

Article



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

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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



Figure S2. Scalar gain for O₃, CH₄ (from left to right) top row, N₂O, HNO₃ middle row and NO₂ and logarithm of H₂O bottom row.



Figure S3. Background vertical error correlation power spectra from 6hr-difference method. These spectral correlations are directly derived from a spherical harmonics representation of the 6-hr difference field, expressed in terms of (n,m), where n is the total wavenumber plotted in the abscissa, and m the zonal wavenumber [62]. The statistics is obtained by averaging over all zonal wave numbers m and over time. Thus the spectral vertical correlation for total wavenumber n, is

$$C_n(\eta,\eta') = \frac{1}{2n+1} \sum_{m=-n}^n c_n^m(\eta,\eta') c_n^{-m}(\eta,\eta') \text{ with } c_n^m = \left\langle \tilde{\psi}_n^m(\eta) \tilde{\psi}_n^m(\eta') \right\rangle, \quad \tilde{\psi}_n^m = \left(\psi_n^m - \left\langle \psi_n^m \right\rangle \right) / \sigma_n^m$$

where the bracket denoted the time mean and η is the model hybrid vertical coordinate which matches pressure in the stratosphere. What is plotted is $\log_{10} C_n(\eta, \eta)$, the spectra of the vertical correlation. From left to right, O₃ and CH₄ top row, N₂O and HNO₃ middle row, and NO₂ and ln(H₂O) lower row.



Figure S4. Background error variance from 6hr-difference method. From left to right, O₃ and CH₄ top row, N₂O and HNO₃ middle row, and NO₂ and log(H₂O) lower row.

-90

-60

0

Latitude (degrees)

30

60

90

-30

-90

-60

-30 0 30 Latitude (degrees)

60

90



Figure S5. Horizontal correlation length. From left to right: O₃, CH₄ top row, N₂O, HNO₃ middle row, and NO₂ and ln(H₂O) bottom row.



Figure S6. Mean analysis increment for O₃, CH₄, N₂O, NO₂ (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_3 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 24hr 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 interactice ozone-radiation run.



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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 Arctice 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.

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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 °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

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Figure S15. LINOZ climatology for September. Ozone in the upper left panel ozone (10⁸ volume mixing ratio), temperature in the upper right panel (°K), overhead ozone column in the lower left panel (units DU).



Figure S16. Same as Figure 19 but at 50 hPa. Contour units are in m/s.



Figure S17. Same as Figure 19 but at 100 hPa. Contour units are in m/s.



Figure S18. Analysis of N₂O (left panel) and O₃ (right panel) at 100 hPa on August 11, 2003, 00 UTC.



Figure S19. 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).



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