Imbalances of non-observed species in variational chemical data assimilation: implications for model assessments?

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Introduction

Four-dimensional data assimilation is a convenient and effective tool to retrieve information on non-observed trace gases. In the stratosphere, this method has been shown to give reliable estimates for ozone and related species based on sparse satellite observations. However, using the SACADA assimilation system, which produces daily chemical fields for the EU MACC project (http://www.gmes-atmosphere.eu), a detailed comparison to independent data has shown that chemical imbalances can deteriorate non-observed species. Here, we present global findings for MIPAS-SACADA and MIPAS-BASCOE analyses for 2003. Comparisons to HALOE, SAGE-2 and ozone soundings show that the Fractional Gross Error for ozone is in general smaller than 15%. Here, we present results of a sensitivity study for October 2003 with respect to assimilated species are analyzed to identify critical species and chemical interactions. We discuss briefly possible implications for the assessment of stratospheric chemistry results based on assimilation models.

Results

Figures below show results of assimilation experiments for with different number of input species. In experiment no. 7 only MIPAS ozone has been assimilated during October 2003 to investigate the impact of source gases H2O and CH4 on reactive species. In the upper stratosphere, when the assimilation of non-ozone species is stopped, H2O rapidly changes (figure 3) with increasing mixing ratios in the southern hemisphere. In the same area, as figure 2 shows, HCl values are also increasing compared to the reference run (assimilation of all MIPAS ESA species). At the end of October, experiment no. 7 shows much higher HCl mixing ratios both in the upper and lower stratosphere of south of approx. 50° S. Changes are mostly pronounced below 10 hPa in the area of the south polar vortex. No HCl deficit is found in MIPAS-BASCOE results. A comparison and evaluation of the respective chemical reactions and their implementation will be part of the MACC-II project starting late in 2011.

Discussion

SACADA results show a strong HCl deficit in the upper stratosphere when all MIPAS ESA species are assimilated. Analysis hints to the assimilation of H2O increasing background concentrations. Whereas effects within the southern polar vortex are clearly linked to heterogeneous reactions (changes also visible in HNO3 and CH4), gas phase reactions (rate constants and reaction channels) probably lead to imbalances above approx. 10hPa in high latitudes. Results show that non-assimilated species are strongly influenced by assimilated species. It is therefore important to compare all chemical related model species when evaluating model results.

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Models and Assimilation Experiments

Assimilation Models	**BASCOE 4.0** [Errera et al., 2010]	**SACADA 2.0** [Elbern et al., 2010]	**Comments**
Coverage/Resolution	37 layer, 0-65km 5° x 3.75° lon-lat grid *hybrid level*	32 layer, 6-65km 250km isocahedron grid *hybrid level*	stratospheric chemistry only lat-lon versus icosaeder grid
Chemistry •*reaction rates* •*photolysis rates* •*source gases*	 *JPL14-2003* *Madronich and Flocke, 1998* *CFC11,CFC12, CH3Br,etc.*	 *JPL15-2006* *Smith, 2007* *CFC11,CFC12,CH3Br,etc.*	 *JPL16 with minor changes* *(see figure below)*
Het. chemistry	Aerosols, Ice, NAT	Aerosols, Ice, NAT, STS	SACADA without sedimentation
Advection	Lin and Rood, FFSL	semi-Lagrange	
Meteo analysis	ECMWF ERA40/ECA	ECMWF ERA40/ECA	
Data assimilation	4D-Var	4D-Var	
Assimilation Data	MIPAS ESA 4.61	MIPAS ESA 4.61	
analysis period *assimilated species*	Apr 2003 – Dec 2003 *O3, H2O, HNO3, CH4, N2O, NO2*	Apr 2003 – Dec 2003 *O3, H2O, HNO3, CH4, N2O, NO2*	reference run (Exp1)
analysis period *assimilated species*		Apr 2003 – Dec 2003 --	free run (Exp2)
analysis period *assimilated species*		Oct 1st – Oct 31, 2003 *ozone*	ozone only run (Exp7)

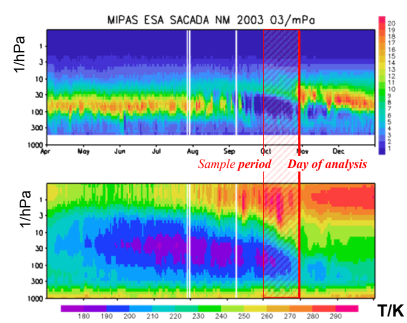

Figure 1: Ozone partial pressure and temperatures above Neumayer Station (ca. 71°S, 8°W) from April to December 2003 as analyzed by MIPAS-SACADA and ECMWF ERA40. The shaded area indicates the sample period used for the additional assimilation experiments 8 and 7. Results presented in this paper are valid for 12:00 GMT on October 28, 2003.

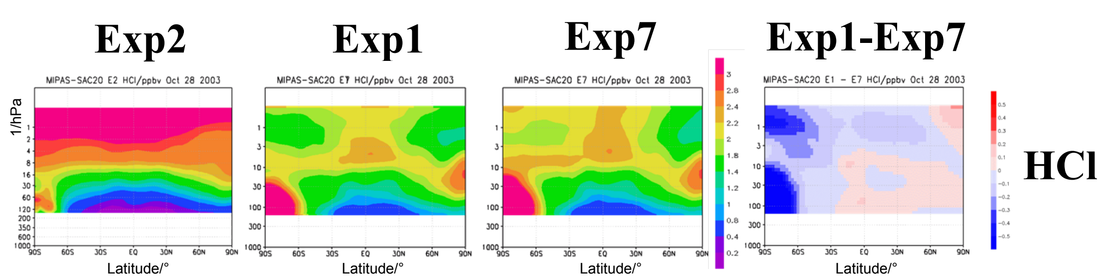

Figure 2: Zonal mean HCl mixing ratios between 146 and 0.3 hPa altitude based on assimilation experiments no. 1 and 7. Experiment no.2 results were derived without assimilation (free run). The plot on the far right side shows the differences between experiments no. 1 and 7, i.e. the impact of assimilating non-ozone species.

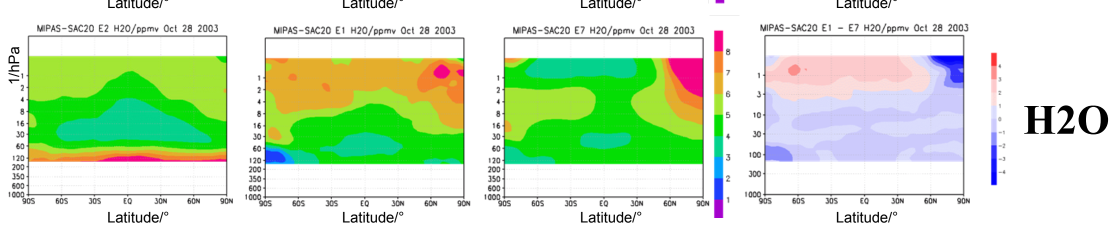

Figure 3: As figure 2 but for zonal mean H2O mixing ratios. Experiment no. 7 shows mainly the impact of *non-assimilating* H2O. Note the strong anti-correlation above 10 hPa with HCl differences of figure 2.

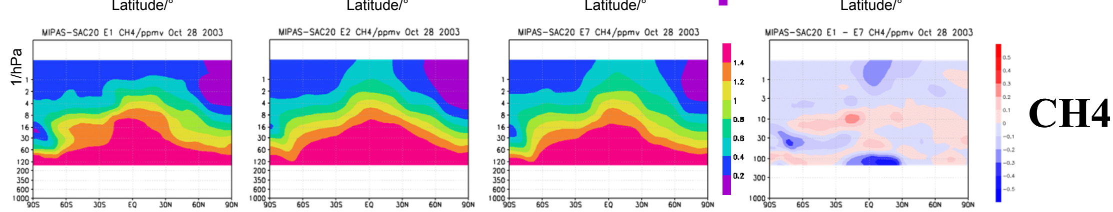

Figure 4: As figure 2 but for zonal mean CH4 mixing ratios. Compared to H2O, absolute changes of CH4 due to assimilation of non-ozone species are rather small. Most differences are found within the southern vortex and near the tropical tropopause.

Acknowledgement:
This study was funded by 7th EU Framework Program. We are grateful to all providers of model and observational data.

Data link:
MIPAS ESA: http://earth.esa.int/dataproducts

References:

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