

# Supplementary Material: Coupled stratospheric chemistry-meteorology data assimilation. Part II: Weak and strong coupling

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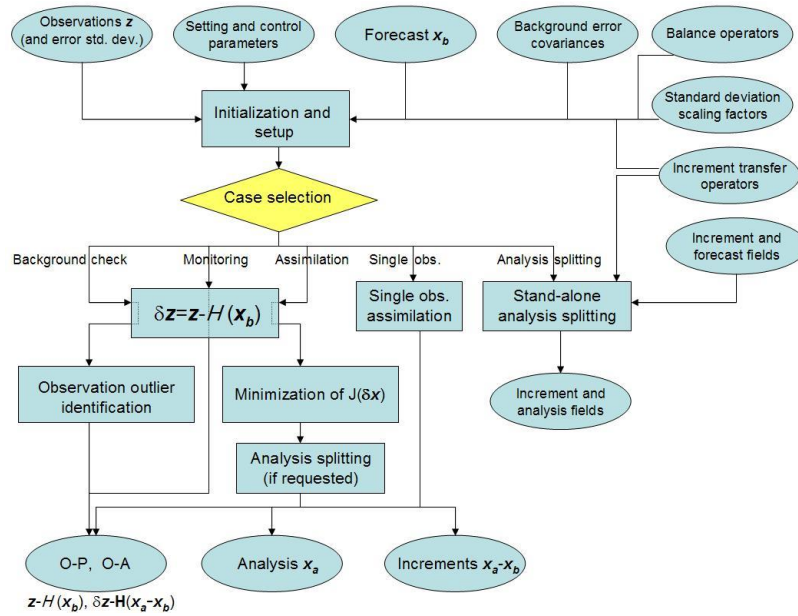
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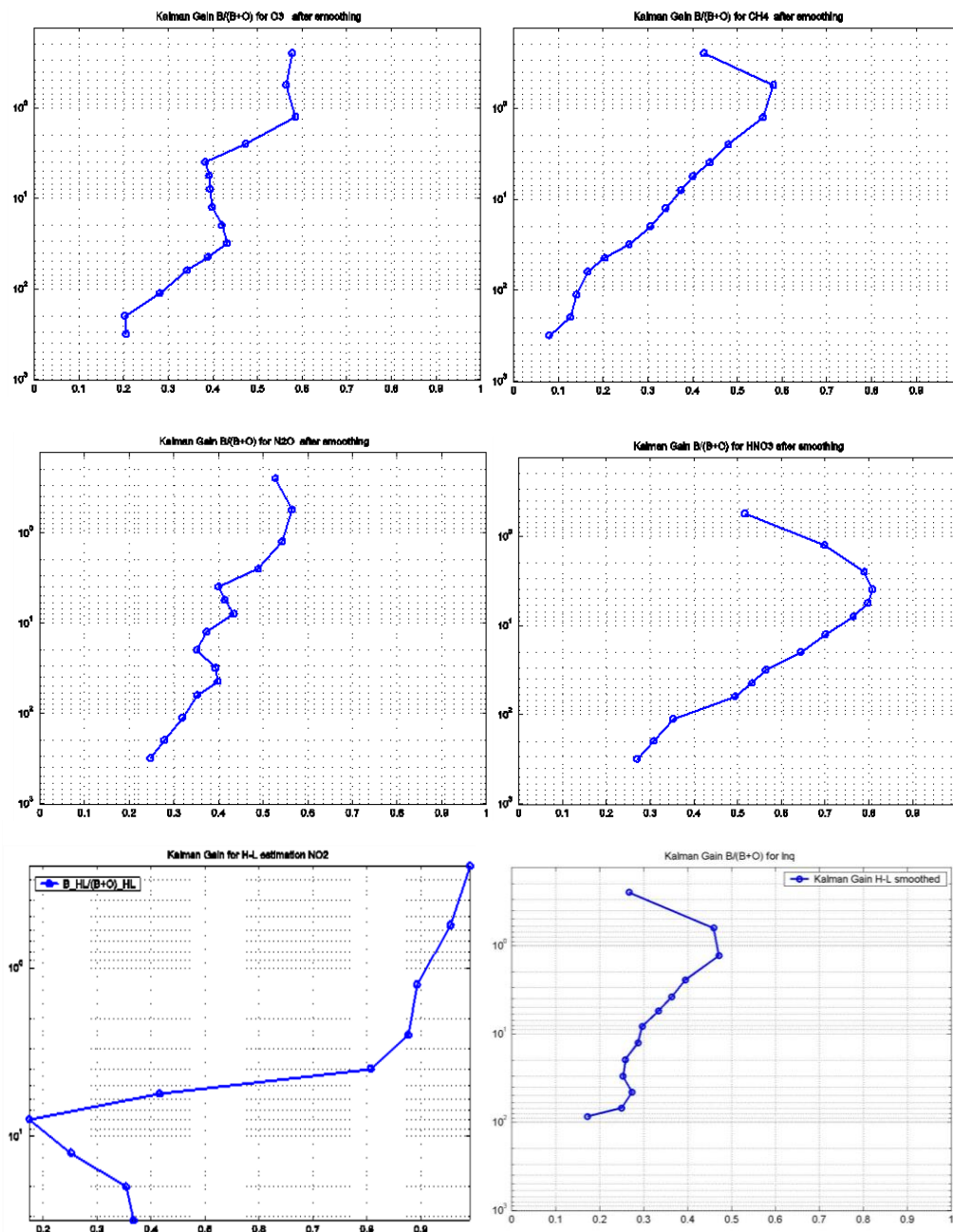
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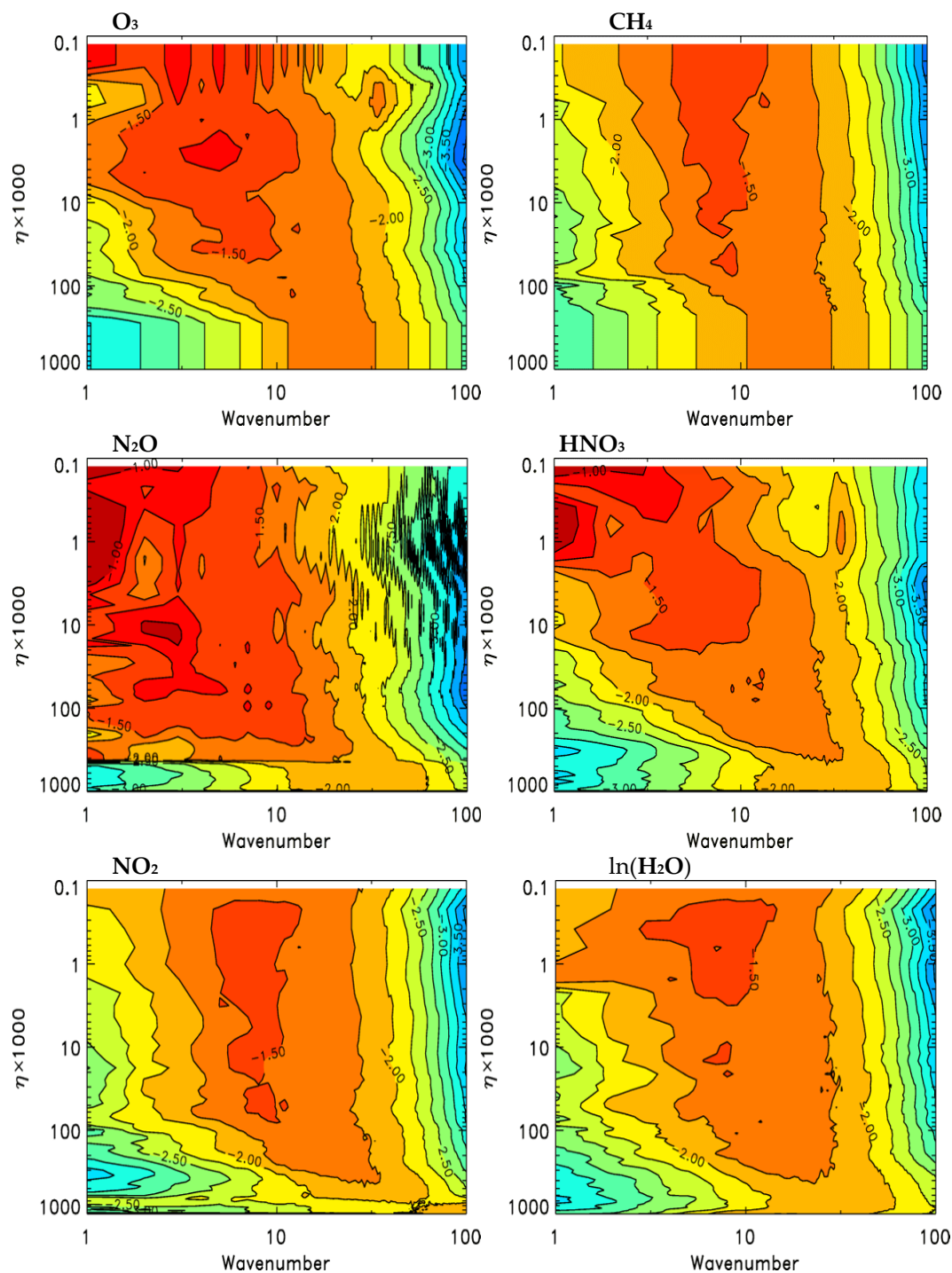
**Figure S1.** Flow chart covering the main steps and options of the 3D-Var-Chem.

Figure S1 provides a summary of some of the main steps and options of the 3D-Var-Chem, omitting here some of the various intermediate steps. As illustrated in this figure, the 3D-Var package can be used not just for (1) general assimilation but as well, and at least, for (2) identification of observation outliers (background check), (3) monitoring (determination of O-P only), (4) testing using single observation experiments, and (5) stand-alone analysis splitting. The term “analysis splitting” that is discussed below in greater detail refers to the process of

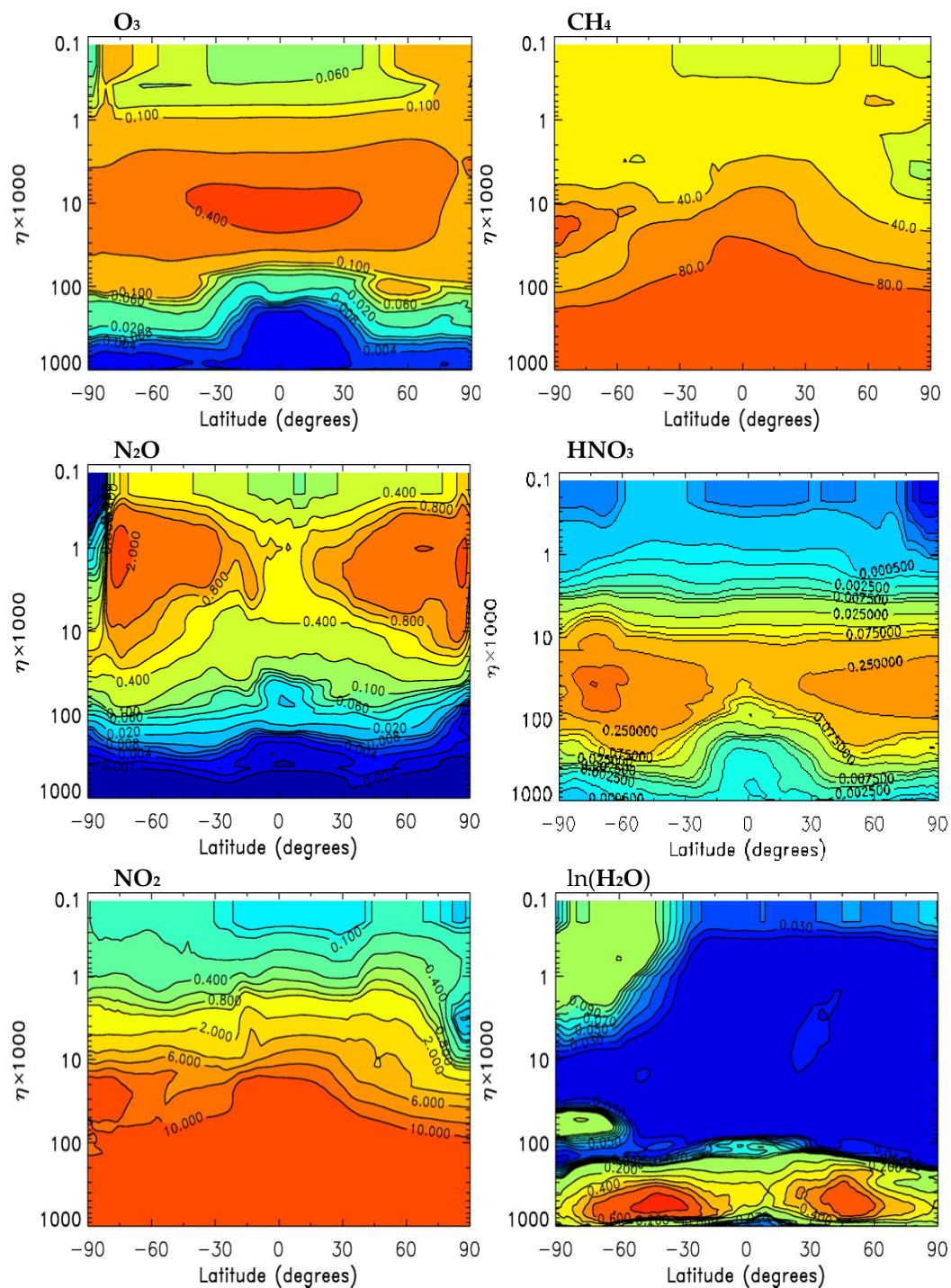
transferring increments for fields where observations were or are available to correlated model state fields for which observations are not available. This and the optional scaling of error standard deviations shown as part of the figure are two of the various features implemented as part of the 3D-Var-Chem.



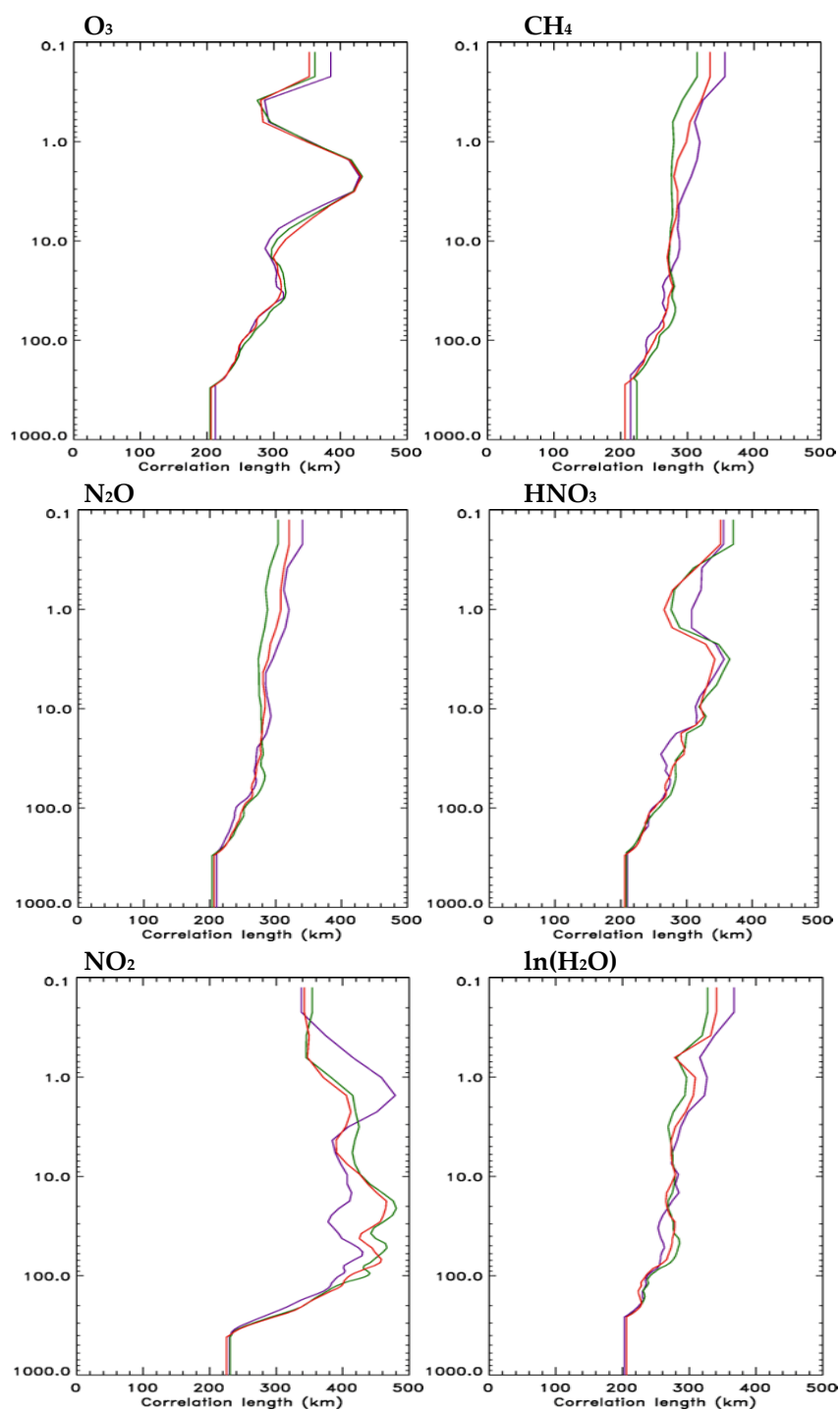
**Figure S2.** Scalar gain for  $O_3$ ,  $CH_4$  (from left to right) top row,  $N_2O$ ,  $HNO_3$  middle row and  $NO_2$  and logarithm of  $H_2O$  bottom row.



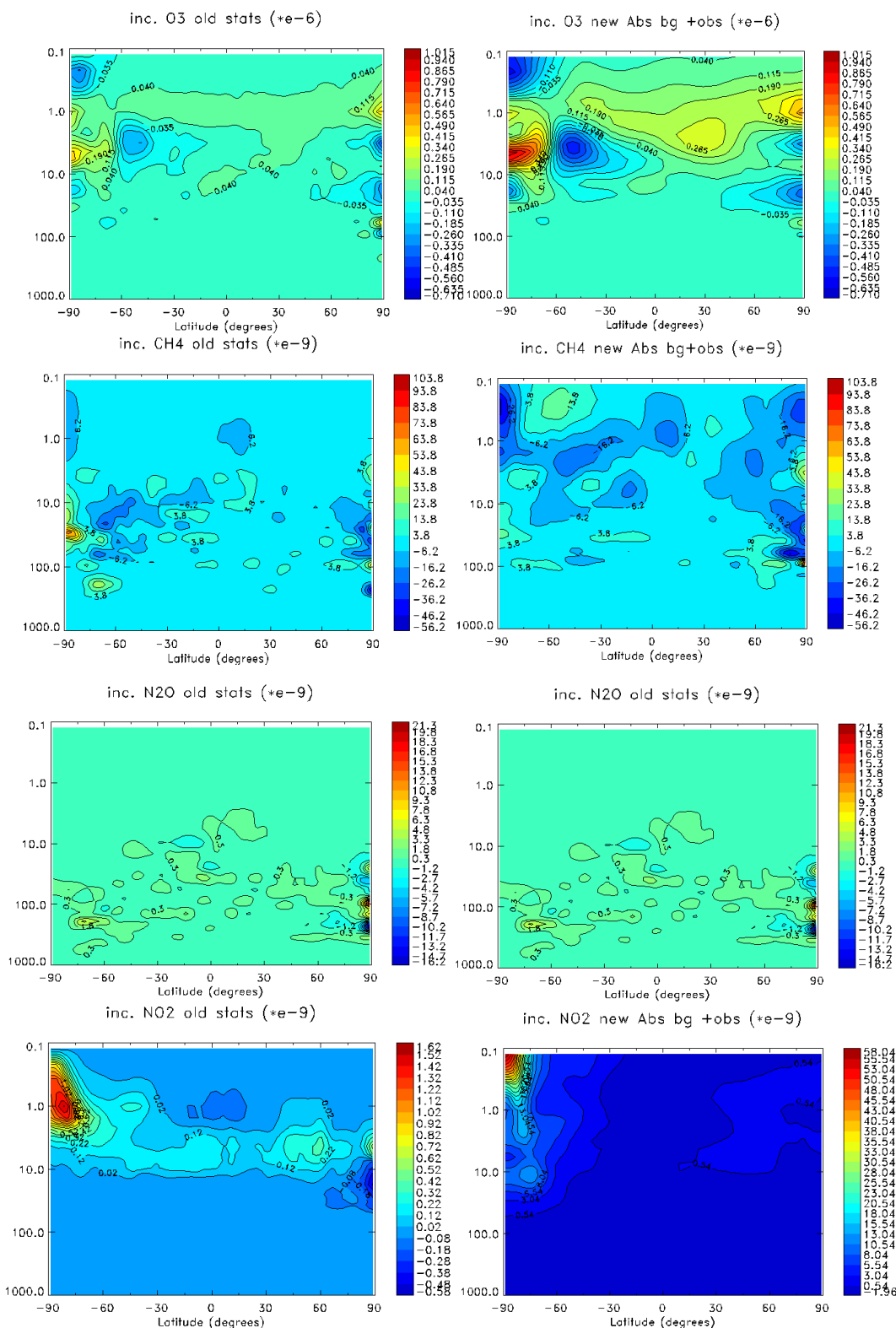
**Figure S3.** Background error correlation spectra from 6hr-difference method. From left to right, O<sub>3</sub> and CH<sub>4</sub> top row, N<sub>2</sub>O and HNO<sub>3</sub> middle row, and NO<sub>2</sub> and ln(H<sub>2</sub>O) lower row.



**Figure S4.** Background error variance from 6hr-difference method. From left to right, O<sub>3</sub> and CH<sub>4</sub> top row, N<sub>2</sub>O and HNO<sub>3</sub> middle row, and NO<sub>2</sub> and log(H<sub>2</sub>O) lower row.

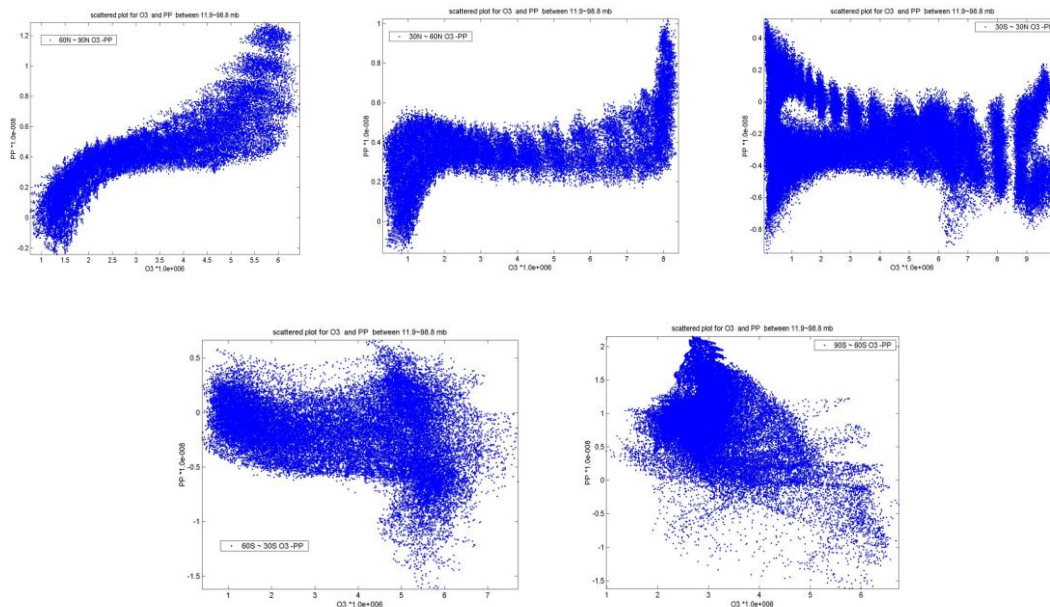


**Figure S5.** Horizontal correlation length. From left to right:  $O_3$ ,  $CH_4$  top row,  $N_2O$ ,  $HNO_3$  middle row, and  $NO_2$  and  $\ln(H_2O)$  bottom row.

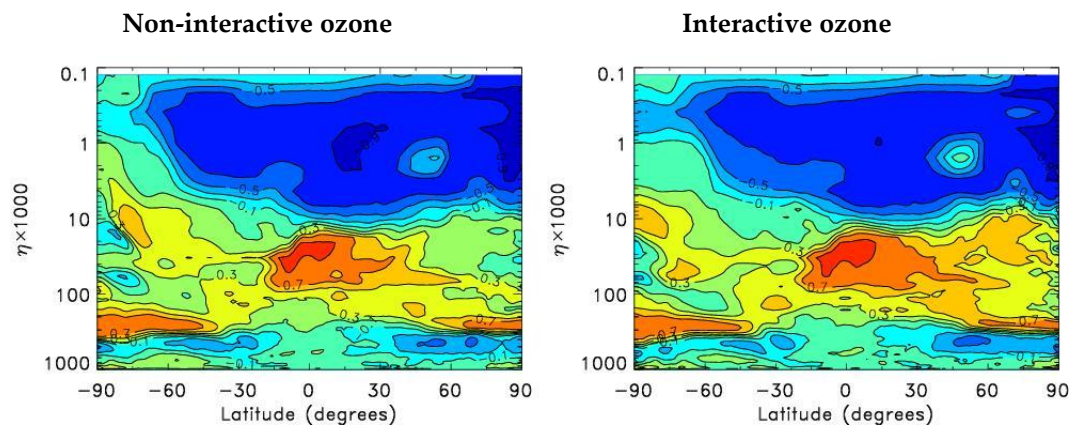


**Figure S6.** Mean analysis increment for O<sub>3</sub>, CH<sub>4</sub>, N<sub>2</sub>O, NO<sub>2</sub> (from top to bottom) for the period of August 17 to September 5, 2003. Left panel using the first guess or old error statistics. Right panel using the new error statistics consisting in CQC error correlation and HL error variances.



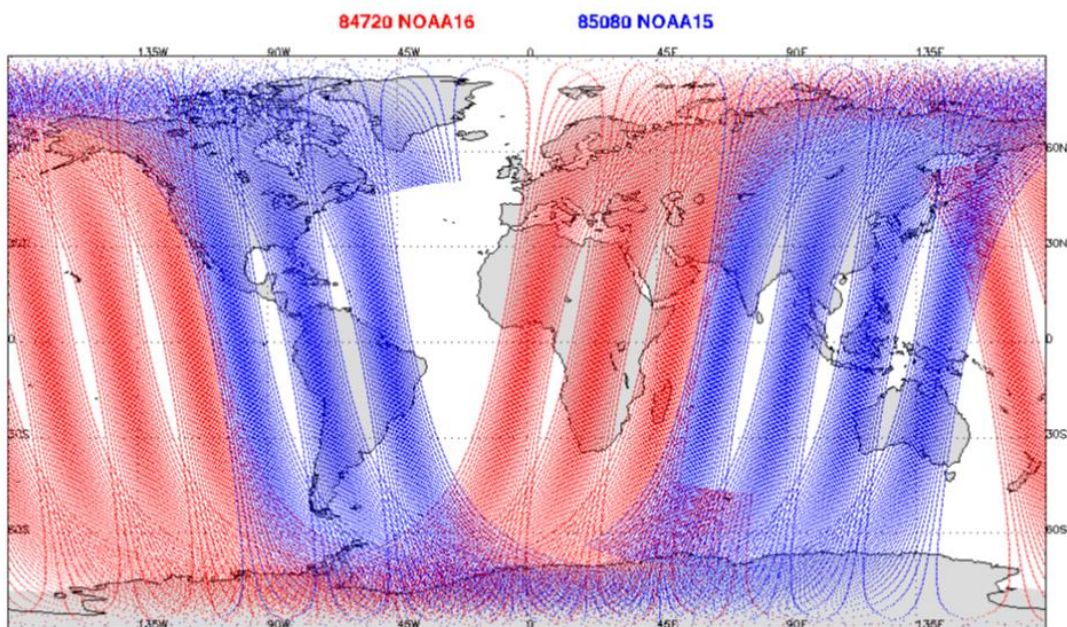


**Figure S7.** Scatter of O<sub>3</sub> and streamfunction values between 10 and 100 hPa for the month of March 2003.



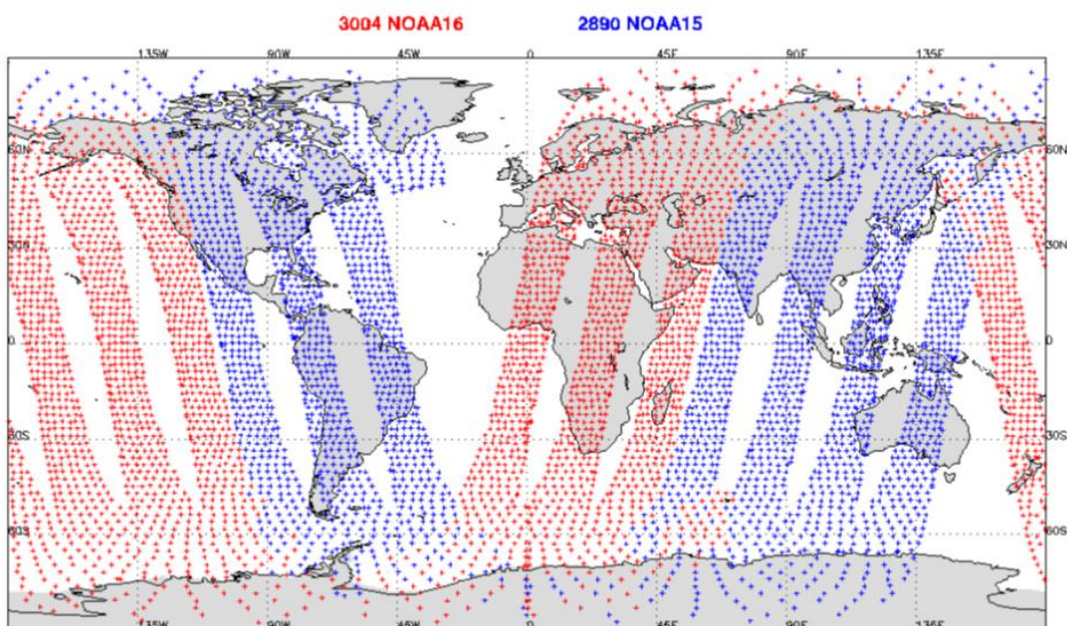
**Figure S8.** Cross-correlation between ozone and temperature derived from the 24-hr difference (i.e. CQC) method for July 2003. Left panel is for a non-interactive ozone-radiation run of GEM-BACH and right panel for an interactive ozone-radiation run.

# ATOVS Observations decoded



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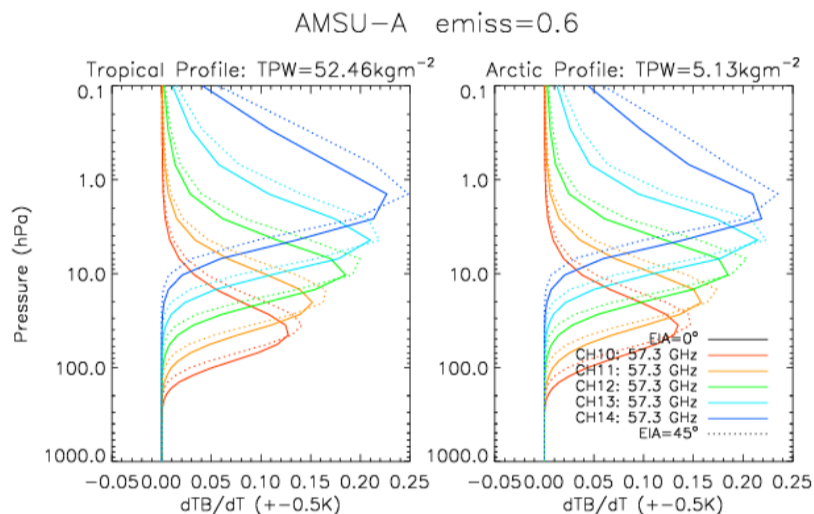
## ATOVS Observations after thinning



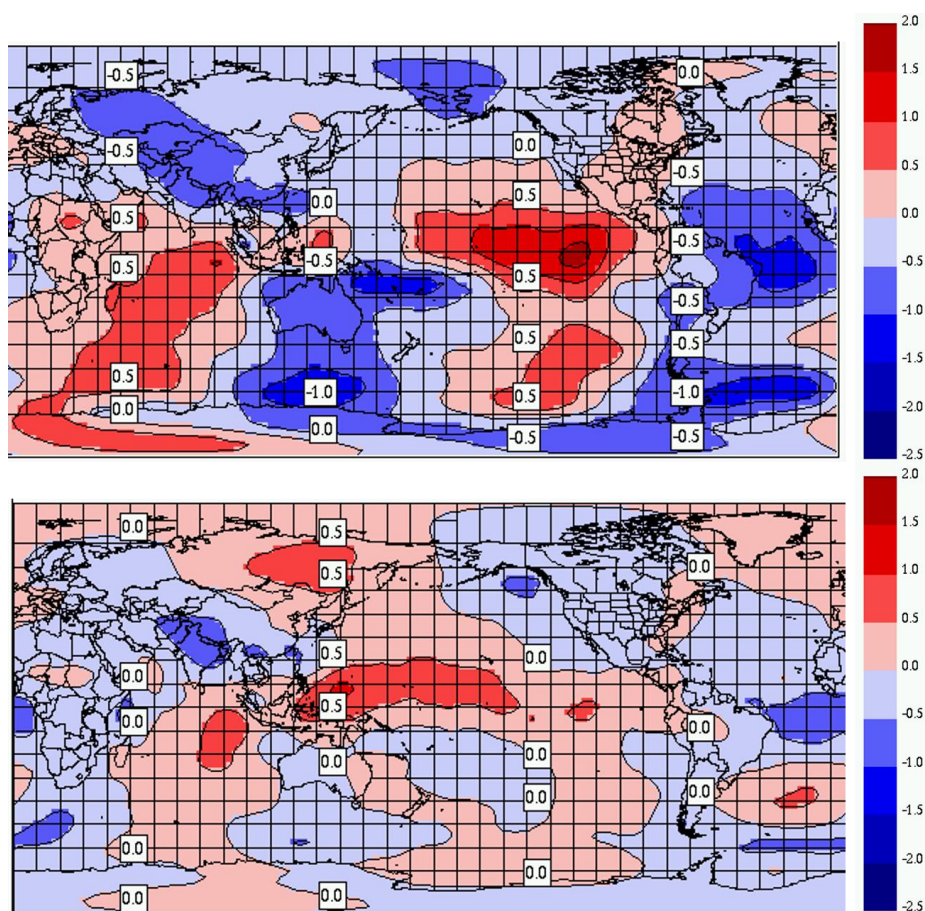
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**Figure S9.** Horizontal coverage of AMSU-A profiles in 6 hours. Upper panel are all profiles, lower panel are the thinned profiles used for data assimilation.

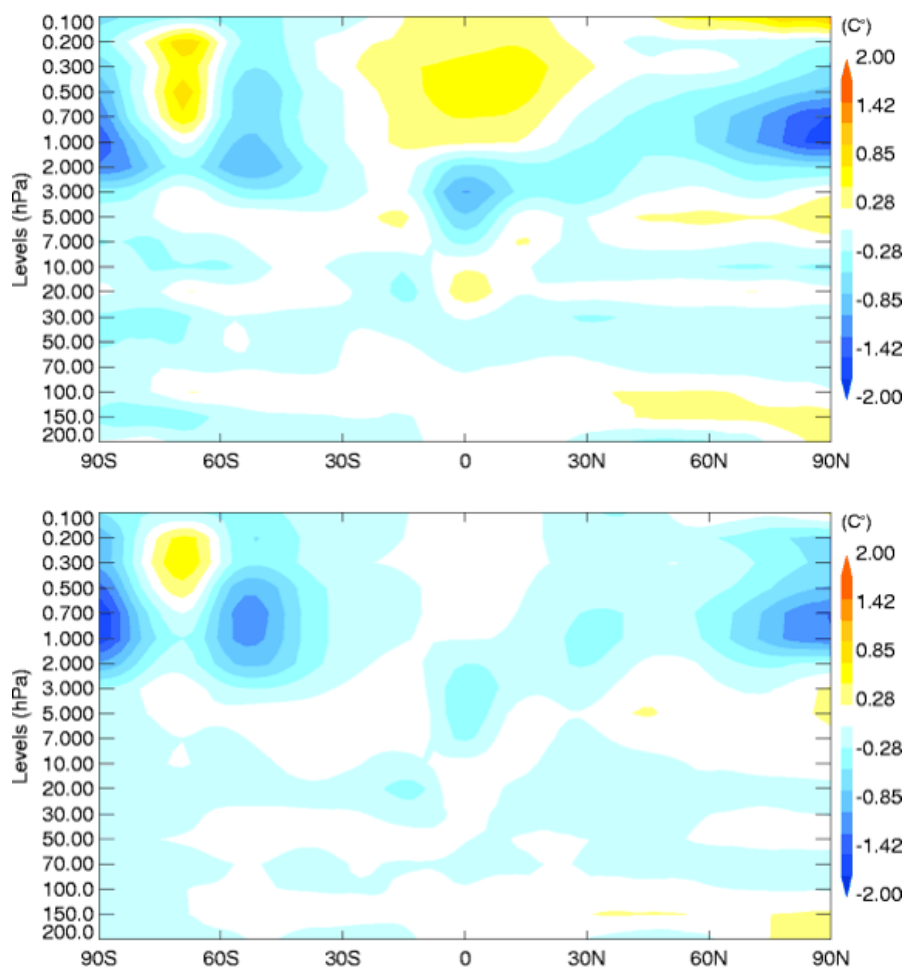




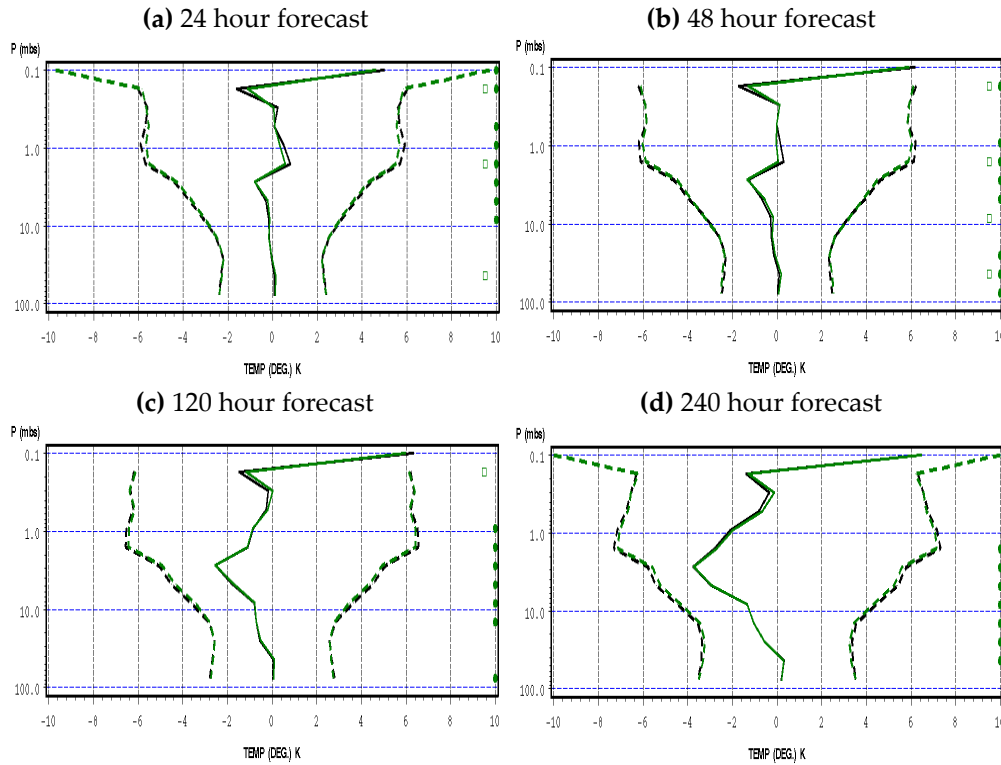
**Figure S10.** Sensitivity matrix of brightness temperature over temperature for channels 10-14 of AMSU-A. Left are profiles for Tropical air mass, right profiles for Arctic air mass. Solid curves are for nadir measurements and dotted lines



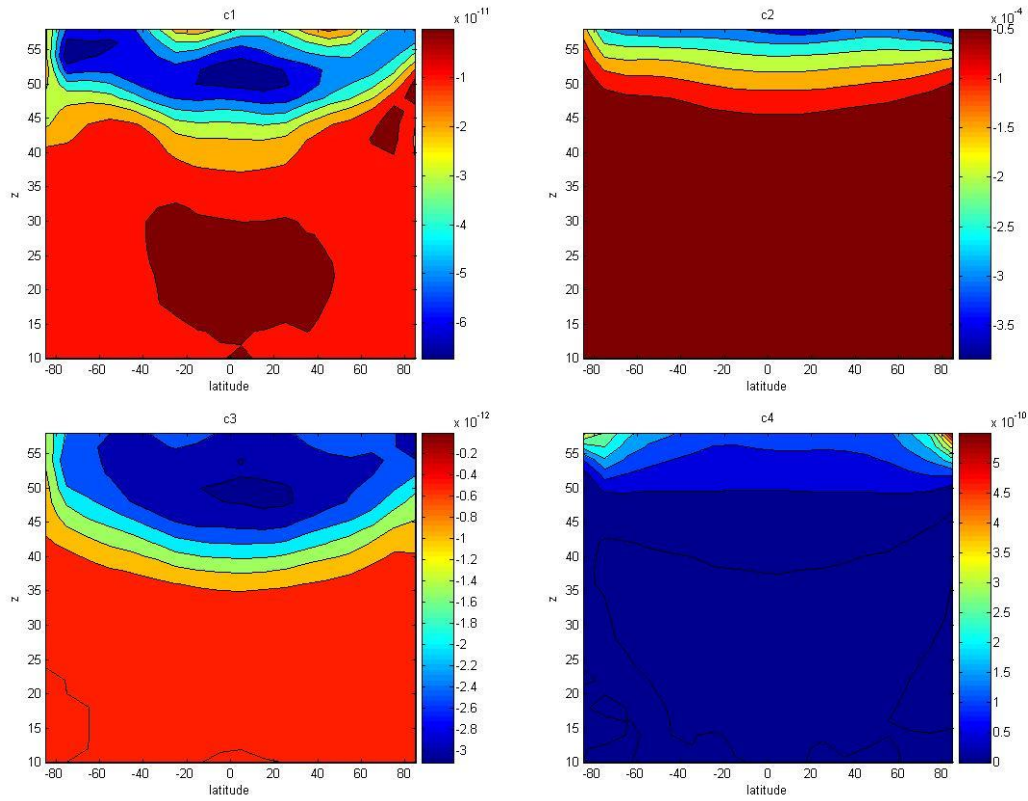
**Figure S11.** Mean analysis increment at 10 hPa for the month of September 2003. Upper panel using the standard AMSU-A bias correction. Lower panel using the new AMSU-A bias correction based on assimilation of MIPAS temperature only in the stratosphere.



**Figure S12.** Zonal mean analysis increment for September 2003. Upper panel using the standard AMSU-A bias correction. Lower panel using the new AMSU-A bias correction based on assimilation of MIPAS temperature only in the stratosphere.

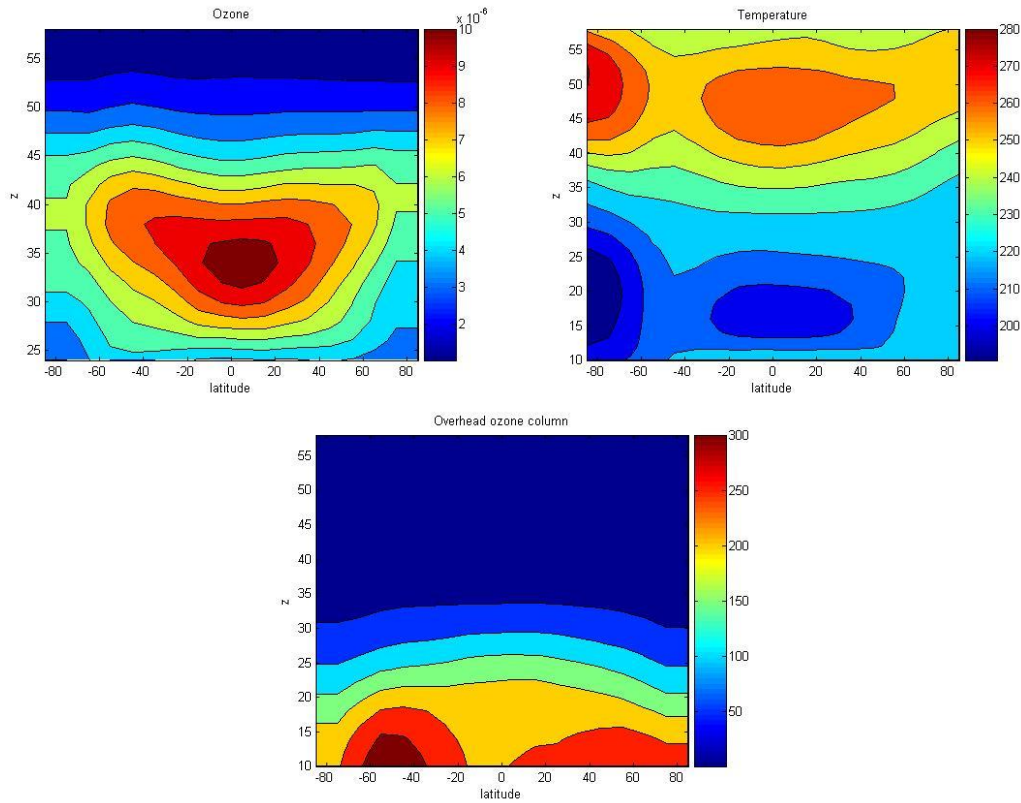


**Figure S13.** Global verification of observation-minus-forecast temperatures for different forecast lead time. In green, is the assimilation of MIPAS temperatures and AMSU-A with no stratospheric channels, and in black is the assimilation of MIPAS temperatures with all the AMSU-A channels. Verification is made against MIPAS temperatures. Panel (a) is the verification using a one day forecast, panel (b) a two day forecast, panel (c) a five day forecast, and panel (d) a 10 day forecast.

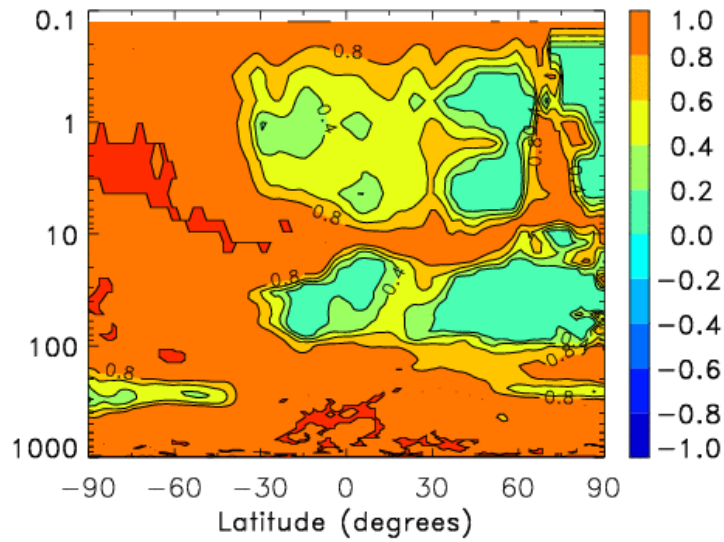


**Figure S14.** Coefficients of the LINOZ scheme for September. Upper left panel  $c_1$  ( $10^{-11}$  volume mixing ratio  $s^{-1}$ ), upper right panel  $c_2$  ( $10^{-4} s^{-1}$ ), lower left panel  $c_3$  ( $10^{-12}$  volume mixing ratio  $^{\circ}K^{-1}$ ), lower right panel  $c_4$  ( $10^{-10}$  volume mixing ratio  $DU^{-1}$ ). The pressure altitudes (km) are  $z = 16 \log_{10}(10^5/p)$  where the pressure  $p$  is in Pa





**Figure S15.** LINOZ climatology for September. Ozone in the upper left panel (units  $10^{-8}$  volume mixing ratio), temperature in the upper right panel ( $^{\circ}\text{K}$ ), overhead ozone column in the lower left panel (units DU).



**Figure S16.** Ratio of unexplained variance to the total variance for the balance operator  $\mathbf{A}^{CQC-NMC}$ .

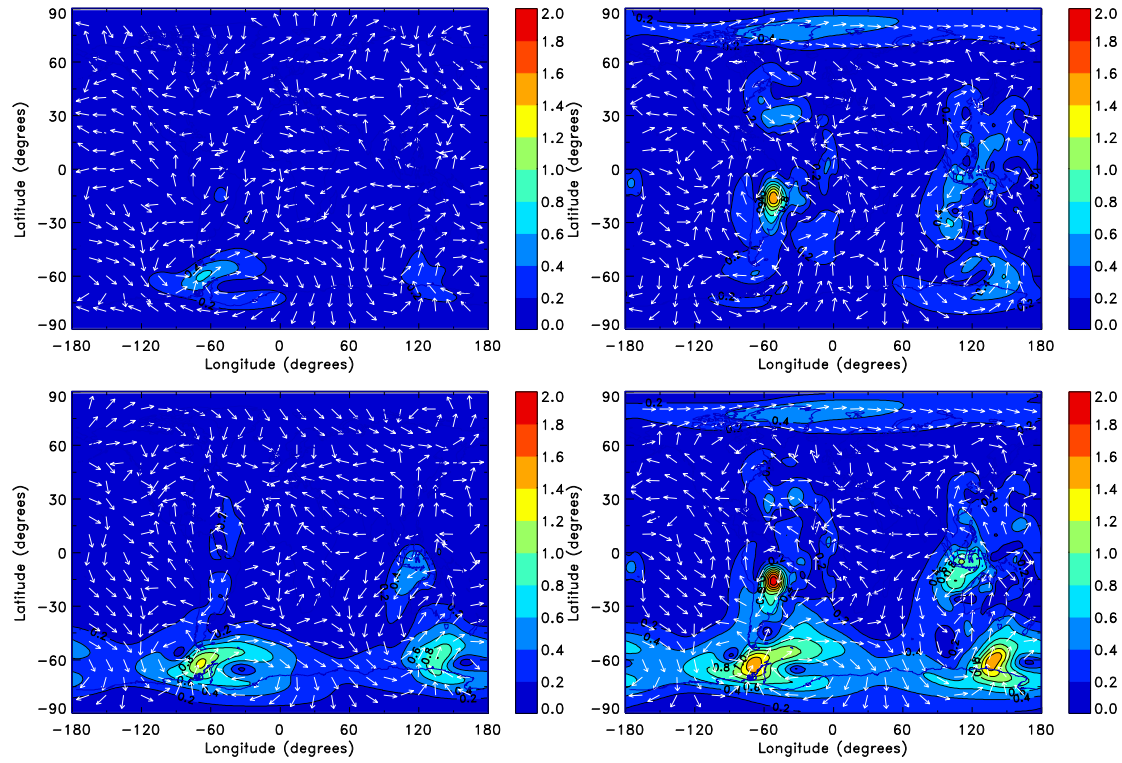


Figure S17. Same as Figure 19 but at 50 hPa

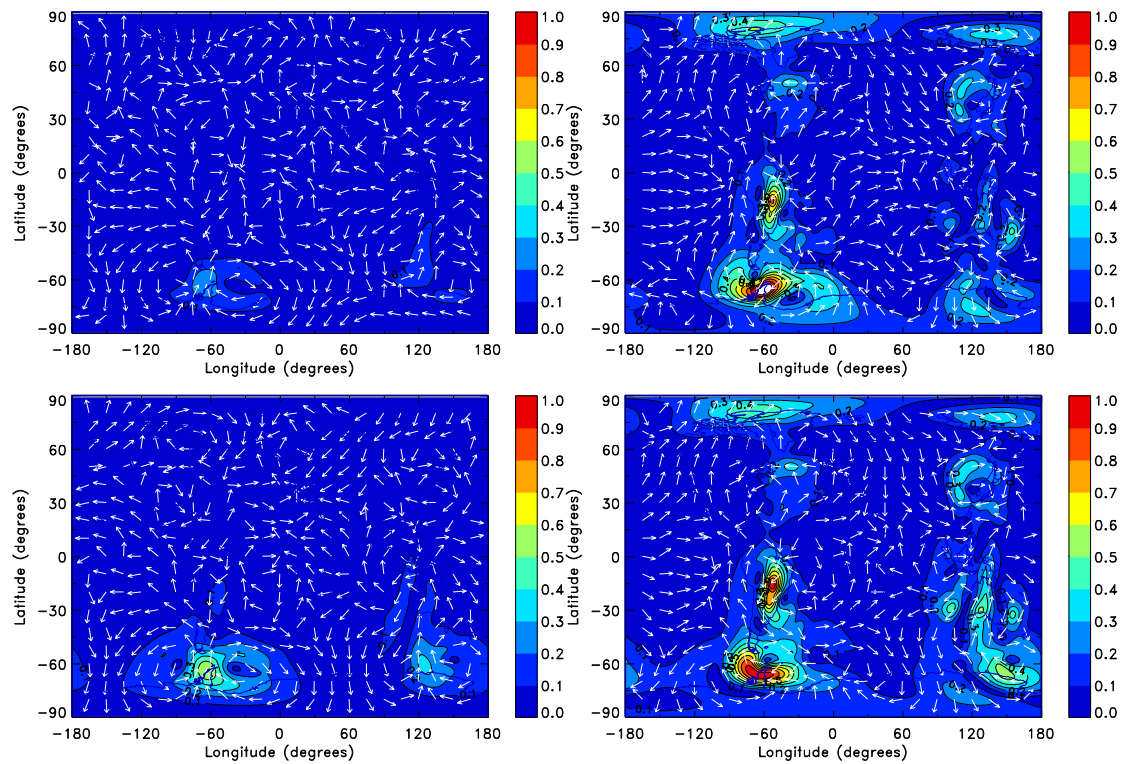
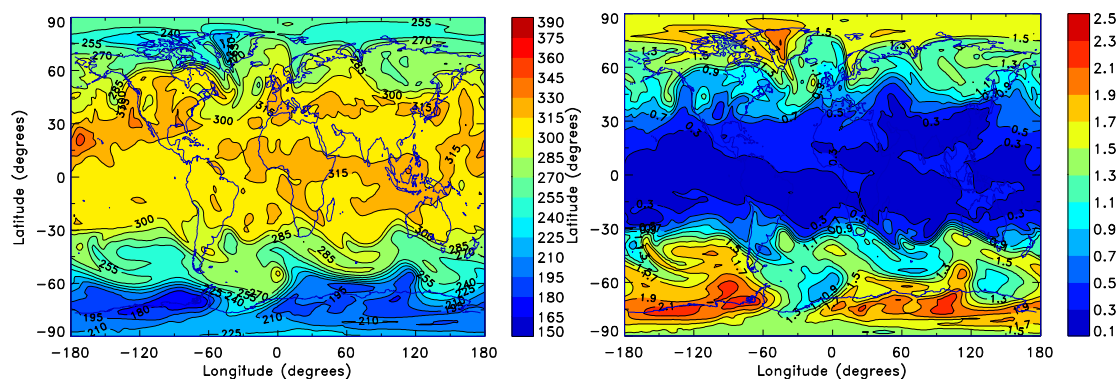
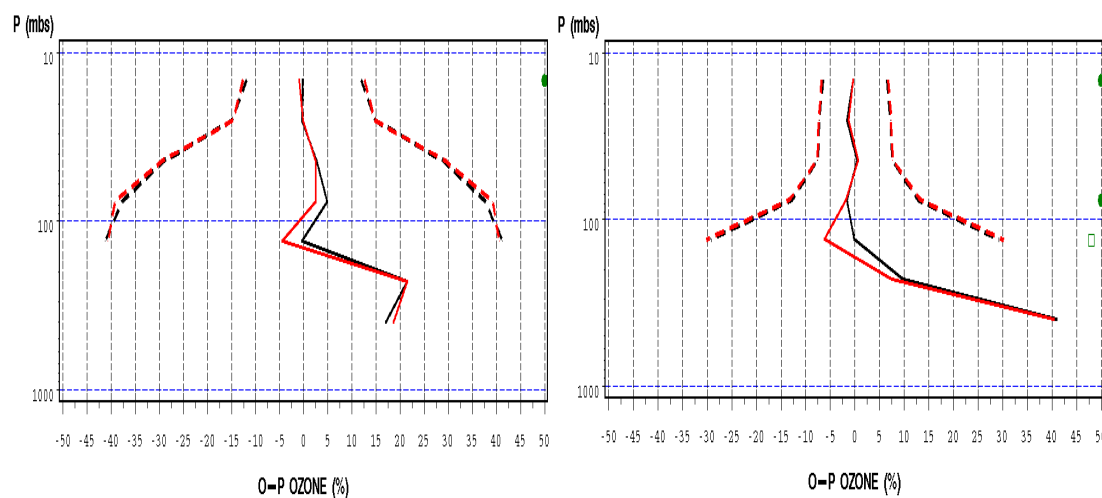


Figure S18. Same as Figure 19 but at 100 hPa



**Figure S19.** Analysis of N<sub>2</sub>O (left panel) and O<sub>3</sub> (right panel) at 100 hPa on August 11, 2003, 00 UTC.



**Figure S20.** OmP ozone comparison against MIPAS for the 3D-Var assimilation cycle (black) and 4D-Var (red) for the period September 20 to October 5, 2003 over the South Pole region (left) and Southern Hemisphere mid-latitudes (right).