breaking event. We conclude that the advection of variance plays only a marginal role in improving the performance of trace constituent assimilation systems. Rather, the primary mechanism for optimality lies in flow-dependent error correlations. They create instantaneous spatial corrections, reducing further the variance over the observed region and extending the region of influence of the observations. These results suggest that, in effect, the information content in the error correlations is far greater than in the error variances.

An assessment of the covariance modeling for the initial, model, and representativeness errors showed that the relative error formulation improves the forecast error variance over a scheme that uses uniform error variance. No significant improvement, as measured by the error variance, was detected between experiments conducted with FOAR and SOAR correlation models. We argue that the choice of a correlation model should primarily be based on the desired spectral characteristic of the analysis correction.

An assimilation experiment using the standard Kalman filter algorithm was also compared with experiments using our Kalman filter formulation, which uses the properties of the continuum covariance evolution problem. The results show that the variance loss described in section 3 of Part I does in effect degrade the performance of the standard Kalman filter algorithm in data assimilation. The numerical discretization error alone was found to be of a size comparable to the model error covariance obtained with our Kalman filter formulation, which now appears to be primarily due to physical modeling errors, that is, errors due to the winds, and errors due to physical and chemical effects neglected with our two-dimensional tracer transport model. We argue that the use of the continuum formulation for evolving the error covariance can substantially improve the performance of a Kalman filter system by eliminating the model error covariance due to numerical discretization.

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