Numerical Weather Prediction

Towards a Constituent Assimilation System - Assimilation of MIPAS methane observations at the Met Office

Forecasting Research Technical Report No. 501

David R. Jackson and Alan J. Geer

email:nwp_publications@metoffice.gov.uk

Towards a Constituent Assimilation System - Assimilation of MIPAS methane observations at the Met Office

David R. Jackson and Alan J. Geer[1,*]

[1]: DARC, University of Reading, Reading, UK

[*]: Current affiliation: ECMWF, Reading. UK

Document Change History

First version, David Jackson	12/02/2007
Revised draft for dissemination, David Jackson	08/03/2007
Updated after comments from M Keil	12/03/2007
Updated after comments from A Geer	22/03/2007
Final version, David Jackson	26/03/2007

Abstract

In this report we demonstrate the capability for the Met Office ozone assimilation scheme to be extended to assimilate other constituent data by performing experiments to assimilate Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) methane data. The approach used is to modify the existing ozone assimilation code to be appropriate for methane.

We perform two experiments. Both are run between 23 September and 31 October 2003. The two runs use background error standard deviations that are 5% (run 5PC) and 1% (run 1PC), respectively, of the climatological background. Run 5PC produces a fairly realistic representation of certain features of the methane field, such as the 'double peak' structure in the low latitude upper stratosphere. This double peak is absent from run 1PC. However, particularly in the southern hemisphere stratosphere, there is unrealistic vertical structure in the run 5PC analyses, which is a consequence of vertical noise in the MIPAS data. Moreover, the bias between the analyses and independent data from the Halogen Occultation Experiment (HALOE) is often larger for run 5PC than for 1PC.

Improvements to the analysis could come from the following areas: using bias correction of the MIPAS data, instead of no bias correction; removal of erroneous vertical structure in the MIPAS data prior to assimilation; adoption of more sophisticated methods of representing the background error covariances to replace the empirical approach used in the experiments described here.

1 Introduction

In recent years, considerable progress has been made in developing the capability to assimilate ozone data in the Met Office NWP system. Jackson and Saunders (2002) and Jackson (2004) document the ozone assimilation scheme. The scheme has been successfully used to assimilate data from various research satellite instruments (Lahoz et al, 2005; Geer et al, 2006a,b, 2007; Jackson, 2007), and the possibility of adding an ozone assimilation capability to the operational Met Office NWP system is being considered (Mathison et al, 2007).

The ability to assimilate constituents in addition to ozone may well be required in the future as the need for accurate analyses and forecasts of air quality grows. Devenish (2006) has outlined the issues and requirements for chemical data assimilation for air quality forecasting. As a first step towards a generic constituent assimilation system, in this report we show that the Met Office ozone assimilation scheme can be successfully modified to assimilate methane observations.

Methane is one of the most important anthropogenic greenhouse gases. Increases in methane since pre-industrial times have contributed 20% to the total radiative forcing due to well-mixed greenhouse gases (e.g IPCC, 2001) In addition to this direct forcing there are also indirect greenhouse effects through chemistry - increased methane leads to higher levels of tropospheric ozone and stratospheric water vapour. Furthermore, stratospheric methane is an excellent tracer of atmospheric transport, since its source is located at the surface and its sink is essentially in the stratosphere via photolysis and chemical reactions with OH.

The outline of this report is as follows. A description of the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) methane assimilated, and the Halogen Occultation Experiment (HALOE) methane data used to validate the results, appears in Section 2, and a description of the assimilation system is in Section 3. Experimental results are in Section 4 and conclusions and suggestions for future work appear in Section 5.

2 Methane Datasets Used

In the data assimilation experiments described in this paper, methane data from the MIPAS instrument are assimilated. MIPAS methane profiles are available from 12-60km. The retrieval algorithm for the MIPAS data has undergone a number of revisions and in this report the MIPAS methane profiles assimilated are version 4.61 retrievals (see Raspollini et al, 2006). The total error in these retrievals is approximately 10% near the tropopause, 10-20% in the 15-45km region, and rising to 30 % between 45 and 60 km (Raspollini et al, 2006).

Camy-Peyret et al (2004) compared version 4.61 MIPAS methane profiles with balloon, aircraft, ground-based and satellite observations. They found that, overall, MIPAS measures methane reliably, with a precision of better than 15%. In addition, there is a systematic positive bias of MIPAS methane with respect to the other datasets in the upper troposphere / lower stratosphere above 100 hPa. Figure 1 illustrates this bias compared to Halogen Occultation Experiment (HALOE) observations in the July 2002 to March 2004 period. Maximum biases of over 0.3 ppmv are seen. Further comparisons between HALOE and MIPAS methane are shown in Juckes (2006). He shows MIPAS methane is 0.05 ppmv higher than HALOE methane at 850 K, which is in approximate agreement with Figure 1. Camy-Peyret et al also noted that the MIPAS retrieval algorithm generates oscillating or 'zig-zag' profiles in the upper troposphere / lower stratosphere, which is seen as a large rms difference between MIPAS and the correlative measurements. These oscillations are also discussed in Lahoz et al (2007).

In Section 4, the assimilation results are evaluated by comparison with independent data from HALOE. The HALOE instrument provides high-quality vertical profiles of methane derived from solar occultation experiments. The vertical resolution of the profiles is approximately 1.3 km. Like MIPAS, the retrieval algorithm for HALOE data has undergone many upgrades and version 19 HALOE retrievals are used here. The HALOE methane profiles have been validated by Park et al. (1996). They found that the combined systematic and random uncertainty of single methane profiles is between 11 and 19% in the lower stratosphere and is between 6 and 27% in the upper stratosphere. The agreement with correlative measurements is typically better than 15%, and systematic biases are smaller than those found with MIPAS.

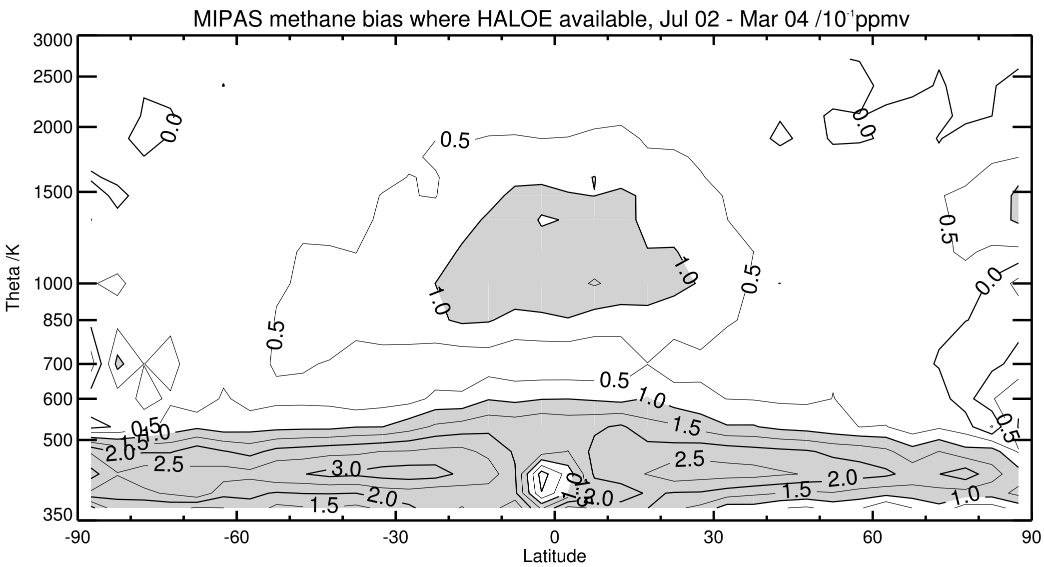

Figure 1: *Equivalent latitude / theta section of bias between MIPAS and HALOE data for July 2002 - March 2004 period. Units: 0.1 ppmv.*

3 The Met Office Data assimilation system

The Met Office NWP system has recently been extended to allow the assimilation of ozone (Jackson and Saunders, 2002, Jackson, 2004), but ozone is not assimilated operationally. In this report, the ozone assimilation system is modified so that methane data are assimilated instead of ozone. This is a quick and easy way of demonstrating that the ozone assimilation scheme can be easily adapted to assimilated other constituents. The assimilating forecast model has a horizontal resolution of 3.75^o longitude by 2.5^o latitude and 50 levels in the vertical, from the surface to $\sim$0.1 hPa. The model dynamical equations, including the transport scheme, have a semi-Lagrangian formulation (Davies et al, 2005). The data assimilation uses 3D-Var (Lorenc et al, 2000) and methane is assimilated univariately.

The background methane field is calculated using the tracer transport equation. In addition to this transport, chemical destruction of methane (and production of water vapour) by methane oxidation is represented by a parametrization scheme. The scheme is based on that used at ECMWF (Untch et al., 1998, ECMWF, 2004)) and uses pressure-varying rate coefficients based on data that appear in Brasseur and Solomon (1984). The ozone assimilation scheme uses an ozone photochemistry parametrization in this part of the code and so, in the methane assimilation experiments shown here, this parametrization is replaced by the methane oxidation scheme.

The initial conditions for the assimilation experiments are as follows. The mass and wind fields are taken from the daily stratospheric analyses that were produced operationally by the Met Office at that time (eg Swinbank et al, 2004). Initial conditions for methane are taken from the zonal mean of all MIPAS data for 23/09/2003.

The methane background error standard deviation is calculated from the annual mean MIPAS methane climatology for 2003, which appears in Figure 2. It was assumed that the background error standard deviation is a percentage of the climatological field. Originally, the standard deviation was chosen to be 10% of the climatology, but assimilation trials that used this value failed only a few days into the trial, possibly because of the large vertical oscillations seen in the MIPAS retrieved profiles. In the end, background error standard deviations that were 1% and 5% of the 2003 climatology were used. These values were selected to enable sufficient information from the MIPAS data to be added to the analysis, whilst at the same time suppressing much of the vertical noise in the MIPAS profiles.

In the absence of any other information, the methane background error correlations used were the same as the correlations used for the ozone assimilation. This may be a reasonable approximation, at least in the lower and middle stratosphere, since at these levels both methane and ozone are very much dynamical tracers whose distributions are controlled by the atmospheric transport. In the upper stratosphere and above, ozone is controlled by photochemistry, and so applying ozone correlations to methane may be a poorer assumption at these levels.

While this approach to deriving methane background error covariances is empirical, it should be pointed out that few other systems have assimilated methane, and of those that do, the background error covariances are equally empirical. If the work reported here continues later, there is scope to ‘bootstrap’ the covariances and recalculate them using the NMC method (Parrish and Derber, 1992) or the approach outlined by Polavarapu et al (2005).

4 Results

Figure 3 shows zonal mean methane analyses for both runs for two dates, 06/10/2003 and 26/10/2003. On both dates, run 5PC shows evidence of a ‘double peak’ in low latitude methane in the upper stratosphere. At these levels, methane is greater in the subtropics than at the equator, and this pattern

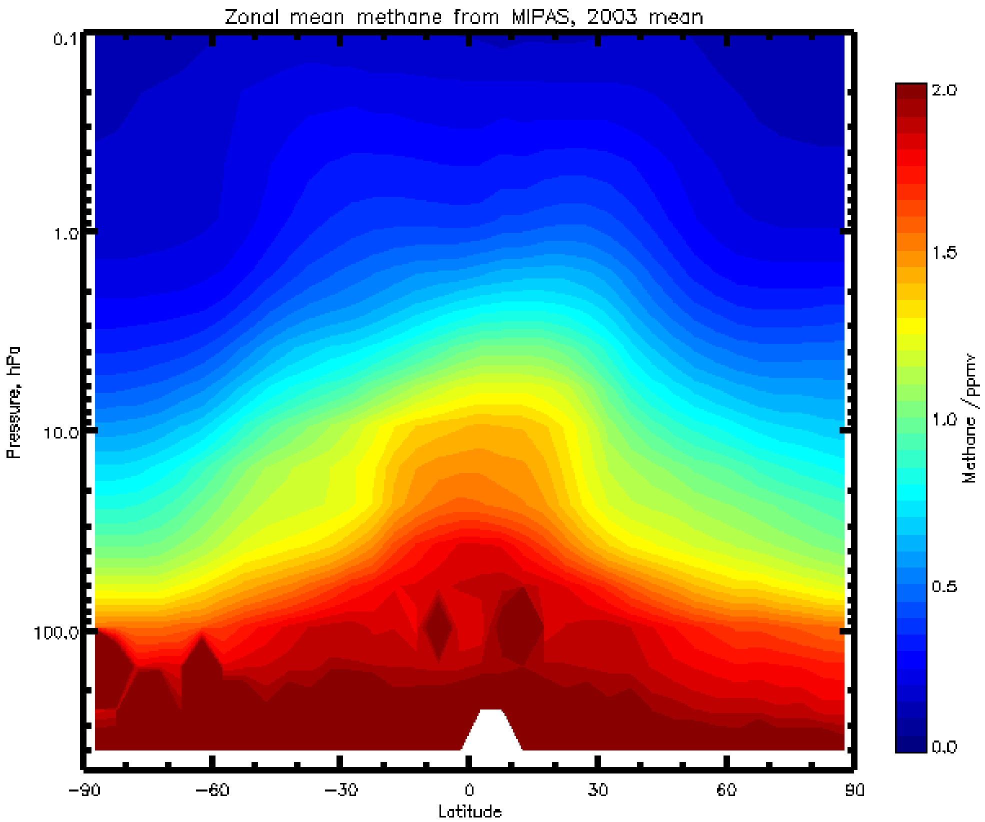

Figure 2: *Zonal mean methane for 2003, calculated from MIPAS observations.*

is due to the mean meridional circulation induced by the westerly phase of the semi annual oscillation (eg Gray and Pyle, 1986). There is little or no evidence of this double peak in the initial conditions or in the run 1PC analyses, so this suggests the double peak is not well simulated by the forecast model, but that is is represented by the MIPAS observations, since run 5PC gives a greater weight to these observations in the analysis than run 1PC does.

Although this is an encouraging result, Figure 3 also shows that there is an improbable bulge in high methane for run 5PC in the tropics near 20 km, which is likely due to an erroneous feature in the MIPAS data. In addition, there is a lot of vertical noise in the analysis fields in run 5PC, particularly in the southern extratropical lower stratosphere. This noise in the MIPAS retrievals has been noted by Camy-Peyret et al (2004). In contrast, this vertical noise is not seen in the run 1PC fields. The analysis increment on the same days (Figure 4) also shows the pattern of vertical noise for run 5PC, but not for run 1PC. Therefore, it appears that the greater weight given to the observations in run 5PC results in the vertical noise from the MIPAS observations being added to the analysis.

The analysis increments also show that in the lowermost stratosphere for run 5PC there are large negative increments in the extratropics and a smaller, but noticeable positive increments at low latitudes. This suggests that the background methane field over-estimates, and under-estimates, methane at these respective latitudes. Similar biases have been noted in ozone assimilation experiments (Jackson, 2007), but with opposite-signed errors, since the equator to pole gradient in the lowermost stratosphere for ozone is the opposite sign to that for methane. A possible explanation is that the meridional transport in the background field is too rapid here, resulting in excessive transport of high methane tropical air to the extratropics, and of low methane extratropical air to low latitudes. This bias is seen in run 1PC because that analysis gives a lot of weight to the biased background field, but in run 5PC the bias is

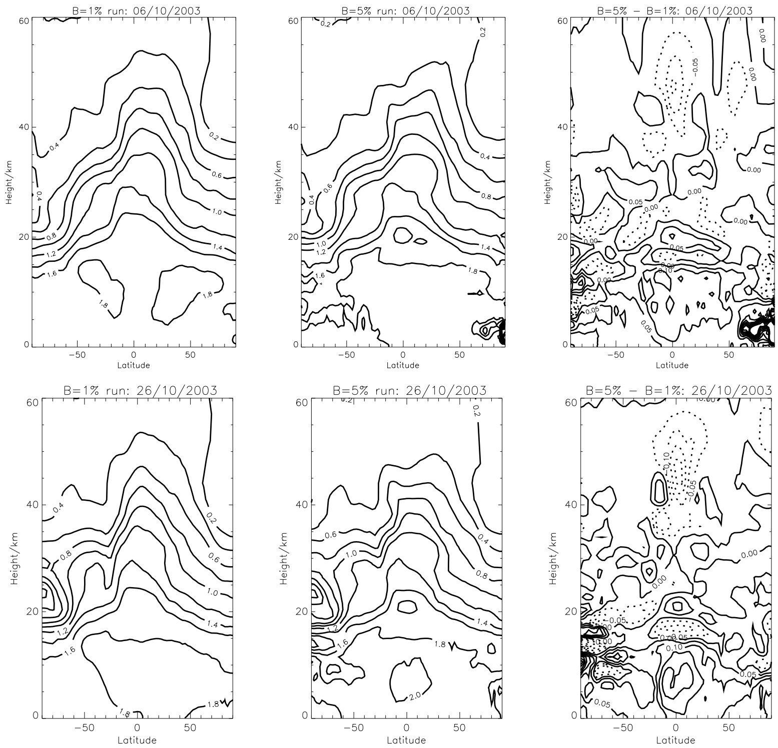

Figure 3: *Zonal mean methane analyses from run 1PC (left), run 5PC (centre) and run 5PC minus run 1PC (right) for 06/10/2003 (top) and 26/10/2003 (bottom). Units: ppmv. Contour interval: 0.2 ppmv (left and centre plots), 0.05 ppmv (right plots). Negative values are represented by dashed contours.*

corrected by some degree by the MIPAS analysis increments.

Mean errors calculated with respect to HALOE data (Figure 5) show that in the middle to upper stratosphere the bias in run 5PC is greater than in run 1PC. Generally, run 5PC methane is too low, whereas the run 1PC bias is close to zero. This is consistent with Figure 3, which shows run 5PC methane is lower than corresponding run 1PC values at these levels everywhere except the subtropics. Note, however, that at the middle strtaosphere and above the standard deviation of the HALOE - analysis differences is almost always smaller for run 5PC than for run 1PC. Given that the run 5PC bias is larger here, this suggests that run 5PC represents the spatial and temporal variability of the HALOE observations better, and thus that the double peak seen in the run 5PC fields in Figure 3 is realistic. Given that the bias between HALOE and MIPAS data is generally quite small here (Figure 1) this makes the increased bias in Figure 5 in run 5PC hard to explain. It is perhaps related to the small number of HALOE data available for the comparison used in Figure 5 and is thus a representativeness problem.

Another clear difference is in the middle stratosphere near 30 km, where run 5PC methane is greater than run 1PC methane. This difference leads to a reduced bias with respect to HALOE in the extratropics and an increased bias at low latitudes. A further clear difference between the runs is seen in the extratropics near 20-25 km, where run 5PC values are smaller than the run 1PC values and the HALOE - analysis differences are greater. The relative differences between the run 5PC and 1PC biases in Figure 5 near 30 km may be explained by the bias between HALOE and MIPAS (see Figure 1). However, in the 20-25 km region things are not so simple, since if the HALOE v MIPAS bias were reflected in the HALOE - analysis differences in Figure 5 then these differences would be more positive for run 1PC than for run 5PC. However, in fact in the extratropics the opposite is happening.

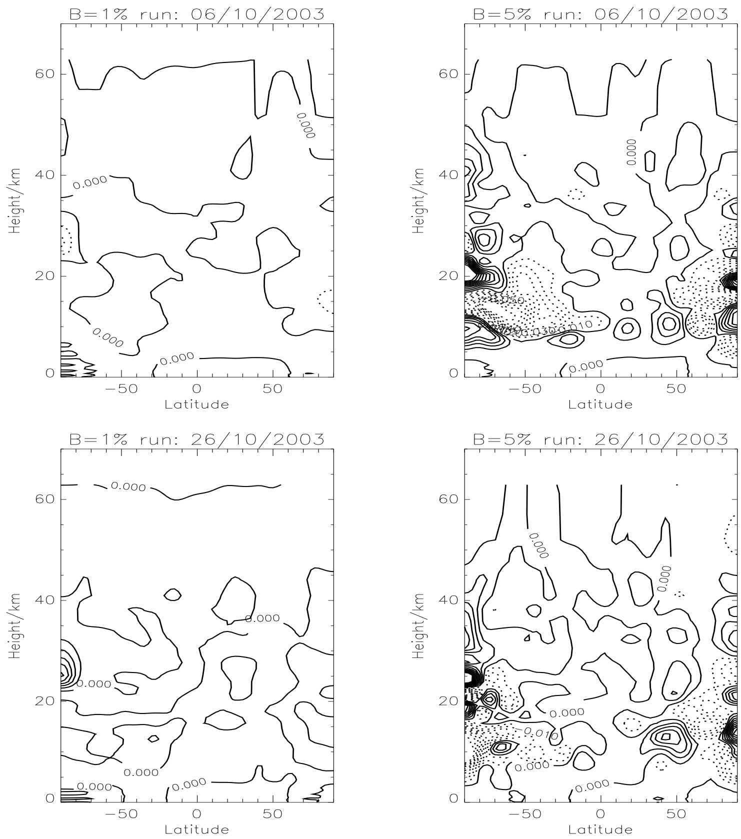

Figure 4: *Zonal mean methane analysis increments from run 1PC (left), and run 5PC (right) for 06/10/2003 (top) and 26/10/2003 (bottom). Units: ppmv. Contour interval: 0.01 ppmv. Negative values are represented by dashed contours.*

At lower and mid stratospheric levels, differences between the standard deviations of the HALOE - analysis differences are not always systematic or easy to explain. An exception is the larger standard deviation for run 5PC seen in the southern extratropics, which arises from the fact that the vertical noise seen in run 5PC at those locations is unrealistic and is not seen in the HALOE fields.

5 Possible Future work

The results presented here show that when MIPAS methane data are assimilated, the assimilation scheme does a reasonable job in representing the methane field. However, issues with vertical noise and bias in the MIPAS retrievals affect the quality of the retrievals. Currently, the only way to address these issues is to make the background error variance small, but then that means that much useful information from the MIPAS data is not being included in the analysis (eg lack of evidence for a double peak in the tropical upper stratosphere in run 1PC), and that the analysis is affected by biases in the model background.

There are three areas in which the assimilation work could be taken forward to address these issues.

1. **Removal of MIPAS vertical oscillations** Code supplied by Quentin Errera (BIRA, Brussels) could be used to remove erroneous vertical oscillations in the MIPAS profiles in the observation

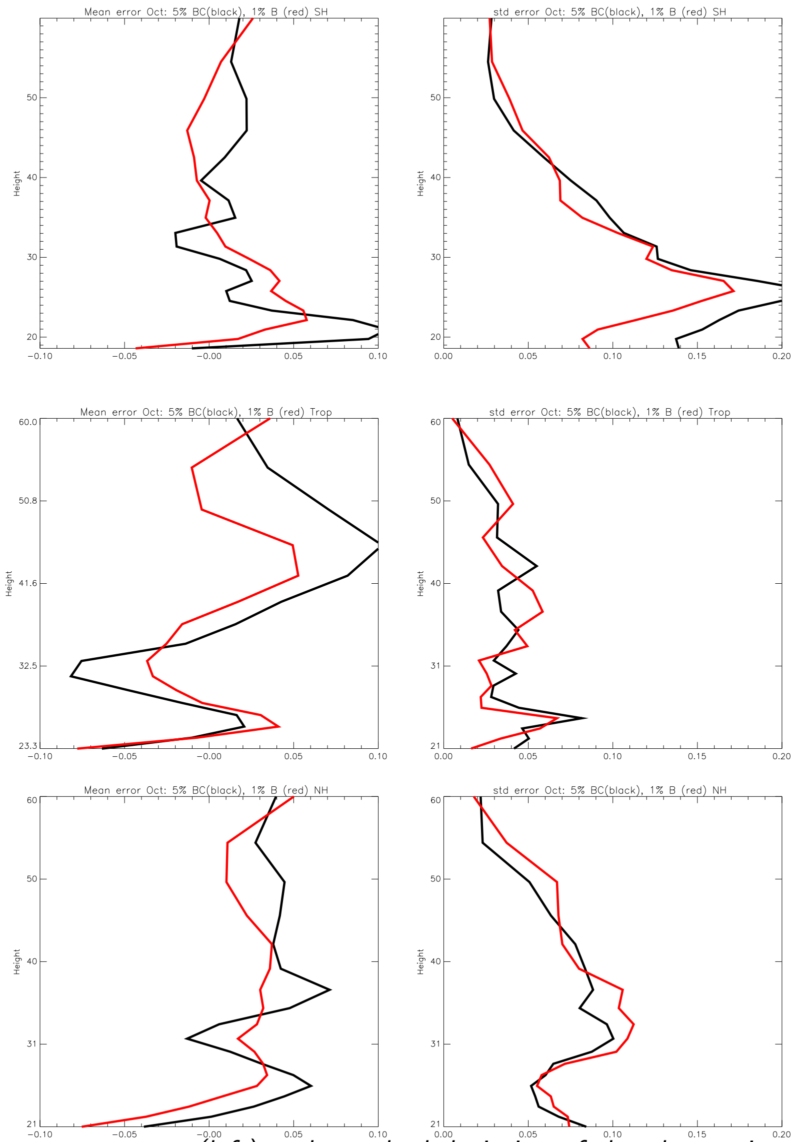

Figure 5: *Methane mean errors (left) and standard deviation of the observation minus analysis differences (right), calculated with respect to HALOE observations. Results are for October 2003 for the southern extratropics (top), tropics (middle) and northern extratropics (bottom). Run 5PC results are in black and run 1PC results are in red. Units: ppmv.*

processing step. This would address problems with the analysis seen here, particularly for run 5PC in the southern lower stratosphere.

2. **Bias correction** The MIPAS - HALOE differences shown in Figure 1 could be subtracted from the MIPAS observations prior to assimilation. Furthermore, once variational bias correction for satellite radiances is developed and better understood, this technique could also be extended to apply to apply to the MIPAS data.

3. **New background error covariance calculations** The current method of calculating the background error variance is very ad hoc and the error correlations used are appropriate for ozone, not methane. A possible way forward would be to run an assimilation trial with the current covariances, and with oscillation removal and bias correction applied, and use the statistics from it to re-calculate the covariance matrix using the NMC method. Another, quicker, approach would be to run a monthly long forecast and calculate error covariances from 6 hourly differences (after Polavarapu et al, 2005).

6 Summary

In this report the Met Office ozone assimilation was modified in order to assimilate MIPAS methane observations. The modification was quite simple and involved replacing the ozone photochemistry parametrization in the background field calculation with a methane oxidation parametrization and ensuring that the ozone field in the initial conditions was replaced by a methane field. In addition, background error standard deviations were calculated by setting this standard deviation to a certain percentage of a climatological methane field.

Two experiments were run, in which the background error standard deviation was 1% and 5% of the climatological field. With the higher background error standard deviation, features observed by MIPAS but not represented in the background field, such as a double peak in the low latitude upper stratosphere, were better represented. In addition, it appears that there may be a bias related to transport errors in the lowermost stratosphere. In run 5PC this was addressed, although this did not necessarily lead to a reduction in the calculated analysis bias against HALOE data, possibly because of the sparsity of HALOE data available for comparison.

A drawback of using the 5% background error standard deviation is that problems associated with the MIPAS retrievals manifested themselves in the analysis. This included an unrealistic bulge of high methane in the tropics near 20 km, and erroneous vertical oscillations, which were most apparent in the southern stratosphere. These features can be suppressed by using a smaller background error standard deviation, but if future assimilation experiments are to be carried out, it very important that the erroneous vertical oscillations and the MIPAS biases should be removed in the observation processing step prior to performing the assimilation.

This work has shown that the ozone assimilation scheme can be easily modified to assimilate methane. In principle it should be straighforward to modify the ozone code into a generic, scalable constituent assimilation code that can be used for air quality and other studies. It should be noted that the addition of many constituents to the assimilation scheme is computationally expensive (perhaps an extra 10% to forecast model costs and and extra 20% to assimilation costs per extra constituent). However, with the introduction of increased computer power in coming years the issue should become more tractable and it will be feasible for an air quality assimilation system to be developed that will advance current air quality modelling work currently taking place using the Unified Model (the AQUM project).

References

Brasseur, G. and Solomon, S. (1984) *Aeronomy of the middle atmosphere*, D Reidel Publishing Co., Dordrecht, 452pp

Camy-Peyret, C., Payan, S., Dufour, G., Oelhaf, H., Wetzel, G., Stiller, G. P., Glatthor, N., Blumenstock, T., Blom,C.E., Keim, C., Miluteit, S., Engel, A., Pirre, M., Moreau, G.; Catoire, V.; Bracher, A.; Weber, M.; Bramstedt, K. (2004) Validation of MIPAS CH4 profiles by stratospheric balloon, aircraft, satellite and ground based measurements., *Proc. ACVE-2 meeting*, 3-7 May 2004, Frascati, Italy, 2004, ESA SP-562.

Davies, T., Cullen, M.J.P., Malcolm, A.J., Mawson, M.H., Staniforth, A., White, A.A., and Wood, N. (2005) A new dynamical core for the Met Office's global and regional modelling of the atmosphere. *Quart J. Royal. Meteor. Soc.* **131** 1759-1782

Devenish, B. (2006) Chemical data assimilation for air quality forecasting, Met Office Forecasting Research Technical Report 494

ECMWF (2004) IFS documentation CY28r1. Available from http://www.ecmwf.int/research/ifsdocs/CY28r1/index.html

Geer, A. J., Peubey, C, Bannister, R, Brugge, R, Jackson, D.R, Lahoz, W.A, Migliorini, S, O'Neill, A and Swinbank, R (2006a) Assimilation of stratospheric ozone from MIPAS into a global general circulation model: the September 2002 vortex split. *Quart. J. Roy. Meteor. Soc.* **132** 231-257

Geer, A. J., Lahoz, W.A., Bekki, S., Bormann, N., Errera, Q., Eskes, H.J., Fonteyn, D., Jackson, D.R., Juckes, M.N.,Massart, S., Peuch, V.-H., Rharmili, S., and Segers, A. (2006b) The ASSET intercomparison of ozone analyses: method and first results *Atmos. Chem. Phys.* **7** 5445-5474

Geer, A. J., Lahoz, W.A., Jackson, D.R., Cariolle, D., and McCormack, J.P. (2007) Evaluation of linear ozone photochemistry parametrizations in a stratosphere-troposphere data assimilation system *Atmos. Chem. Phys.* **7** 939-95

Gray, L.J. and Pyle, J. A. (1986) The Semiannual oscillation and equatorial tracer distributions. *Quart J. Royal. Meteor. Soc.* **112** 387-407

IPCC (2001) Climate Change 2001: The scientific basis. Edited by Houghton, J.T., Ding, Y., Griggs, D.J. et al. Cambridge University Press, UK and New York, NY, USA.

Jackson, D.R. (2004) Improvements in ozone data assimilation at the Met Office, Met Office Forecasting Research Technical Report 454

Jackson, D.R. (2007) Assimilation of EOS MLS ozone observations in the Met Office Data Assimilation System. To be submitted to *Quart. J. Roy. Meteor. Soc.*

Jackson, D.R. and Saunders, R. (2002) Ozone data assimilation: preliminary system, Met Office Forecasting Research Technical Report 394

Juckes, M.N. (2006) An annual cycle of long lived stratospheric gases from MIPAS. *Atmos. Chem. Phys. Discuss.* **6** 9389-9429

Lahoz, W.A, Brugge, R, Jackson, D.R, Migliorini, S, Swinbank, R, Lary, D and Lee, A (2005) An Observing System Simulation Experiment to evaluate the scientific merit of wind and ozone measurements from the future SWIFT instrument. *Quart. J. Roy. Meteor. Soc.* **131** 503-523

Lahoz, W.A., Geer, A.J., and Orsolini, Y.J. (2007) Northern Hemisphere stratospheric summer from MIPAS observations *Quart. J. Roy. Meteor. Soc.* **133** 197-211

Lorenc, A. C., Ballard, S.P., Bell, R.S. et al (2002) The Met. Office global three dimensional data assimilation scheme, *Quart. J. Roy. Meteor. Soc.* **126** 2991-3012

Mathison, C., Jackson, D.R, and Keil, M (2007) Methods of improving the representation of ozone in the Met Office Model. *NWP Technical Report 502*

Parrish, D.F and Derber, J.C (1992) The National Meteorological Center's spectral statistical-interpolation analysis system. *Mon. Weather Rev.* **120** 1747-1763

Park, J. H.,Russell, J.M. III, Gordley, L.L,Drayson, S.R., enner,D.C., McInerney,J., Gunson, M.R., Toon, G.C., Sen, G.B, Blavier, J.-F.,Webster, C.R., Zipf, E.C., Erdman, P., Schmidt, U., and Schiller, C. (1996) Validation of Halogen Occultation Experiment CH4 Measurements from the UARS, *J. Geophys. Res.* **101** 10,183-10,203

Polavarapu, S, Ren, S, Rochon, Y, Sankey, D, Ek, N, Koshyk, J and Tarasick, D (2005) Data assimilation with the Canadian Middle Atmosphere Model. *Atmos.-Ocean* **43** 77-100

Raspollini, P., Belotti, C., Burgess, A., et al (2006) MIPAS level 2 operational analyses, *Atmos. Chem. Phys.* **6** 5605-5630

Swinbank, R., Keil, M., Jackson, D.R., and Scaife, A.A. (2004) Stratospheric Data Assimilation at the Met Office - progress and plans. ECMWF workshop on Modelling and Assimilation for the Stratosphere and Tropopause 23-26-June, 2003.

Untch, A., and Simmons, A.J. and others (1998), Increased stratospheric resolution in the ECMWF forecasting system. *ECMWF Newsletter*, 8, 2-8