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Impact of Interaction between Assimilated and Non-Assimilated Constituents – Assimilation Experiments with MIPAS Measurements

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Introduction

In chemical data assimilation, the assimilated species normally only represent a small subset of chemical variables in a GCCM (or CTM). These assimilated species interact with each other as well as with unassimilated constituents through model chemistry. The inconsistency between model and measurements disturbs the balances among species as dictated by model chemistry and a 'chemical shock' occurs adversely affecting model forecasts. One of the main sources of inconsistency between model and measurements is the processes that are not resolved or represented by the model.

We conducted a series of data assimilation experiments with a coupled dynamical-stratospheric chemistry model (GEM-BACH) and a 3-D variational assimilation (3D-Var) system with data retrieved from the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) instrument. The assimilation experiments coincides with a period of energetic particle precipitation (EPP). This provided a good opportunity to evaluate the response of the chemistry model as part of an assimilation system when faced with a situation where there is a significant mismatch between observations and model chemistry.

During EPP, highly energetic electrons and protons influence the production of odd oxygen (HOx) and active nitrogen (NOx=NO +NO2) which are transported down from the mesosphere to the upper stratosphere under favorable conditions of general circulation. This can affect ozone chemistry through chemical catalytic cycles. Evidence of high amounts of upper stratospheric/mesospheric polar NOx and anomalous values of HNO3 as measured by the MIPAS/ENVISAT mission have been documented in the recent literature (Funke et al., 2005, Stiller et al., 2005, Orsolini, 2006). GEM-BACH does not have a provision to simulate any geomagnetic effect and direct impacts caused by EPP resulting in larger than usual biases in error residuals between observation and model (OmP) in the absence of chemical assimilation. A. Robichaud et al. (2009, submitted to ACP) evaluated the spatial-temporal evolution of the first and second statistical moment of OmP of targeted chemical constituents in the mid and upper stratosphere/stratopause region (output from the same system as discussed in this work but with assimilation of a slightly different version of MIPAS retrieval data) with and without chemical assimilation and computed the ozone polar loss caused by EPP and subsequent SPE (solar proton event) in 2003. It shows that, by assimilating MIPAS data, the system can well compensate for the mismatch between observation and model due to processes not accounted for by the model. Also see this paper for a review of the processes and related publications.

Here we present results of univariate assimilations of MIPAS measurements of O3, NO3, HNO3 and CLONO2, either assimilated separately or in different combinations. This presentation will

- demonstrate the possible effectiveness of chemical data assimilation in compensating for the deficiency in model chemical and /or physical process,
- evaluate the impact of the assimilated species on non-assimilated species, and
- demonstrate the importance of proper combinations of species to be assimilated.

Model , Assimilation System and Data

A comprehensive global coupled chemical-dynamical general circulation model (CGCM) was developed relying on the stratospheric version of the Canadian GEM (Global Environmental Multi-scale) model and a comprehensive interactive stratospheric chemistry package developed originally at Belgium Institute for Space Aeronomy (BIRA). This is a result of a productive collaboration between research and operational institutions from Canada and Belgium on the project 'Coupled Chemical-Dynamical Data Assimilation' sponsored by ESA and lead by Dr. R. Ménard. The model has 80 vertical levels including 27 in the stratosphere and is integrated at a high horizontal resolution of 1.5° X 1.5° (a grid of 240X120) with a lid at 0.1 hPa. The applied 3D-Var-FGAT system is an extension of Environment Canada's operational 3D- and 4D-Var system (see Gauthier at al. 1999a and 1999b) with FGAT enabling assimilation of chemistry constituents.

The conventional dynamical (meteorological) assimilation was done in a separate run with error statistics built using the NMC method. The resulting dynamical fields are used to refresh the dynamics every 6 hours during the chemistry assimilation runs. The background error statistics for chemical species use correlations calculated from consecutive 6-hour forecast differences and background and observation error standard deviation derived using the Hollingsworth and Lonnberg (1986) innovation-based approach. MIPAS is a slow downward limb scan Fourier spectrometer which measures the complete spectrum of limb emission in the frequency interval 680-2410 cm^{-1} and offers a very good geographical and temporal coverage; a spectrum is acquired every 4.6 seconds at each of the 17 tangent altitudes giving about 1000 profiles per day from 68 km to 6 km with vertical resolution of 3 km in stratosphere but lower in the mesosphere. It provides day and night measurements pole to pole which allows investigating the Arctic and the Antarctic areas during the polar vortex season. Particularly interesting is the capability of observing at the same time HNO3 and NO2 in the polar night making possible the assessment of the evaluation of chemical transformation within the NOy family occurring during EPP events. Two versions of MIPAS retrieved profile datasets are available: one from the non-linear least square fit called Optimized Retrieval Model (ORM) and is referred to as MIPAS-ESA, the other from IMK (Institut für Meteorologie und Klimaforschug, at Karlsruhe, Germany) and is referred here to as MIPAS-IMK. For a description of both datasets and related literature please refer to Ménard et al. (2007) which also includes most of the interpretations indicated in this presentation. Both datasets are used in separate assimilation runs. Comparison of the results from MIPAS-ESA and MIPAS-IMK is beyond the scope of this presentation.

Abstract

The interaction between assimilated and non-assimilated constituents has been assessed using a coupled chemistry-dynamics 3-D variational data assimilation system. Profiles of stratospheric O3, NO2, HNO3 and ClONO2 retrieved from measurements of the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) instrument have been assimilated both separately and in different combinations. The analysis focused on use of MIPAS retrieval products from the "Institut für Meteorologie und Klimaforschung" (IMK) with references to results obtained using the operational MIPAS offline products. The study illustrates the implication of inconsistencies between measurements and the modeled photochemical processes in context of a distinct geomagnetic event EPP (energetic particle precipitation) during Antarctic winter 2003.

Results

1. Single-species assimilation

a. Assimilating O3 only

Without chemistry assimilation, model O3 has a huge deficit (positive OmP), especially at the upper stratosphere. This is corrected to some extent by increases in O3 volume mixing ratio through assimilating O3 measurements. Assimilating O3 does not have much impact on HNO3, NO3 or CLONO2.

Note for all the OmP plots in this presentation O refers to MIPAS-IMK measurement while P refers to 6-hour forecast from previous analysis valid at the same time.

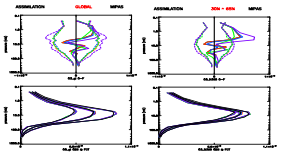

Fig.1a. Global average O3 results. **Upper panel**: mean (solid line) and std. dev (dashed line) of OmP. **Lower panel**: Mean and std. dev. of actual observations (black) and model 6-hr forecasts with assimilation of (1) MIPAS-IMK O3 as VMR (blue), (2) MIPAS-IMK O3 as overhead column densities OCD (red), (3) MIPAS-ESA O3 as VMR (green) and (4) no chemistry assimilation (purple).

Fig.1b. As in fig. 1a but for the mid-latitude northern hemisphere.

b. Assimilating HNO3 only

1) Improvement on HNO3:

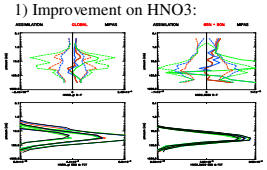

Fig. 2a. Global average HNO3 results. **Upper panel**: mean (solid line) and std. dev. (dashed line) of OmP. **Lower panel**: Mean and std. dev. of actual observations (black) and model 6-hr forecasts with assimilation of (1) MIPAS-ESA HNO3 as VMR (blue), (2) MIPAS-IMK HNO3 as VMR (red) and (3) no chemistry assimilation (green)

Fig. 2b. As in fig. 2a but for the north pole

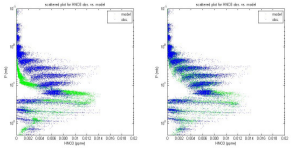

Fig. 3a. Scatter plot of HNO3 volume mixing ratios at the south pole from observations (blue) and model 6-hr forecasts without chemistry assimilation (green).

Fig. 3b. Same as fig. 3a but from observations (blue) and model 6-hr forecasts with HNO3 assimilation (green).

Assimilating HNO3 greatly reduces the deficit in the upper stratosphere and also reduces the surplus in the high troposphere/lower stratosphere to some extent. This is true for both the N.H. and S.H..

2) Impact on O3 and NO2 from assimilating HNO3

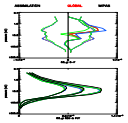

Fig.4. As in fig. 2a (global) but for O3.

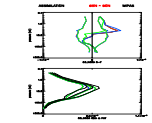

Fig. 4b. As in fig. 2b but for O3 at the north pole.

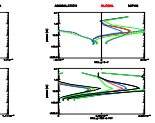

Fig. 5. As in fig. 3a (global) but for NO2.

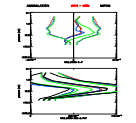

Fig. 5b. As in fig. 3b but for NO2 at the north pole.

Assimilating HNO3 significantly increases the upper stratosphere O3 deficit (depleting O3) in the N.H., including the north pole, but decreases the deficit in the S. H.. It also reduce surplus or create small deficit at high troposphere/lower stratosphere. On the other hand, assimilating HNO3 significantly improves NO2 forecast by reducing deficit in the whole stratosphere both at N.H. and S.H..

c. Assimilating NO2 only

1) Improvement on NO2:

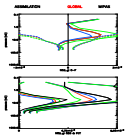

Fig. 6a. Global average NO2 results. **Upper panel:** mean (solid line) and std.dev (dashed line) of OmP. **Lower pannel**: Mean and std. dev. of actual observations (black) and model 6-hr forecasts with assimilation of (1) MIPAS-ESA NO2 as VMR (blue), (2) MIPAS-IMK NO2 as VMR (red) and (3) no chemistry assimilation (green)

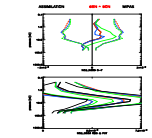

Fig. 6b. As in fig. 6a but for the north pole.

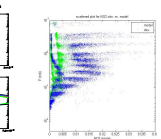

Fig.7a. Scatter plot of NO2 volume mixing ratio at the south pole from observations (blue) and model 6-hr forecasts without chemistry assimilation (green).

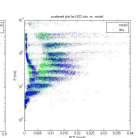

Fig. 7b. Same as fig. 7a but from observations (blue) and model 6-hr forecasts with NO2 assimilation (green).

2) Impact on O3 and HNO3 from assimilating NO2

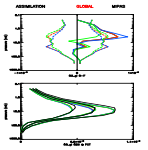

Fig. 8. As in fig. 6a (global) but for O3.

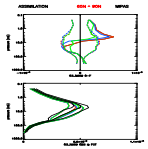

Fig. 8b. As in fig. 6b but for O3 at the north pole.

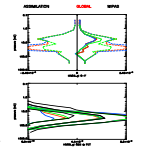

Fig. 9. As in fig. 8a (global) but for HNO3.

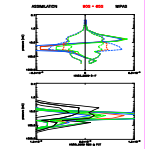

Fig. 9b As in fig. 8b but for HNO3 at the north pole.

Assimilating NO2 greatly deteriorates the O3 deficit in the upper stratosphere but increases its concentrations almost everywhere else. It creates a larger O3 deficit in the upper stratosphere by catalytic destruction. On the other hand, it increases HNO3 almost everywhere in the upper stratosphere but decreases HNO3 (increases deficit) in the lower stratosphere except at the north pole where it significantly increases the already present HNO3 surplus.

d. Assimilating CLONO2 only

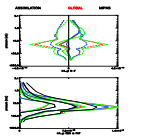

Fig. 10a. Global average CLONO2 results. **Upper panel**: mean (solid line) and std. dev (dashed line) of OmP. Lower panel: Mean and std. dev. of actual observations (black) and model 6-hr forecasts with assimilation of (1) MIPAS-IMK CLONO2 as OCD (blue), (2) MIPAS-IMK CLONO2 as VMR (red) and (3) no chemistry assimilation (green)

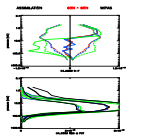

Fig. 10b. As in fig. 10a but for the north pole.

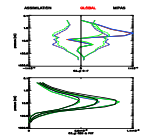

Fig. 11a. As in fig. 10a but for global O3.

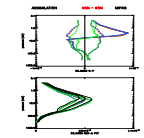

Fig. 11b. As in fig. 10b but for O3 at the north pole.

Assimilating CLONO2 decreases its deficit (adding CLONO2) in the upper stratosphere up to the stratopause, and decreases the surplus (decreasing CLONO2) in the lower stratosphere. The most significant effect is at the north pole lower stratosphere where assimilation works very well in correcting the surplus of CLONO2. As a result, more O3 is depleted in the model in the upper stratosphere and the surplus is increased (more O3) in the lower stratosphere at the north pole.

2. Multiple-species assimilation

a. Assimilating NO2 and O3 together

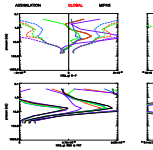

Fig. 12a. Global average NO2 results. **Upper panel**: mean (solid line) and std.dev (dashed line) of OmP. Lower panel: Mean and std. dev. of actual observations (black) and model 6-hr forecasts with assimilation of (1) MIPAS-ESA NO2+O3 as VMR (blue), (2) MIPAS-IMK NO2+O3 as VMR (red), (3) MIPAS-IMK NO2+O3 as OCD (green) and (4) no chemistry assimilation (purple)

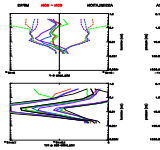

Fig. 12b. As in fig. 1 1a but for NO2 at the north pole.

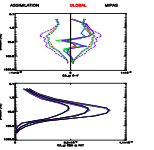

Fig. 13a. As in fig. 12a but for global O3.

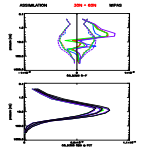

Fig.13b. As in fig. 12a but for O3 at the north pole.

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2. Multiple-species assimilation (cont'd)

Assimilating NO2 and O3 together has about the same effect on each species as assimilating them individually. Especially, it reduces the negative effect of catalytic destruction of O3 by assimilating NO2 alone.

b. Assimilating NO2, O3, HNO3 and CLONO2 together

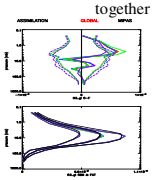

Fig. 14a. Global average O3 results. **Upper panel**: mean (solid line) and std. dev (dashed line) of OmP. **Lower panel**: Mean and std. dev. of actual observations (black) and model 6-hr forecasts with assimilation of (1) MIPAS-IMK NO2+O3+HNO3+CLONO2 as OCD (blue), (2) MIPAS-IMK NO2+O3+HNO3+CLNO2 as VMR (red), (3) MIPAS-IMK NO2+O3+HNO3+CLONO2 as VMR with tuned obs. error (green) and (4) no chemistry assimilation (purple)

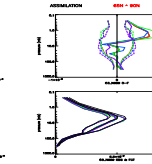

Fig.14b. As in fig. 14a but for the north pole.

Assimilating O3, NO2, HNO3 and CLONO2 together has a similar effect on NO2, HNO3 and CLONO2 respectively as assimilating each of them individually, while the effect on O3 is similar to assimilating CLONO2 individually or in combination with other species. i.e., as long as CLONO2 is assimilated, its O3-destructive effect is dominant.

From the perspective of the single- and multiple-species experiments shown here, NO2 and HNO3 have to be assimilated to capture their abnormally high concentration. At the same time, O3 has to be assimilated to alleviate the enhanced catalytic destructive effect (we note that the model itself has an ozone deficit in spite of the fact that it does not have enough NOx). Our assimilation of CLONO2 has too much destructive effect on O3 indicating that it should be treated with care. e.g. tuning of the variances is needed and cross-correlation with other species and chemical time scales may also need to be taken into account.

Summary and Discussion

The main source of global stratospheric NOx is oxidation of N2O from the troposphere but during the EPP period there is anomalous but continuous transport downward of those chemical constituents from the mesosphere/lower thermosphere (MLT) region into the upper stratosphere. At the same time, anomalously high OH is also produced (not normally available during polar night) which reacts with NO2 to produce high concentrations of HNO3. This mechanism is not present in our GEM-BACH model but through assimilating MIPAS measurements the deficits in the model NO2 and HNO3 are compensated disturbing the balances in model chemistry.

NO2 is transferred to HNO3 through ion cluster chemistry reactions and/or heterogeneous reactions of NOx on sulfate aerosols via N2O5 or (less likely) through gas phase reaction. What we see from figs. 8 and 9 is from heterogeneous reactions and/or gas phase chemistry since GEM-BACH does not include ion cluster chemistry.

In figs. 4 and 5, we see that the impact of assimilating HNO3 on NO2 is to increase it everywhere through photodissociation, which then significantly increases the upper stratosphere O3 deficit with a weaker effect in the lower stratosphere. This can be explained by the fact that the photolysis rate of HNO3 (also CLONO2) producing NO2 plus OH very rapidly at upper altitudes; one should expect a very rapid (~few hours) conversion to these constituents in the upper stratosphere. At 10 hPa, it will be slower (~1 day for HNO3). NO2 then destroys O3 through catalytic reactions (which is consistent with what we see in figs. 8 a and b). This occurs on a very short time scale, especially in the upper stratosphere. So, adding HNO3 destroys ozone everywhere and more rapidly in the upper stratosphere.

One thing we have not discussed is the effect of error statistics applied to each species, which is beyond the scope of this presentation. Clearly the relative impact of each species depend on the relative weight assigned to its forecast and observation errors. For example, from figs. 14 a and b we can see that the green line, which is the result of giving more weight to observations by reducing the observation error std . dev., shows a stronger destructive effect by increasing NO2 and (to a lesser extent) CLONO2. Also the issue of whether univariate variances is appropriate or not needs to be addressed. This should depend on the photochemical time scale of related species.