Royal Netherlands Meteorological Institute
Ministry of Transport, Public Works and Water Management

Determining tropospheric ozone columns from space by assimilation of GOME-2 ozone profiles

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GOME-2 ozone profiles are assimilated with the TM5 chemical transport model using the Kalman filter technique. The tropospheric ozone column can be determined directly from the regular model output or by applying the "residual method". In the residual method the stratospheric ozone column is determined from the assimilation output and subtracted from the GOME-2 total ozone column product. The residual column is an estimate for the tropospheric column. The advantage of this approach is that you combine the actual measurement of the profile (which has limited vertical sensitivity) with the high resolution chemistry (reactions, source, sinks etc) of the chemical transport model.

1. Kalman filter

GOME-2 measurements and TM-5 model output are combined using a Kalman filter approach (figure 1 and equations 1 ∼ 7).

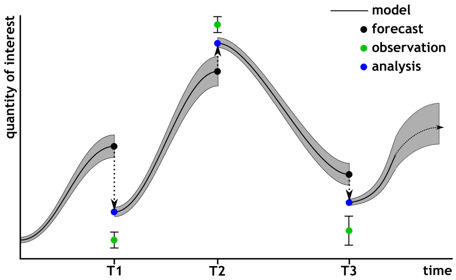

Figure 1: Sequential Kalman filtering. The black line illustrates the model output and the gray area the uncertainty of the model. Observations are indicated by the green dots with error bars. The value of the model result when an observation is available is called the forecast. A weighted average between the forecast and the observation is calculated. This weighted average is called the analysis. The analysis is used as a new starting point for the model calculations.

$$\begin{aligned}
\mathbf{x}_{i+1} &= M(\mathbf{x}_i) + \mathbf{w}_i, \quad \mathbf{w}_i \sim N(\mathbf{0}, \mathbf{Q}_i) && (1)\\
\mathbf{y}_i &= H(\mathbf{x}_i) + \mathbf{v}_i, \quad \mathbf{v}_i \sim N(\mathbf{0}, \mathbf{R}_i) && (2)\\
\mathbf{x}^f_{i+1} &= \mathbf{M}(\mathbf{x}^a_i) && (3)\\
\mathbf{P}^f_{i+1} &= \mathbf{M}\mathbf{P}^a_i\mathbf{M}^T + \mathbf{Q}_i && (4)\\
\mathbf{x}^a_i &= \mathbf{x}^f_i + \mathbf{K}_i\left(\mathbf{y}_i - \mathbf{H}_i\mathbf{x}^f_i\right) && (5)\\
\mathbf{P}^a_i &= (\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\,\mathbf{P}^f_i && (6)\\
\mathbf{K}_i &= \mathbf{P}^f_i\mathbf{H}^T_i\left(\mathbf{H}_i\mathbf{P}^f_i\mathbf{H}^T_i + \mathbf{R}_i\right)^{-1} && (7)
\end{aligned}$$

The covariance matrix $\mathbf{P}$ is too large to handle, its size is the number of elements in the state vector squared. For TM5 this amounts to $(120 \times 90 \times 44)^2$ elements. To reduce $\mathbf{P}$ to something more manageable we parameterize it into a time dependent standard deviation field and a constant correlation field.

The number of elements in a ozone profile (40 for OPERA) is generally much larger than the degrees of freedom (about 5 to 6). We therefore reduce the number of datapoints per profile by taking the singular value decomposition of the AK, and transforming the profiles accordingly. Since it is too costly to assimilate each OPERA pixel one by one, we assimilate a whole track at once.

Finally, we use an eigenvalue decomposition to calculate the $\left(\mathbf{H}_i\mathbf{P}^f_i\mathbf{H}^T_i + \mathbf{R}_i\right)$ matrix inverse in the Kalman filter equation. We truncate it at a number of eigenvalues representing about 98% of the original trace. In total, it takes about 35 hours to assimilate a whole month of data.

2. Results

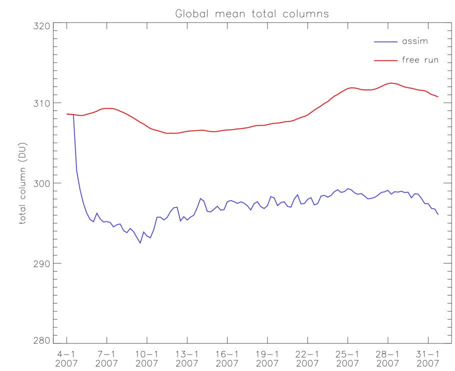

Figure 2: This is a time series of the free (red line) and assim (blue line) model runs starting at the fourth of January, 00 hours. The unit is the global mean total column in DU. Note that in the beginning both runs are exactly the same, this is because no ozone profiles were available until about 15 hours on January 4th. But as soon as ozone profiles are available, the global mean drops by about 15 DU with respect to the free model run.

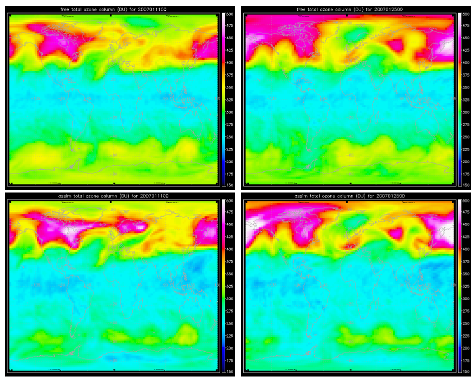

Figure 3: Shown here are two total column plots for each of the model runs, the free run on top and the assimilation run at the bottom. The left column is one week, and the right column is three weeks after the start of the assimilation. The most striking difference is the high ozone column over the south pole in the free run with respect to the assimilation run. This is caused by the model TM5. TM5 uses the Foruin-Kelder climatology to nudge the ozone profile. Since the Fortuin-Kelder climatology contains little ozone hole information, the predicted columns in the free run are higher than in the assimilation run.

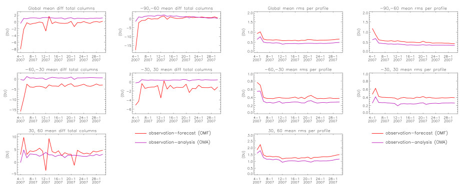

Figure 4: The left two columns show the OmF and OmA mean values. The right two columns show the global mean RMS between observation and forecast and observation and analysis. Both plots show that the analysis is closer to the observation than the forecast, which is to be expected.

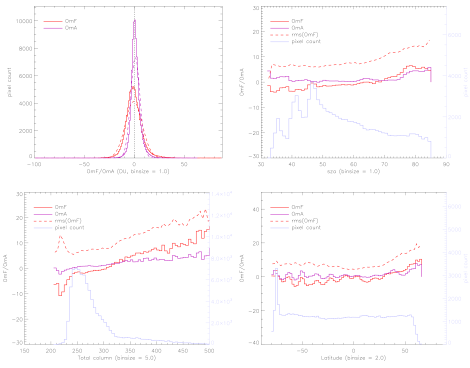

Figure 5: Top left: histogram of OmF and OmA. Both are normally distributed (dashed line is normal distribution with the same mean and sdev), and the OmA distribution is higher and smaller, indicating that observation and analysis are more alike than observation and forecast. OmF/OmA as a function of: SZA (top right), total column (bottom left) and latitude (bottom right).

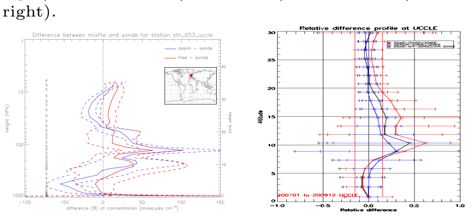

Figure 6: The left plot shows the relative difference between all sondes launched from Uccle in January 2007 and the model output. Please note that there are only five colocations between sonde and model. The right plot shows a picture that was kindly provided by Andy Delcloo, from the RMI in Belgium. They did a validation study for Gome-2 where they collected 3 years of data. It is clear that the OPERA profiles have difficulties in the UTLS region which will be translated into the assimilation process.

3. Conclusion

The assimilation system described here using the Kalman filter works as expected. The low ozone columns over Antarctica are present in the assim run, but not in the free run. The model is pulled towards the observations, the OmF and OmA are normally distributed, and there are no unexpected features in the plots of OmF/OmA against sza, total column or latitude. An improvement with respect to sondes could be made by including better quality OPERA profiles. In the future, we want to use the analysis profiles to calculate stratospheric column, assimilate data for a longer time period and perform a thorough validation study.

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