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Constrained adaptive bias correction for satellite radiance assimilation in the ECMWF 4D-Var system

Wei Han[1] and Niels Bormann[2]

1 CMA, Beijing, China
2 ECMWF, Reading, UK

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Wei Han (CMA),

Niels Bormann (ECMWF)

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Abstract

This memorandum investigates the use of a modified version of Variational Bias Correction in which a constraint is imposed on the size of the bias correction by adding a new term to the variational cost function ("CVarBC"). This novel approach is aimed at situations where significant model bias has previously led to problems with variational bias corrections drifting over time, prompting ad-hoc decisions to provide anchoring information through assimilating certain observations without bias corrections. Two such situations are investigated: upper stratospheric temperature observations from AMSU-A which are presently anchored through assimilating channel 14 without a bias correction; and ozone observations from hyperspectral infrared instruments which are presently anchored by assimilating one channel per instrument without bias correction.

In both situations, CVarBC is able to successfully constrain drift in the bias corrections, while at the same time being able to correct observational bias pattern that were previously ignored when these observations were assimilated without bias correction (e.g., inter-satellite biases or scan-dependent biases in the case of AMSU-A). This leads to a better consistency of the analysis with other observations. In the case of the ozone channels, CVarBC can be used to avoid assuming that single selected channels are unbiased, by instead weakly constraining the bias correction for all ozone-sensitive channels from hyperspectral infrared observations. The new approach leads to a more robust system with benefits for maintenance, particularly for reanalysis applications.

1 Introduction

The adequate treatment of systematic errors in the assimilation of satellite radiances is an essential pre-requisite to the successful use of these observations. Such systematic errors arise either from the observations themselves, for instance, through instrument anomalies or sub-optimalities in the calibration, or from the radiative transfer modelling required during the assimilation. These systematic errors are typically removed before or during the assimilation based on parametric models for the biases (e.g., Harris and Kelly 2001). Today, this is often done in an adaptive way, for instance through Variational Bias Correction (VarBC, e.g., Dee 2004, Auligné et al. 2007). Here, the free parameters of the bias model are estimated as part of the control vector. VarBC estimates bias corrections that are consistent across the observing system, including consistency with other un-biased observations, but also potentially influenced by model bias (Eyre 2016).

Adaptive methods such as VarBC have been very successful for observations sensitive to aspects of the atmosphere that are well-observed by un-biased other observations and for which model biases are small. Un-biased other observations help VarBC to separate model biases from observational biases, and such observations are often referred to as "anchors" for VarBC. However, problems occur, for instance, when the bias correction interacts with the quality control (e.g., Auligné and McNally 2007) or for observations that are sensitive to aspects that are otherwise not well observed and where model biases are strong (e.g., Di Tomaso and Bormann 2011, Eyre 2016). In the latter case, VarBC lacks information to distinguish between model and observational biases, and as a result the bias corrections can drift to unrealistic values, correcting for model biases as well as observational biases. This is undesirable, particularly in a reanalysis context, as it leads to biased analyses. In the ECMWF system, this has been found particularly problematic for upper stratospheric and mesospheric temperature channels (e.g., Di Tomaso and Bormann 2011), observing a region where the ECMWF model exhibits considerable biases. It has also been an issue for the assimilation of ozone channels from infrared instruments (Han and McNally 2010). As shown by Eyre (2016), the effect of aliasing model bias into observational bias corrections increases even in the presence of anchoring observations the more observations are bias-corrected.

To avoid unrealistic drifts in the bias corrections, additional constraints need to be imposed on VarBC. Currently, the method used at ECMWF and elsewhere is to assimilate selected affected channels without a bias correction. For instance, the highest-peaking AMSU-A channel (channel 14) is assimilated without a bias correction, and this successfully anchors the upper stratosphere (e.g., Di Tomaso and Bormann 2011). Selected ozone channels from hyperspectral infrared instruments are also assimilated without bias correction, anchoring the upper tropospheric/lower stratospheric ozone analysis (Han and McNally 2010). The approach to assimilate certain radiance observations without bias correction is of course a very simplistic and pragmatic constraint, based on the hypothesis that the observational biases are much smaller than the model biases for these specific channels. However, the approach neglects that there may be observational bias pattern that should be corrected (e.g., scan-dependent biases or inter-satellite biases in the case of AMSU-A channel 14). Also, assuming that the bias is small can of course be questionable, for instance when biases in the observation operator may be sizeable.

In the present paper, we investigate the use of a modification to VarBC which allows a more flexible constraint on the bias correction, tied to an estimate of the uncertainty in the size of the bias correction. This new approach aims to limit the size of the bias correction, but at the same time allows some structures of the bias to be corrected. This is achieved through a modification to the variational cost function, and we refer to the resulting scheme as “Constrained Variational Bias Correction” (CVarBC).

The structure of the paper is as follows. We first outline the new methodology and introduce the modification to the variational cost function. Next we investigate the application of the new method to AMSU-A channel 14 to replace the current approach of anchoring the upper stratospheric temperature analysis. This is followed by discussions of a more extensive use of the new method for several stratospheric channels. Finally, we also apply the new method to the assimilation of ozone information from hyperspectral infrared observations. Our overall conclusions are provided in the last section.

2 Methodology

The general framework of VarBC is described in detail in Auligné et al. (2007), and here we will only recall the main parts. VarBC uses an appropriately chosen parametric model, h($\mathbf{x}$, $\boldsymbol{\beta}$), usually a function of the atmospheric state $\mathbf{x}$ and some free bias parameters $\boldsymbol{\beta}$ which are to be estimated. The free parameters are estimated during the variational analysis by including them in the general control vector and using the following cost function:

$$\begin{aligned} 2J(\mathbf{x},\boldsymbol{\beta}) = {} & (\mathbf{x}_b-\mathbf{x})^T\mathbf{B}_x^{-1}(\mathbf{x}_b-\mathbf{x}) \\ & +(\boldsymbol{\beta}-\boldsymbol{\beta}_b)^T\mathbf{B}_\beta^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_b) \\ & + [\mathbf{y}-H(\mathbf{x})-h(\mathbf{x},\boldsymbol{\beta})]^T\mathbf{R}^{-1}[\mathbf{y}-H(\mathbf{x})-h(\mathbf{x},\boldsymbol{\beta})] \end{aligned}$$

Here, $\mathbf{x}_b$ is the atmospheric background state from a short-range forecast, with the background error covariance $\mathbf{B}_x$. $\boldsymbol{\beta}_b$ is the background state for the bias parameters (from the previous analysis), with background error covariance $\mathbf{B}_\beta$. $\mathbf{y}$ denotes the observations, with the observation error covariance $\mathbf{R}$ and the observation operator H.

Note that in this standard formulation of VarBC, there is no penalty for the size of the bias correction. While the 2nd term, the VarBC background term, provides a constraint on the modification to the bias parameters for each analysis cycle, the size of the bias correction can nevertheless grow unrealistically over many cycles, provided of course this achieves an overall reduction in the size of the cost function at each minimisation.

For Constrained VarBC, we add an additional term to the variational cost function that penalizes the size of the bias correction, as follows:

$$\begin{aligned} 2J(\mathbf{x},\boldsymbol{\beta}) \;=\; & (\mathbf{x}_b-\mathbf{x})^T\mathbf{B}_x^{-1}(\mathbf{x}_b-\mathbf{x}) \\ & + (\boldsymbol{\beta}-\boldsymbol{\beta}_b)^T\mathbf{B}_\beta^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_b) \\ & + [\mathbf{y}-H(\mathbf{x})-h(\mathbf{x},\boldsymbol{\beta})]^T\mathbf{R}^{-1}[\mathbf{y}-H(\mathbf{x})-h(\mathbf{x},\boldsymbol{\beta})] \\ & + \alpha^2[h(\mathbf{x},\boldsymbol{\beta})-\mathbf{b}_0]^T\mathbf{R}_b^{-1}[h(\mathbf{x},\boldsymbol{\beta})-\mathbf{b}_0] \end{aligned} \tag{1}$$

Here, $\mathbf{b}_0$ is a prior estimate of the bias (in many applications this will be zero) and $\mathbf{R}_b$ provides an estimate of the uncertainty in the prior estimate of the bias. The latter should be linked, for instance, to the uncertainty in the absolute calibration, in contrast to **R** which describes the random component of the observation error. α^2 is a regularization parameter that can be used to determine the relative sizes of the J_O-term (the 3rd term) and the new constraint-term.

As can be seen, the bias correction is now determined through the interaction of three terms: the J_O-term (3rd term), a background term for the bias parameters (2nd term), and the J_{CVarBC} term (4th term). A reduction in the J_O-term, resulting from correcting a bias, will now be associated with an increase in the J_{CVarBC}-term when the bias correction deviates from the pre-scribed value. The resulting solution will reflect the relative size of the observation error **R** and the bias uncertainty $\mathbf{R}_b$: if the assigned error in the size of the bias correction is very small compared to the assigned observation error, the penalty for any deviation from the pre-scribed bias values will outweigh reductions in the J_O-term, and the behavior of CVarBC will be very similar to assimilating the observations with a fixed bias correction. In contrast, if the assigned error in the size of the bias correction is very large compared to the observation error the behavior will be similar to that of a free-running VarBC. Note that the penalty term will act not only on the size of the global mean bias correction, but also on any geographical or other structures in the estimated bias corrections, again dependent on the choice of parameters used for CVarBC. If the prior estimate of the bias is a global constant, CVarBC will potentially also dampen any geographical or other structures in the estimated bias corrections.

The gradient of the cost function with respect to the bias parameters now becomes:

$$\begin{aligned} & \nabla_{\boldsymbol{\beta}} J(\mathbf{x},\boldsymbol{\beta}) \\ & = \mathbf{B}_\beta^{-1}(\boldsymbol{\beta}-\boldsymbol{\beta}_b) - \mathbf{P}^T\mathbf{R}^{-1}[\mathbf{d}-\mathbf{P}\boldsymbol{\beta}] + \alpha^2\mathbf{P}^T\mathbf{R}_b^{-1}[\mathbf{P}\boldsymbol{\beta}-\mathbf{b}_0] \\ & = (\mathbf{B}_\beta^{-1} + \mathbf{P}^T\mathbf{R}^{-1}\mathbf{P} + \alpha^2\mathbf{P}^T\mathbf{R}_b^{-1}\mathbf{P})\boldsymbol{\beta} - (\mathbf{B}_\beta^{-1}\boldsymbol{\beta}_b + \mathbf{P}^T\mathbf{R}^{-1}\mathbf{d} + \alpha^2\mathbf{P}^T\mathbf{R}_b^{-1}\mathbf{b}_0) \end{aligned} \tag{2}$$

Here we assume a linear bias model $h(\mathbf{x},\boldsymbol{\beta}) = \mathbf{P}\,\boldsymbol{\beta}$ with **P** a matrix of (possibly state-dependent) predictors, and $\mathbf{d} = \mathbf{y} - H(\mathbf{x})$. This is required during the minimization of the cost function during the variational analysis.

The above modification to the variational cost function and its gradient has been implemented in the ECMWF 4d-Var system. In the following, we will investigate its behavior using the two areas where currently selected channels are assimilated without bias corrections, ie the upper stratospheric/lower mesospheric temperature analysis and the upper tropospheric/lower stratospheric ozone analysis.

3 CVarBC for upper stratospheric temperature-sounding channels

The ECMWF model exhibits considerable temperature biases over the upper stratosphere/lower mesosphere region. This can be seen, for instance, from zonal means of differences between forecasts and analyses at various forecast ranges (e.g., Figure 1, left). Past experimentation has shown that this model bias leads to unrealistic drifts in the bias corrections for the stratospheric AMSU-A channels which are sensitive to these regions (see Figure 1, right for AMSU-A weighting functions). To counter-act this effect, AMSU-A channel 14 is assimilated without a bias correction.

In the following, we address two objectives: Firstly, we re-examine the behavior of VarBC in the absence of an upper stratospheric anchor, as the behavior might have changed as a result of changes to the model bias since the introduction of VarBC. Secondly, we investigate replacing the “hard” anchor of assimilating AMSU-A channel 14 without a bias correction with the “soft” anchor of using CVarBC for AMSU-A channel 14. The motivation for using CVarBC in this context is that it should allow at least the partial correction of some known bias pattern in AMSU-A channel 14, such as scan-dependent biases or inter-satellite biases.

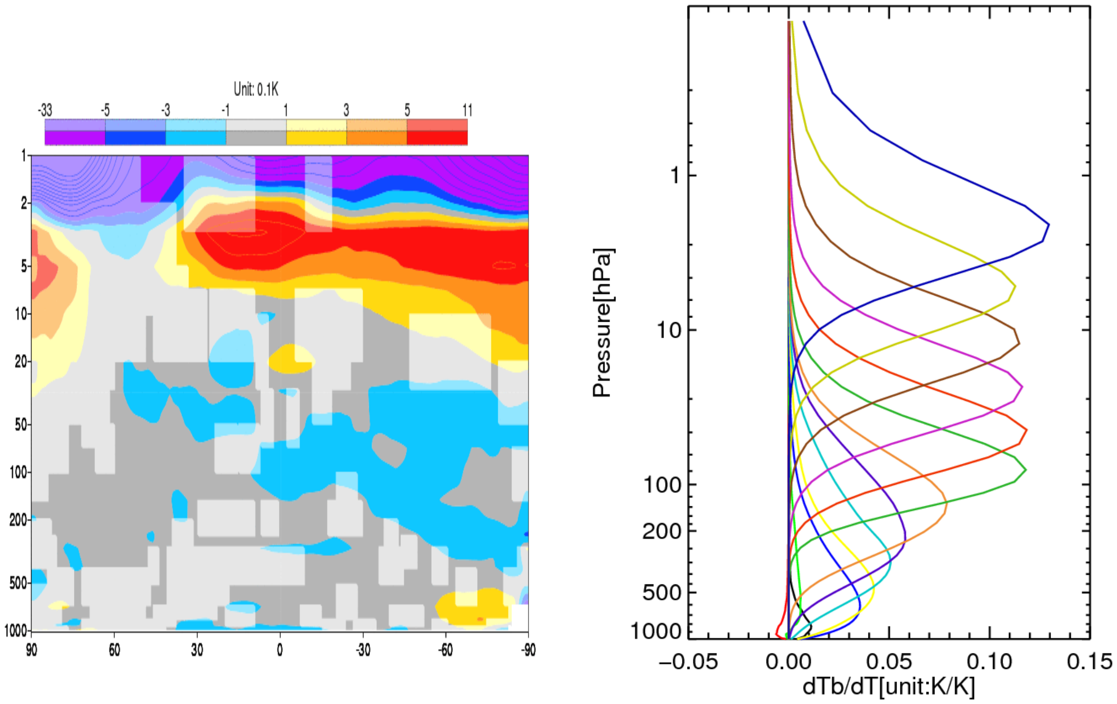

Figure 1: Left: Zonal mean of the difference between the operational ECMWF 1-day temperature forecast and the analysis for December 2014 – February 2015. Note that the unit is 0.1 K; deeper colours indicate statistically significant differences at the 95 % level. Right: AMSU-A weighting functions for a standard atmosphere profile.

3.1 Experiments

To investigate the use of CVarBC for AMSU-A channel 14, we conducted the following three experiments with the ECMWF assimilation system:

Control: Use of VarBC as in operations, including assimilation of AMSU-A channel 14 without a bias correction.

VarBC: As Control, but we use unconstrained VarBC for AMSU-A channel 14. This is to investigate whether the problem of VarBC drifting to unrealistic bias corrections still exists in the present operational system.

CVarBC14: As Control, but we use CVarBC for AMSU-A channel 14.

The bias model for AMSU-A channel 14 for the VarBC and the CVarBC14 experiment consists of a constant offset and a third-order polynomial in the scan-angle, designed to allow the correction of inter-satellite and scan-dependent biases. An air-mass component as used for the other AMSU-A sounding channels could have been added, but for these first experiments we decided not to include this for channel 14, in order to retain a constraint on the geographical structure of the bias correction. The bias correction was initialized by setting the global offset to the mode of the background departures of the first cycle. For other AMSU-A sounding channels, all three experiments use the standard operational bias model, which uses in addition an air-mass component based on a linear model with four layer thicknesses as predictors.

The additional CVarBC-parameters for AMSU-A channel 14 were as follows: The pre-scribed bias value was set to 0 K, the same for all satellites. The uncertainty in this bias estimate was assumed to be $R_b = (1.4\ K)^2$ and hence the same value as the observation error used for this channel and broadly in-line with estimates of the calibration accuracy. The regularization parameter α was set to 0.3, following some experimentation.

In the VarBC and the CVarBC14 experiment, we relaxed the background constraint on the adjustments to the VarBC parameters for AMSU-A channel 14 compared to the operational setting. This is because previous experiments with the operational settings have shown that the drift of VarBC towards model bias tends to be fairly slow, stabilizing only after about one year of experimentation. Such long experimentation was not practical for these first investigations. Relaxation of the background constraint accelerates this drift, but is not expected to affect the final value the variational bias correction converges to. In the operational configuration, the error variance for the bias coefficients is set to 5000 times the observation error variance of the observation in question, whereas in our experiments it is set to 10 times the observation error variance.

The experiments cover the periods 2 December 2014 to 29 April 2015 and 1 June – 31 August 2015 and use 12-h 4d-Var, with a spatial model resolution of TL511 (~40 km), an incremental analysis resolution of TL255 (~80 km) and 137 levels in the vertical.

3.2 Results

Estimated bias corrections

The temporal evolution of the bias correction for AMSU-A channel 14 on NOAA-18 and METOP-A is shown in Figure 2 for the VarBC and the CVarBC14 experiment. In the free VarBC experiment, the bias correction drifts to values of around -2.3 K for NOAA-18 and -1.6 K for METOP-A over the course of the 5 months, with no clear sign that the bias correction has stabilized at this level. Such large bias corrections are thought to exceed the absolute radiometric accuracy for this channel. The behavior demonstrates that the problem of VarBC erroneously correcting for model biases is still present in the ECMWF system.

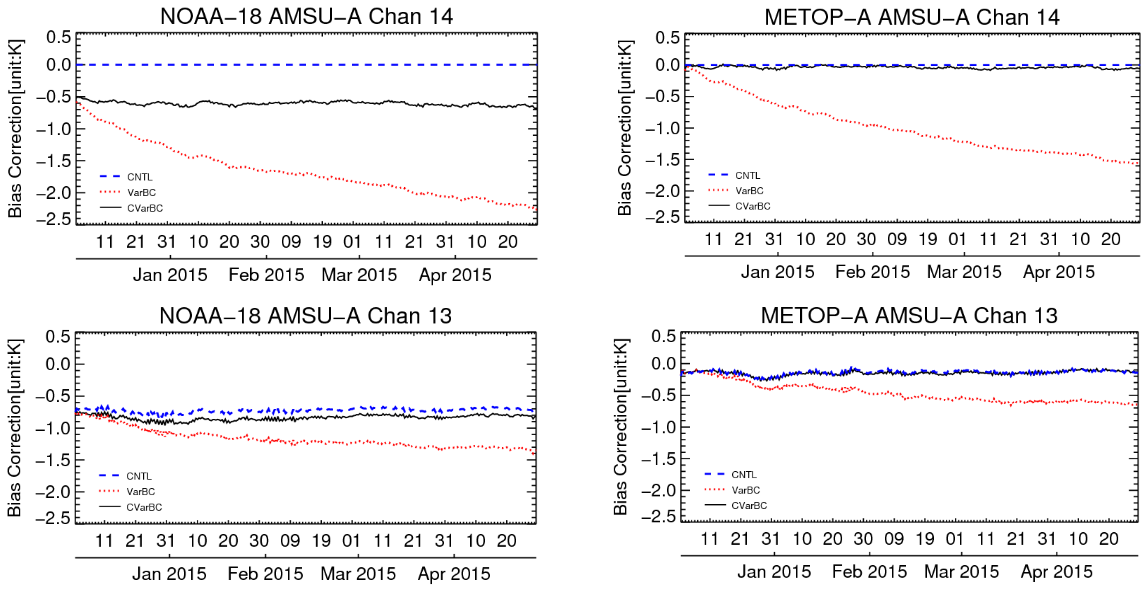

Figure 2: Temporal evolution of the global mean bias correction for the Control (blue dashed), the VarBC (dotted red) and the CVarBC14 experiment (solid black) for NOAA-18 (left) and METOP-A (right) AMSU-A channels 13 (bottom) and 14 (top).

In contrast, the constraint imposed on the size of the bias correction in the CVarBC14 experiment is successful in limiting the drift in the bias correction. The mean bias correction stabilizes quickly, with a value of around -0.6 K for NOAA-18 and around zero for METOP-A. Note that the different treatment of the bias correction in channel 14 also affects neighboring channels, such as channel 13 (Figure 2, bottom). For NOAA-18, the value of the bias correction for channel 14 in the CVarBC14 experiment is different from the zero bias correction imposed in the Control, but it appears nevertheless more reasonable than the value obtained with the free VarBC given the radiometric accuracy of the data.

Figure 2 highlights that CVarBC correctly identifies different biases for the two satellites shown – a clear advantage over imposing the same bias correction for both instruments. This is further highlighted in Figure 3 which displays the mean bias corrections for different assimilated AMSU-A instruments at the end of the assimilation experiment.

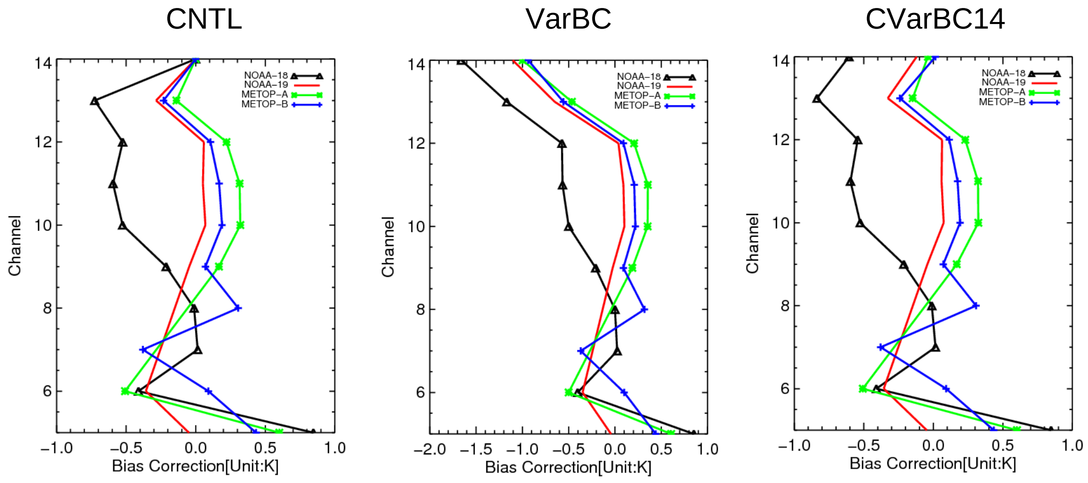

Figure 3: Global mean bias correction for assimilated AMSU-A channels from different satellites for the Control (left), VarBC (middle) and CVarBC14 experiment (right). The statistics have been calculated for the period December 2014 to February 2015.

AMSU-A radiances, model biases, information from any available anchoring observations, and the imposed penalty on the size of the bias correction.

The bias corrections applied in the CVarBC14 experiment also correctly identify scan-dependent biases that are otherwise ignored in the Control experiment. For instance, channel 14 on the NOAA-18 AMSU-A shows a sloping bias-pattern as a function of scan-position before bias correction, and this is removed after bias correction in the CVarBC14 run (*Figure 4*). This is again a very positive finding, and it was one of the motivations for introducing CVarBC.

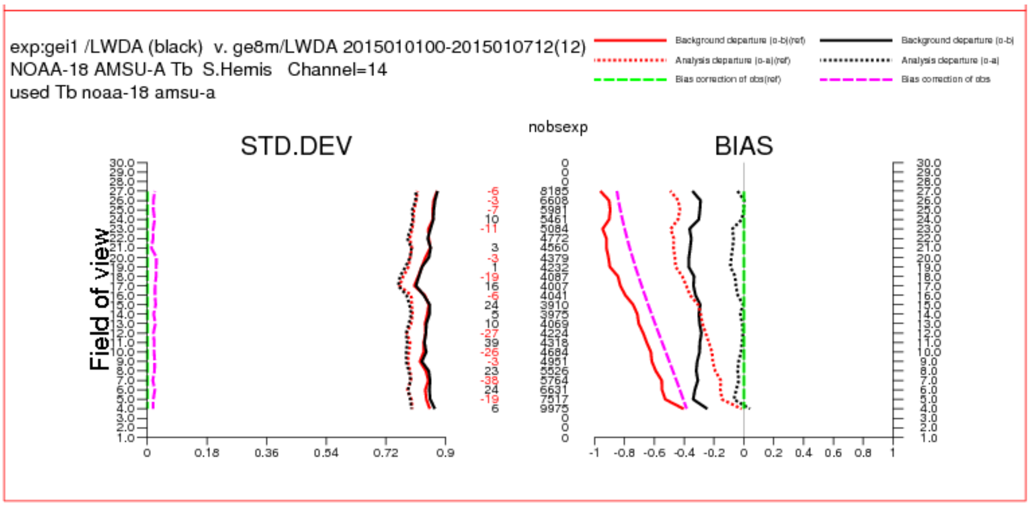

Figure 4: Departure characteristics for NOAA-18 AMSU-A channel 14 as a function of scan-position, in terms of standard deviation (left) and bias (right). Solid lines show the statistics for FG-departures, dotted for analysis departures (both after bias correction), with black indicating results from the CVarBC14 experiment, red the Control. Dashed cyan and green lines mark the bias correction applied in the CVarBC14 experiment and the Control, respectively. The statistics cover the period 1-7 January 2015.

The finding that CVarBC successfully corrects for scan-dependent or inter-satellite biases will, however, depend on the choice of parameters used in the CVarBC14 configuration. As noted earlier, the J_{VarBC} term of the cost function also penalizes any structure in the bias corrections that differs from zero, and may hence also dampen, for instance, corrections for scan-dependent biases or inter-satellite biases. It appears that in the present configuration this effect is small: the differences in the bias corrections estimated for different satellites in the CVarBC14 experiment are very similar to those obtained in the free VarBC experiment. Similarly, the slope of the scan-dependent bias correction in the CVarBC14 experiment is very similar to that of the free VarBC experiment. It appears that for the parameter choice used in these experiments, the reduction in the J_O term resulting from correcting the scan-biases or inter-satellite biases is outweighed by the associated increase in the J_{VarBC}-term. This is a very positive finding, as it makes CVarBC a powerful tool to identify and correct for such bias pattern, and any changes in them over time, a considerable advantage also from a maintenance perspective.

Analysis impact

The CVarBC14 experiment shows overall a greater consistency of the assimilation for the upper stratosphere/lower mesosphere compared to the Control. This can be seen, for instance, from a reduction in the standard deviation of background or analysis departures for the upper-most ATMS channels (Figure 5). Channels 12-15 of ATMS are equivalent to channels 11-14 of AMSU-A, and they are assimilated using the standard free VarBC configuration in the three experiments considered here. They thus provide an unconstrained diagnostic for our bias correction changes. Related to the smaller background departures are smaller increments above 10 hPa in the CVarBC14 experiment compared to the Control, as shown in *Figure 6*. These reductions are most likely a reflection of the better treatment of scan-dependent and inter-satellite biases, as this removes inconsistencies otherwise present in the Control experiment. Note that, not surprisingly, the free VarBC experiment fares even better in this regard, as it further reduces the influence of the AMSU-A channel 14 on any bias structures, albeit at the expense of not correcting model biases.

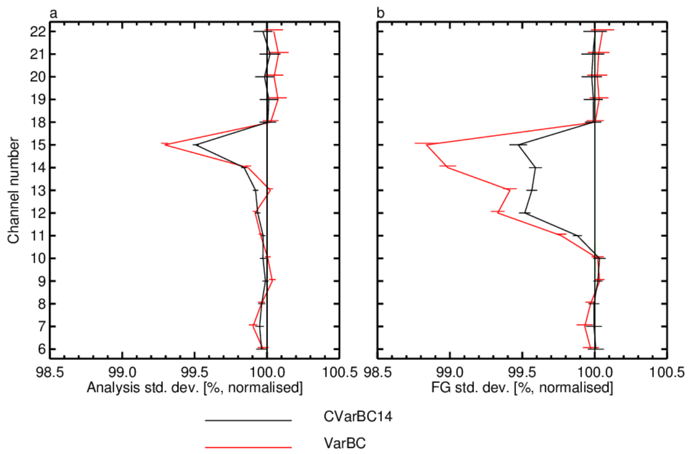

Figure 5: Standard deviations of analysis departures (left) and background departures (right) for used ATMS data, normalised by the values of the Control experiment, for the CVarBC14 experiment (black) and the VarBC experiment (red). Horizontal bars indicate statistical significance intervals (at the 95 % confidence level). Results have been combined for the two seasons considered here.

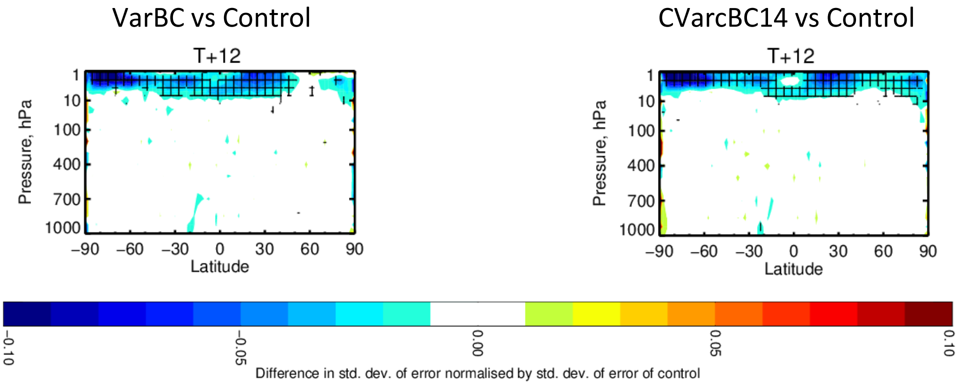

Figure 6: Normalised difference in the zonal mean standard deviation of the temperature increments for the VarBC experiment and the Control (left) and the CVarBC14 experiment and the Control (right). The differences are normalised by the values of the Control and negative values (blue) indicate smaller increments compared to the Control. The period covered is January-April 2015. Cross-hatching indicates statistically significant differences at the 95 % level.

The different treatment of the biases in channel 14 AMSU-A leads to changes in the mean temperature analyses in the three experiments. Reflecting the weighting function of this channel, the changes are mainly confined to levels above 5 hPa, as can be seen in *Figure 7* (right), but changes of a few tenths of a degree are present down to about 50 hPa. In the CVarBC14 experiment, the changes in the zonal mean temperature analysis compared to the Control are within ± 1 K up to 0.05 hPa, and hence relatively modest compared to the more drastic changes of ± 4 K in the free VarBC experiment (cf *Figure 7*, left).

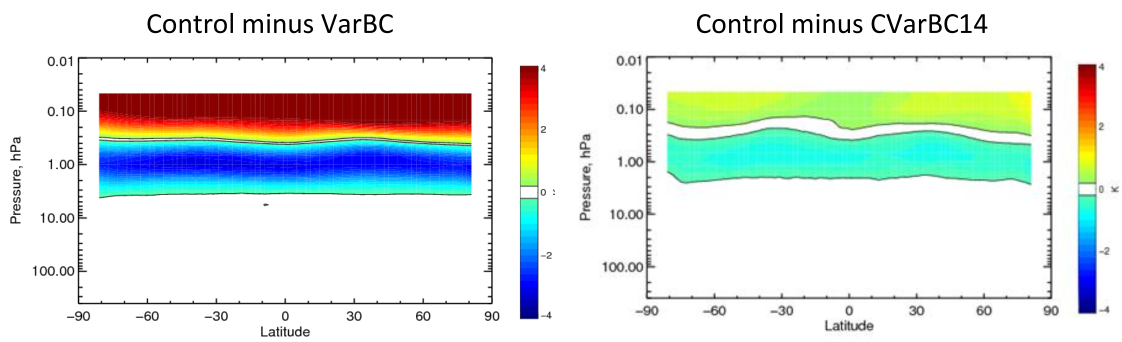

Figure 7: Zonal mean temperature difference between the Control and the VarBC experiment (left) and the Control and the CVarBC14 experiment (right) for December 2014 - February 2015. Negative values (blue) indicate a warming compared to the Control.

Radiosonde-temperature

GPSRO bending angles

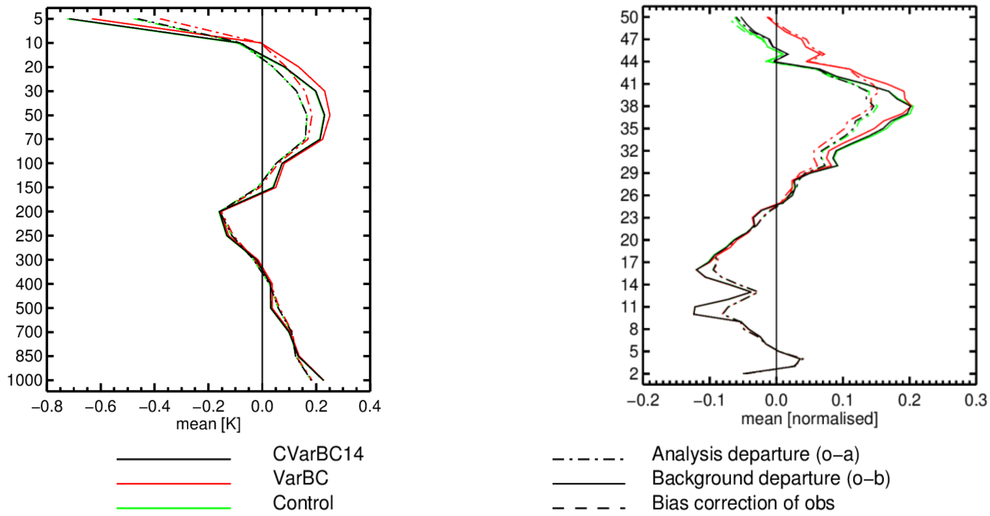

Figure 8: Global mean observation minus background (solid) or analysis (dash-dotted) for radiosonde temperatures (left) and GPSRO bending angles from all assimilated satellites (right). The period covered is December 2014 to April 2015.

It is difficult to validate these changes to the bias characteristics of the analyses, due to the limited number of observations with reliable bias characteristics for these levels. The only other assimilated data are temperature observations from radiosondes (up to 5 hPa) and bending angles from Global Positioning System (GPS) radio occultation (RO) measurements, the latter with relatively poor sensitivity above around 36 km height (~5 hPa). The radiosondes suggest slightly smaller biases for the Control and the CVarBC14 experiment between around 50-10 hPa compared to the VarBC experiment, whereas the VarBC experiment shows the smallest biases at 5 hPa. It is worth noting that the bias pattern at 10 hPa and above is very different from the one reported earlier for the ECMWF system in Di Tomaso and Bormann (2011) who show positive biases of around 0.8 K throughout these levels. This reflects changes in the bias characteristics of the forecast model since these investigations. In contrast to the results for the radiosondes, GPS RO bending angles indicate smaller biases above 40 km (~4 hPa) in the Control and the CVarBC14 compared to the VarBC experiment, with a very minor advantage for the CVarBC14 experiment.

The analyses have also been assessed against temperature retrievals from the Microwave Limb Sounder (MLS, Froidevaux et al. 2016). These may of course have their own bias characteristics, but they are one of the few datasets available that give temperature information with good global coverage in the upper stratosphere/lower mesosphere. Qualitatively consistent with the radiosonde temperature observations or the bias estimates shown in *Figure 1*, the MLS observations suggest a warm bias in the Control experiment between 10-2 hPa and a cold bias at levels around 1 – 0.3 hPa (*Figure 9*). The warm bias is slightly stronger in the 5-2 hPa range in the CVarBC14 experiment, but the changes are small compared to the biases of the Control against MLS (cf *Figure 7*). The VarBC experiment shows an even stronger bias at these levels. Above these levels, the situation is less clear, and none of the three experiments compare particularly well with MLS, reflecting that no observations are assimilated with strong sensitivity and vertical resolution at these levels.

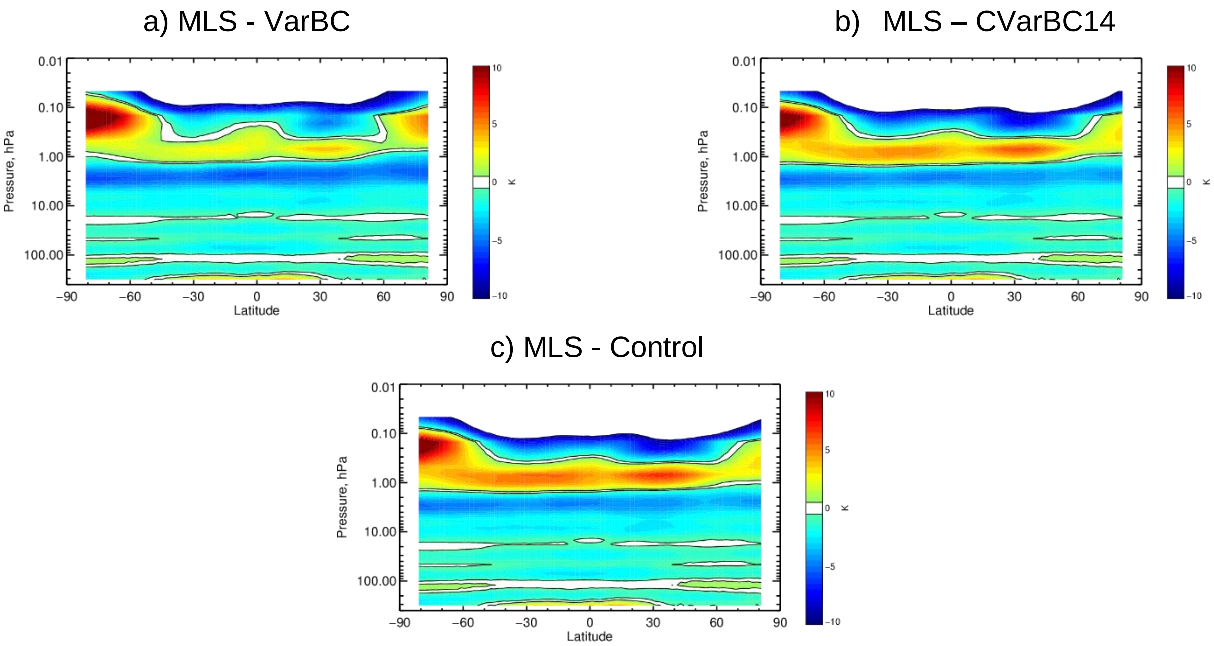

Figure 9: Zonal mean temperature differences between MLS retrievals and analyses for the three experiments considered here. The period covered is December 2014 - February 2015. Positive values (red) indicate warmer values for the MLS retrievals compared to the analyses.

In summary, the above analysis suggest that the CVarBC14 experiment and the Control lead to overall rather similar bias characteristics for the upper stratospheric temperature analysis, with a slight advantage for the CVarBC14 experiment when compared to the limited number of observations available for this region. This might suggest that CVarBC14 estimates a better global mean bias correction for AMSU-A channel 14 than the zero bias correction imposed in the Control. It is likely that this result is dependent on the particular size and sign of the model and observational biases, together with the particular parameter choice used in CVarBC14. This is because the information added to separate model and observational bias in the CVarBC14 experiment is limited, and primarily confined to an estimate of the uncertainty of the bias correction together with allowing for certain bias structures to be estimated. More importantly, the differences in the mean analyses between the Control and the CVarBC14 experiment are generally small compared to our ability to estimate temperature biases at these levels, and the CVarBC14 experiment hence constrains the stratospheric model biases similarly well as the Control.

Forecast impact

The forecast impact in the CVarBC14 experiment is overall positive for temperature in the upper stratosphere, but more neutral over the troposphere (Figure 10). There is some indication of a positive impact beyond day 5 for the CVarBC14 experiment in the troposphere over the winter hemisphere in both seasons (not shown), but this is mostly not statistically significant. For the upper stratosphere, forecast verification is again difficult, given the sparsity of observations, but the reduction in the standard deviation of the forecast error is considered a positive aspect.

Note that the VarBC experiment also performs well by the measures shown in Figure 10. This is because the verification is performed against the own analysis, and this does not capture the drifts in the bias of the analyses. The CVarBC14 experiment shows a clear advantage for these aspects, as demonstrated earlier. Note as well that the dominant signal in the forecast error in the upper stratosphere for all three experiments is the model bias that leads to a gradual increase in the mean temperature bias at these levels (Figure 11). Interestingly, this increase is strongest in the free VarBC experiment, whereas the Control and the CVarBC14 experiment fare similar in this respect.

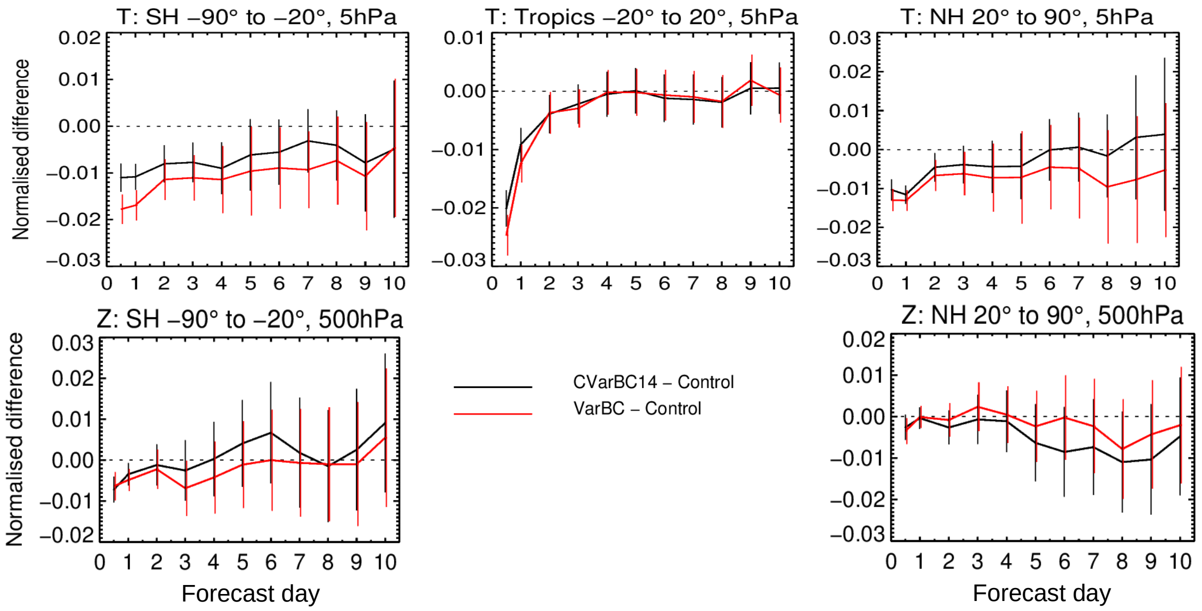

Figure 10: Top row: Normalised difference in the standard deviation of the temperature forecast error at 5 hPa vs the Control as a function of forecast range for the Southern Hemisphere (left), the tropics (middle) and the Northern Hemisphere (right). Black indicates results for the CvarBC14 experiment, red for the VarBC experiment, with vertical bars depicting 95 % confidence intervals. Bottom row: As top, but for the geopotential at 500 hPa for the Southern Hemisphere (left) and the Northern Hemisphere (right). Each experiment has been verified against its own analysis, and the results over the two seasons considered here have been combined, from up to 478 forecasts.

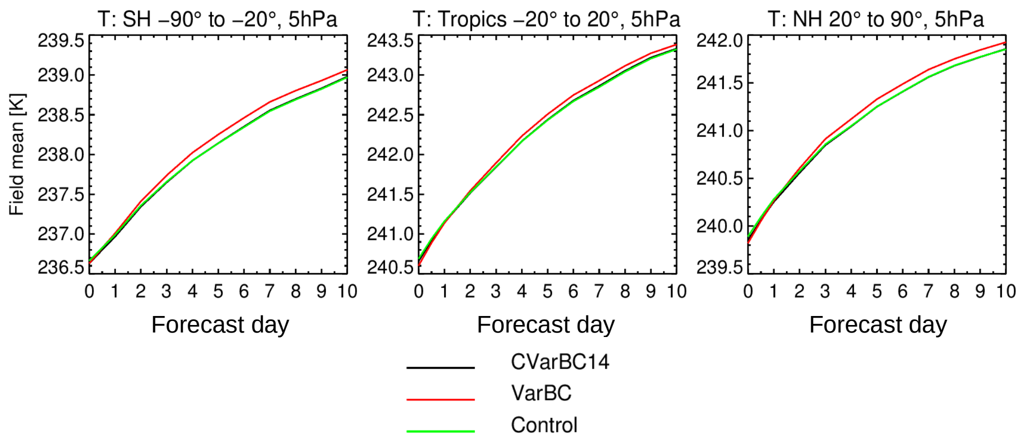

Figure 11: Mean temperature error at 5 hPa as a function of forecast range for the Southern Hemisphere (left), the tropics (middle) and the Northern Hemisphere (right), as verified against each experiments own analysis.

3.3 Extension to several AMSU-A channels

The above analysis has shown that using CVarBC for AMSU-A channel 14 is a viable alternative to assimilating this channel without a bias correction, with some benefits in terms of the corrected bias structures and the consistency of stratospheric temperature analysis. We will now briefly summarise preliminary work that explores further possibilities in this area opened up by CVarBC. In particular, we investigate constraining several upper stratospheric temperature channels from AMSU-A, to further aid the identification of model bias.

In addition to the CVarBC14 experiment introduced above, we conducted two further experiments:

CVarBC13-14: As CVarBC14, but additionally constrain the bias correction for channel 13. The pre-scribed bias value for channel 13 was set to 0 K, the same for all satellites, and R_b = (0.85 K)^2 (same as the observation error used for this channel), α = 0.2.

CVarBC12-14: As CVarBC14, but additionally constrain the bias correction for channels 12 and 13. The pre-scribed bias values for both channels was again set to 0 K, the same for all satellites, and R_b = (0.5 K)^2 for channel 12 and R_b = (0.85 K)^2 for channel 13 (same as the observation error used for these channels), with α = 0.1.

The two additional experiments otherwise use the same set up and period as the experiments introduced in the previous section. Also, the bias model for channels 12 and 13 is unchanged, that is, it consists of a global offset, and air-mass bias correction, and a scan-dependent bias correction.

Results

The CVarBC12-14 and CVarBC13-14 experiments share many of the characteristics of the CVarBC14 experiment when compared to the Control. That is, they also show bias corrections that identify inter-satellite differences in the bias and scan-dependent bias corrections for the channels treated through CVarBC. For channels 12 and 13, this is similar to their earlier treatment through free VarBC (not shown).

The additional constraint on the bias corrections does, however, affect the bias characteristics of the upper stratospheric temperature analysis. This is most noticeable in comparisons to GPSRO bending angle observations which show smaller biases for the CVarBC12-14 and CVarBC13-14 experiments (*Figure 12a*). In particular, the additional CVarBC experiments reduce some of the vertical structure of the bias above 30 km previously present in the Control or the CVarBC14 experiment. Some of the bias changes are also supported by radiosonde temperature observations, but the vertical information above 10 hPa (~30 km) is very limited here (*Figure 12b*). The CVarBC13-14 experiment overall shows the smallest biases against GPSRO or radiosondes. This CVarBC12-14 experiment identifies less of the vertical structure, despite constraining more channels. This may be due to choosing a smaller value for α in this case (ie imposing a weaker constraint for each channel). The interaction between the choice of channels to constrain and the strength of the constraint would need further investigation. In any case, the present results suggest that the upper-most AMSU-A channels can add some information on vertical characteristics of model bias, and these are currently mostly ignored in the Control or CVarBC14 by treating all channels except channel 14 through free VarBC.

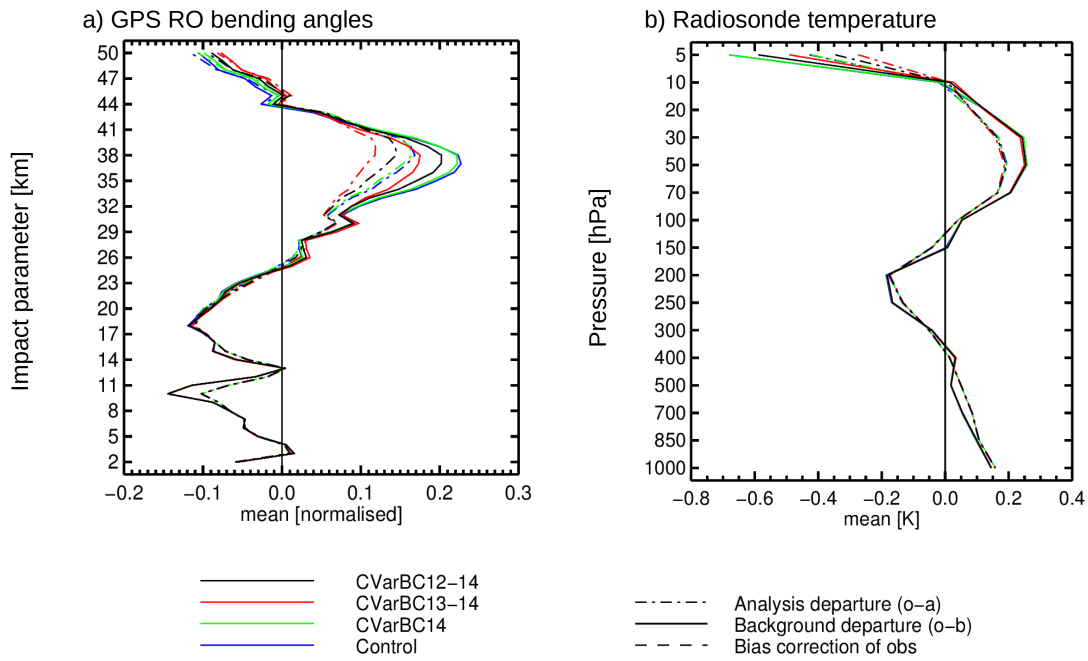

Figure 12: a) Mean departure for GPS RO bending angles over the Northern Hemisphere, normalized by the observation error used in the assimilation system, for the different assimilation experiments as indicated in the legend. Statistics have been calculated over the period December 2014 to February 2015. b) Mean departure for radiosonde temperature observations over the Northern Hemisphere.

The fit to other assimilated observations is otherwise mostly not statistically significantly changed when CVarBC is extended to other AMSU-A stratospheric channels. The only exception are FG-departures for ATMS which show a small, but statistically significant degradation for most channels when the CVarBC treatment is extended to other channels, particularly in the CVarBC12-14 case (*Figure 13*). This behaviour is not fully understood, but it appears that addressing upper stratospheric bias characteristics can have some effect throughout the atmospheric column.

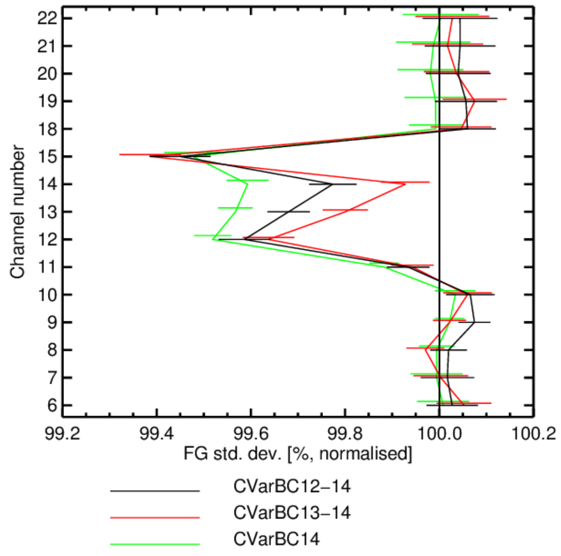

Figure 13: Global standard deviation of FG-departures for ATMS brightness temperatures, normalised by the values of the Control experiment. The three colours indicate the three experiments as given in the legend, and horizontal bars indicated 95 % confidence intervals. Statistics over the two seasons have been combined.

The forecast impact of extending the use of CVarBC to different channels is similar to that seen in the CVarBC14 experiment compared to the Control, that is, positive for temperature in the upper stratosphere, but more neutral over the troposphere.

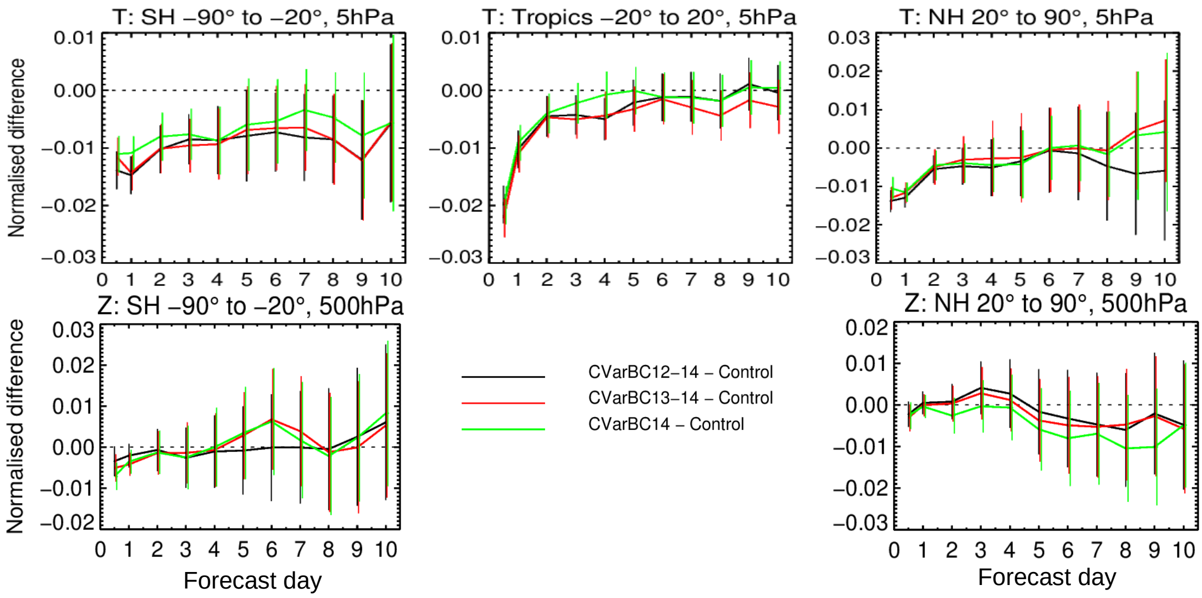

Figure 14: As Figure 10, but for the three experiments versus the Control as indicated in the legend.

3.4 Discussion

In summary, our experiments with applying CVarBC to upper stratospheric temperature sounding channels from AMSU-A showed the following results:

- When applied to channel 14 only, CVarBC is successful in constraining the drift in bias correction otherwise observed in a free-running VarBC experiment, while at the same time being able to correct for inter-satellite or scan-dependent biases.
- This leads to smaller increments in the upper stratosphere compared to an experiment in which channel 14 is assimilated without a bias correction, and mean temperature analyses that compare similarly well to other assimilated and independent observations.
- The use of CVarBC can be extended to other upper stratospheric channels, with other assimilated observations providing some suggestion of benefits in terms of correcting for the vertical structure of model biases in this case. However, when doing so some minor effects are also noted elsewhere in the atmosphere and this behaviour is not yet fully understood.

Overall, it appears that applying CVarBC to AMSU-A channel 14 is a viable and safe alternative to the current practice of assimilating AMSU-A channel 14 without a bias correction, with the benefit of being able to address inter-satellite and scan-dependent biases. If inter-satellite biases or scan-dependent biases were stable, these could of course also be treated more simply in a static way. But the application of CVarBC reduces the need for maintenance in this respect, and this is considered a positive aspect. The latter is particularly beneficial for reanalysis applications, where long periods with several different instruments/satellite are treated fairly rapidly.

4 CVarBC for infrared ozone channels

The use of ozone information from infrared radiances is another area where model biases combined with a lack of sufficient anchoring observations have in the past led to an unrealistic drift of variational bias corrections. The only other observations with some profile information currently assimilated in the operational ECMWF NWP system are retrievals from SBUV, and these are assimilated without bias correction and serve as a partial anchor. However, as discussed in Dragani and McNally (2013), additional anchoring needs to be provided, and this is currently achieved by assimilating selected ozone channels of the hyperspectral infrared instruments (IASI, AIRS, CrIS) without bias corrections. These anchor channels were chosen on the basis of the ozone sensitivity and are successful in preventing unrealistic drifts.

Recent work has, however, highlighted considerable bias uncertainty for the selected ozone channels arising from uncertainty in the spectroscopy. This is highlighted in Figure 15 which shows mean biases (before bias correction) between observations and background equivalents for ozone-sensitive IASI channels calculated with two different versions of spectroscopy/line-by-line models. One is based on kCarta (as currently applied at ECMWF in operations), whereas the other uses the updated spectroscopy available with LBLRTM v12. The model background fields and observations are the same in both cases, only the radiative transfer calculations differ. The anchor channel currently used for IASI is channel 1585, which shows some of the largest differences in bias (of around 0.7 K) in these comparisons, which would lead to considerable changes in the ozone analysis if the same anchor was used with the different spectroscopy. Similarly, during a recent upgrade of the assumed observation error covariance matrix used for IASI, Bormann et al. (2015) found it necessary to change the ozone anchor channel when more weight is given to the ozone channels. Both experiences indicate draw-backs when anchoring the ozone analysis through choosing a single channel as a hard anchor, as it does not allow for unavoidable biases arising from the radiative transfer.

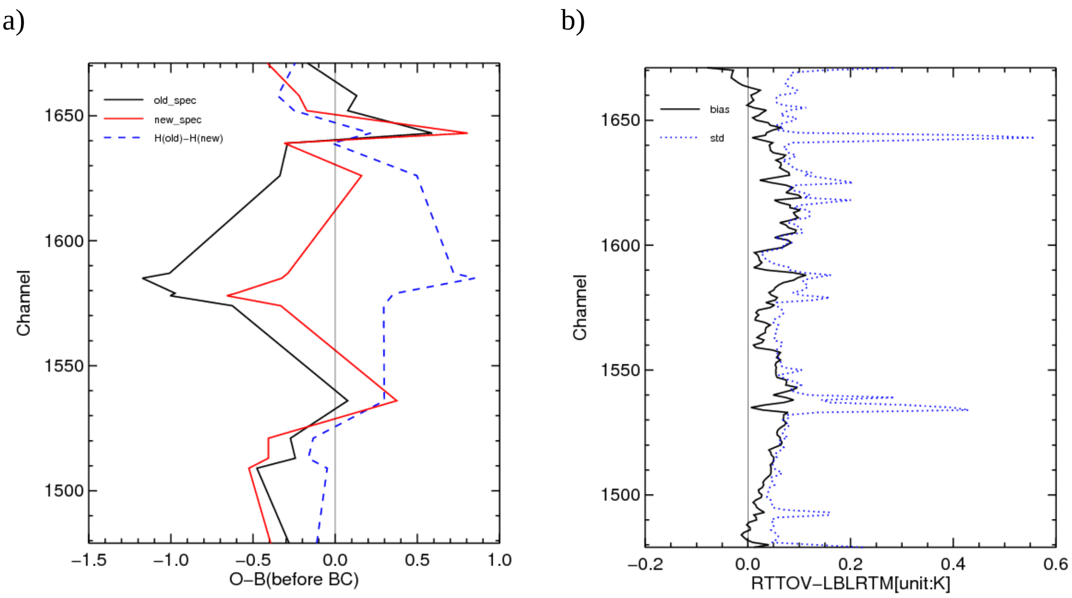

Figure 15: a) Mean difference between observations and background equivalents (before bias correction, K) for IASI ozone channels from Metop-A using old (black) and new (red) spectroscopy. Also shown is the difference between the two radiative transfer calculations (dashed blue). b) Differences between RTTOV and line-by-line model simulations from LBLRTM for IASI ozone channels in terms of bias (black) and standard deviation (dotted blue) for a diverse set of profiles.

4.1 Experiments

In the following we investigate the use of CVarBC for ozone channels as an alternative to assuming that a single channel is unbiased. As it is not clear that one particular channel is expected to be less biased, we decided to apply CVarBC to all ozone-affected channels of the assimilated hyperspectral infrared instruments, and we set the a-priori estimate $\mathbf{b}_0$ for the bias correction to zero. Treating all ozone channels through CVarBC acknowledges that there is uncertainty about the bias characteristics for all these channels. The choice is also motivated by the finding that there are considerable differences in the bias characteristics between different ozone-sensitive channels (Figure 15), and a-priori it is not clear which of these biases are due to radiative transfer bias or due to biases in the model ozone fields. Setting $\mathbf{b}_0$ to zero for all these channels of course still assumes that the overall bias over the ozone band is close to zero. The $\mathbf{R}_b$ matrix together with α in equation (1) should reflect the uncertainty in our a-priori estimate of the bias correction. The largest source of observation-related bias is considered to be the ozone spectroscopy for these channels. The choice of $\mathbf{R}_\mathrm{b}$ and α should therefore reflect estimates of the accuracy of the spectroscopy for different channels. In the absence of other information on this, we instead set these parameters to empirically determined values, linked to the specification of the observation errors.

The following assimilation experiments were conducted over the period June-August 2015, using ECMWF’s 12-hour 4DVAR assimilation system:

Control: Similar to operations, but using an updated observation error covariance matrix for IASI and channel 1574 as ozone anchor channel for IASI. This is the same configuration as described as “NewR” experiment in Bormann et al. (2016), and it will be the operational configuration for IASI in the next update of the operational ECMWF system.

CVarBCO3_1: As Control, but treating the ozone channels of IASI, AIRS, and CrIS using CVarBC. The channels and parameter choices are given in Table 1. For all three instruments, $\mathbf{R}_b$ is assumed to be diagonal, with the error standard deviation similar to the assumed observation error standard deviations, and α = 0.5 for most channels. A slightly smaller value of α has been chosen for two IASI channels, as these exhibit stronger uncertainty resulting from the fast parameterizations used in RTTOV, so a weaker constraint is imposed on these.

CVarBCO3_2: As CVarBC, but using α = 0.2 instead of α = 0.5, thus imposing a weaker constraint on the bias correction to test the sensitivity to this parameter choice.

Table 1: Parameter choices for CVarBC experiments for ozone.

	IASI (Metop-A & -B)	AIRS	CrIS
Range of channel numbers treated by CVarBC	1479 – 1671 (16 selected channels)	1012 – 1123 (20 selected channels)	590 – 685 (17 selected channels)
Parameter choice CVarBCO3_1 experiment	$R_b = (0.5\ K)^2$ α = 0.5, except for 1536 and 1643 for which α = 0.1	$R_b = (2.0\ K)^2$ α = 0.5	$R_b = (1.2\ K)^2$ α = 0.5
Parameter choice CVarBCO3_2 experiment	$R_b = (0.5\ K)^2$ α = 0.2, except for 1536 and 1643 for which α = 0.1	$R_b = (2.0\ K)^2$ α = 0.2	$R_b = (1.2\ K)^2$ α = 0.2

In these experiments, the bias correction model used for most of the ozone channels for all instruments is a linear model with a global constant and four layer thicknesses as airmass-predictors, combined with a third order polynomial in the scan angle to handle scan-dependent biases. The only exception is the treatment of CrIS in the Control experiment, for which the air-mass component is excluded, as is currently done in the operational use of CrIS. The CVarBC experiments bring the use of CrIS ozone channels in line with the other hyperspectral instruments in this regard. All experiments were conducted at a spatial resolution of T_L511 (≈40 km), with a T_L255 (≈80 km) incremental analysis resolution, and 137 levels in the vertical, and in the context of the full observing system.

4.2 Results

Performance of bias correction

Figure 16 summarizes the performance of the bias correction for IASI, AIRS and CrIS ozone channels for the three experiments, in terms of the mean bias correction, and the mean FG and analysis departure after bias correction. For AIRS and CrIS, there are sizeable changes to the mean bias correction for the anchor channels (i.e., channel 1088 at 9.623 µm for AIRS, and channel 626 at 9.61 µm for CrIS), and as a result large differences in the mean departures after bias correction. In contrast, the anchor channel for IASI shows only a relatively small change, a result of using an anchor channel that has recently been updated for this instrument. As expected, the bias corrections are now weakly anchored over all channels, and this leads to an overall shift in the bias corrections for all channels. For IASI and AIRS this is relatively small for the channels that are not anchored in the Control (typically -0.2 K), whereas for CrIS it is a little stronger. All adjustments to the bias corrections occur fairly quickly, over the course of a few days, after which the bias corrections are stable (not shown).

The applied bias corrections show considerable spectral structure, and, as expected, the size of this is sensitive to the strength of the applied soft anchoring. In CVarBCO3_1 with the stronger constraint, the spectral structures of the bias corrections are somewhat dampened compared to CVarBCO3_2. Interestingly, at the same time CVarBCO3_1 shows more spectral structure in the mean FG departures after bias correction, with stronger non-zero departures. However, the difference between the mean analysis and FG departures for these structures is relatively small, suggesting that only a small proportion of these non-zero mean FG departures are converted into analysis increments. This may indicate that the spectral structures originate primarily from radiative transfer biases, rather than forecast model biases (as the latter could be corrected through analysis increments). Consistent with this interpretation, the shape of the spectral bias structures is similar to the differences in the bias between the two spectroscopies shown in *Figure 15*. It is also noteworthy here that CVarBCO3_2 overall shows mean departures after bias correction that are consistently closer to zero for the various channels than in CVarBCO3_1, indicative of a more consistent bias correction in the experiment with the weaker constraint.

In this context it is worth pointing out that the bias correction for the HIRS ozone channel (channel 9) is also closer to zero for the CVarBC experiments, with global mean bias corrections of 0.2 K, 0.1 K and 0.05 K for the Control, the CVarBCO3_1 and the CVarBCO3_2 experiments, respectively. The bias correction for HIRS channel 9 is allowed to adjust freely with VarBC, and the smaller bias corrections give a further indication of good consistency with other observations.

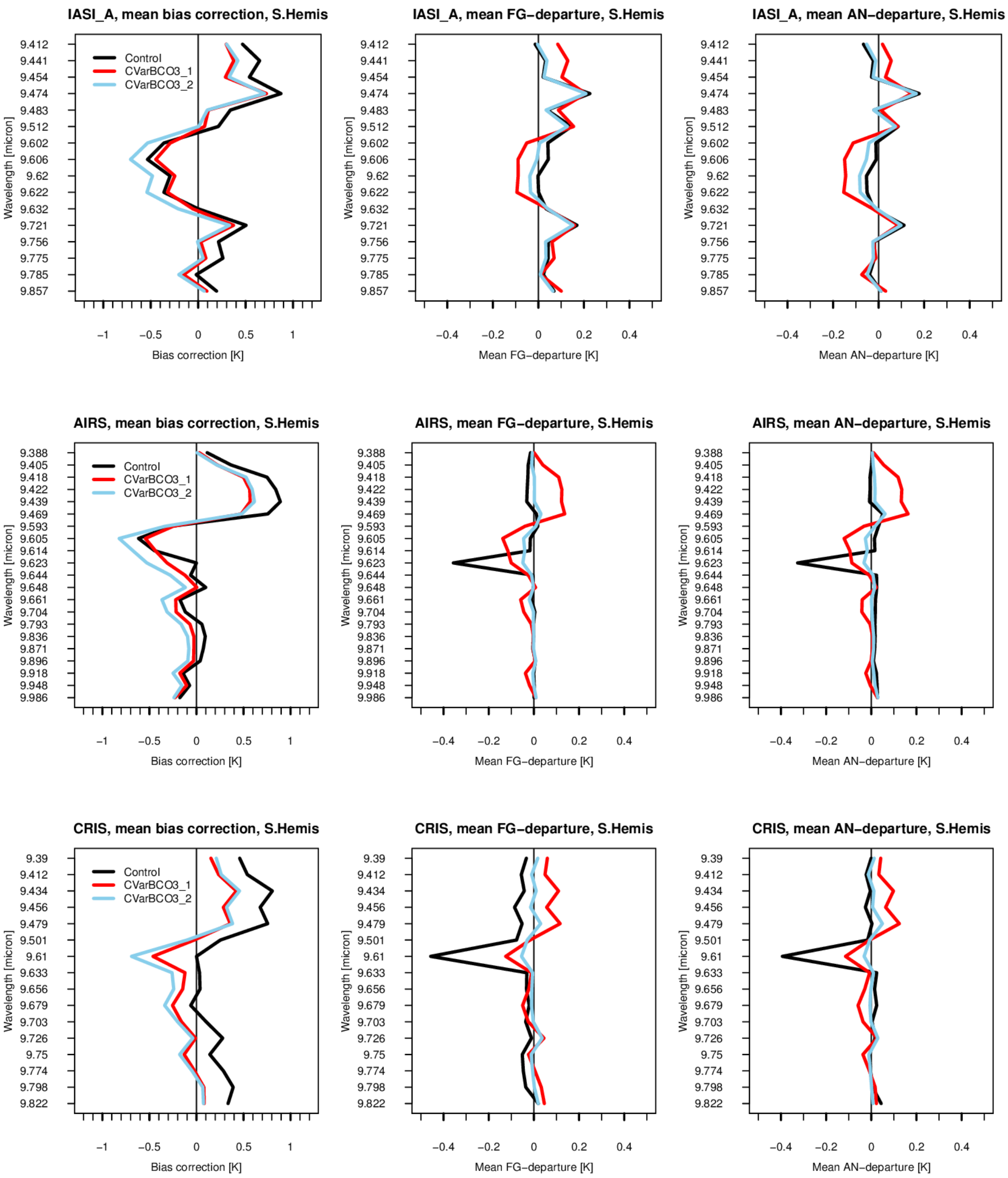

Figure 16: Mean bias corrections (left column), mean FG-departures after bias correction (middle column), and mean analysis departure (right column) for the ozone channels from IASI from Metop-A (top row), AIRS (middle row), and CrIS (bottom row) for August 2015 over the Southern Hemisphere.

Analysis and forecast impact

The modifications to the bias correction for the ozone channels of hyperspectral IR observations lead to small, but statistically significant reductions in the standard deviations of FG departures for the affected channels (*Figure 17*). This is considered to be a positive aspect, as it indicates a better consistency between the short-range forecast and the observations and their treatment in the assimilation system. The reduction is largest for the CrIS ozone channels, where it reaches up to 10 %, most likely primarily a result of allowing an air-mass component in the bias correction model. For AIRS and IASI, the reductions are typically 1 % for the ozone channels for the CVarBCO3_2 experiment, and a little less for the CVarBCO3_1 experiment. The CVarBCO3_2 experiment with the weaker anchoring performs again better in this respect.

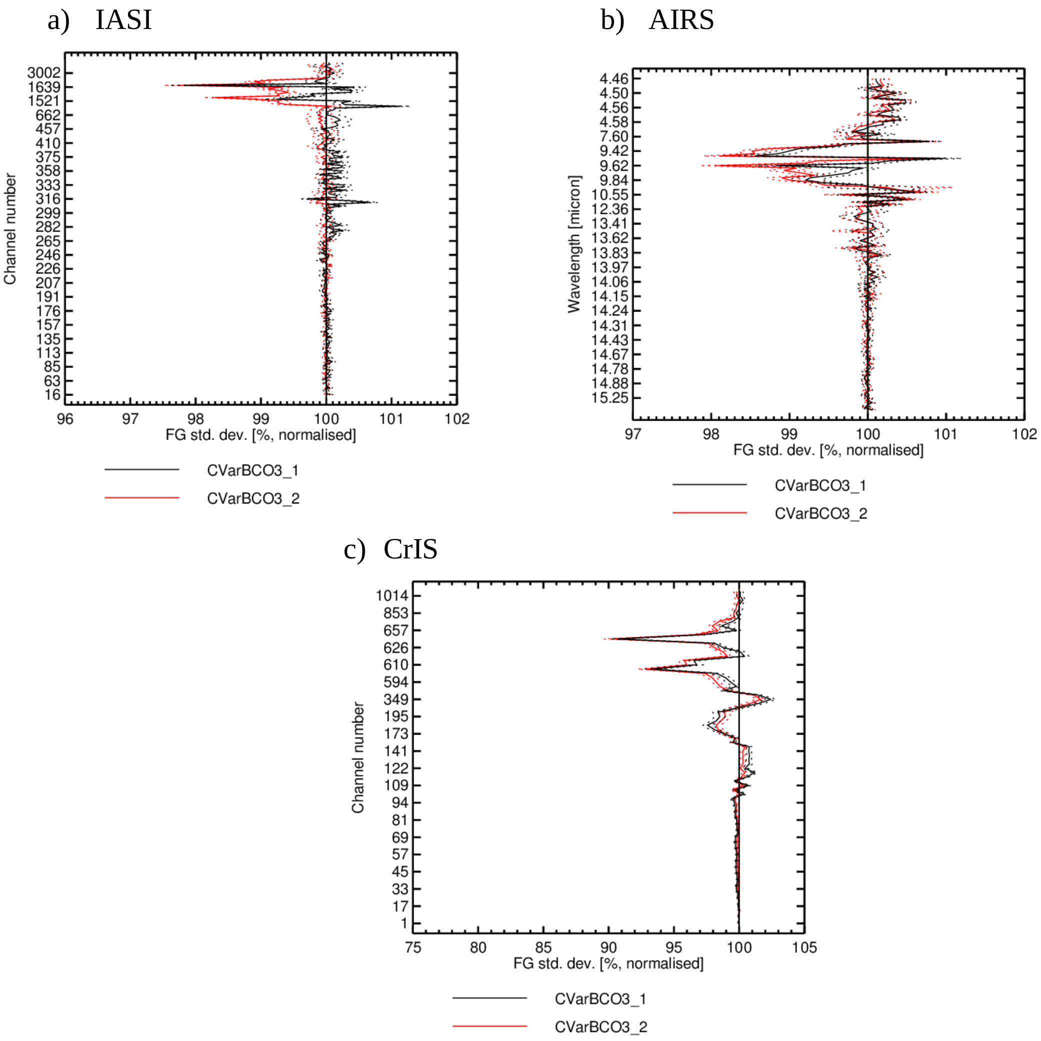

Figure 17: a) Normalised standard deviation of FG-departures [%] for assimilated IASI observations as a function of channel number (global). The values have been normalised by equivalent values of the Control. Black lines indicate results from the CVarBCO3_1 experiment, red lines indicate results for the CVarBCO3_2 experiment. Dotted lines indicate significance intervals at the 95 % level. b) As a), but for AIRS. c) As a), but for CrIS.

The CVarBC experiment with the weaker constraint also shows a good performance when assessed against independent, but also assimilated SBUV retrievals. In terms of biases, these observations indicate little difference between the CVarBCO3_2 experiment and the Control, but the CVarBCO3_1 experiment shows somewhat larger biases around 25 – 65 hPa and below 250 hPa (*Figure 18*). The CVarBCO3_1 and CVarBCO3_2 experiments both show statistically significant benefits over the Control in terms of the standard deviation of FG-departures for SBUV retrievals (*Figure 19*), with reduction in the CVarBCO3_2 experiment of 2 – 5 % in the extra tropics. While the benefits are relatively small, the results further suggest that CVarBC offers a viable alternative to anchor the ozone analysis and the associated variational bias correction.

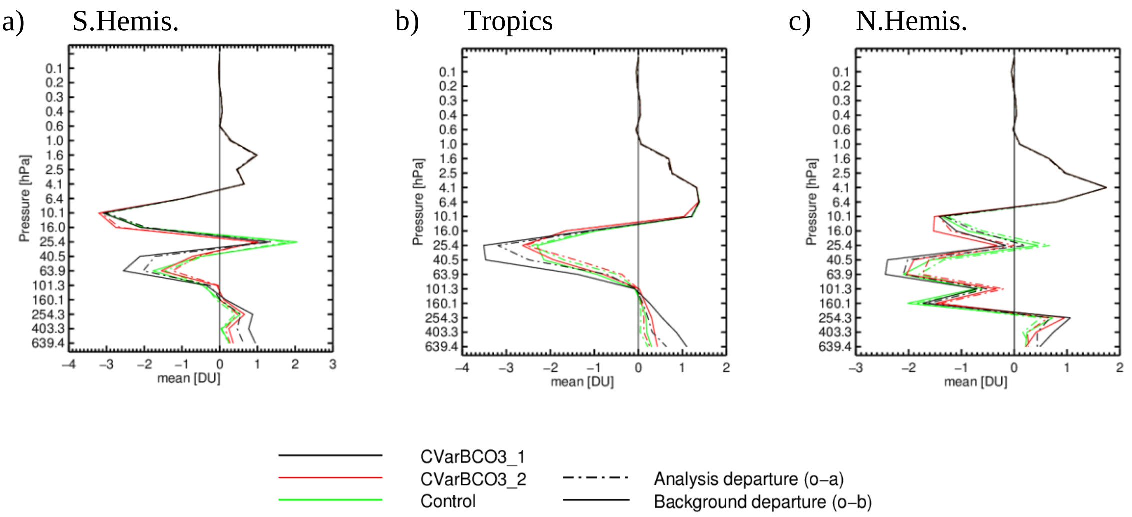

Figure 18: Mean departure for SBUV ozone retrievals from NOAA-19 for a) the Southern Hemisphere, b) the Tropics, and c) the Northern Hemisphere, covering June to August 2015. Solid lines indicate statistics for background departures and dash-dotted lines indicate analysis departures, with the three experiments as given in the legend.

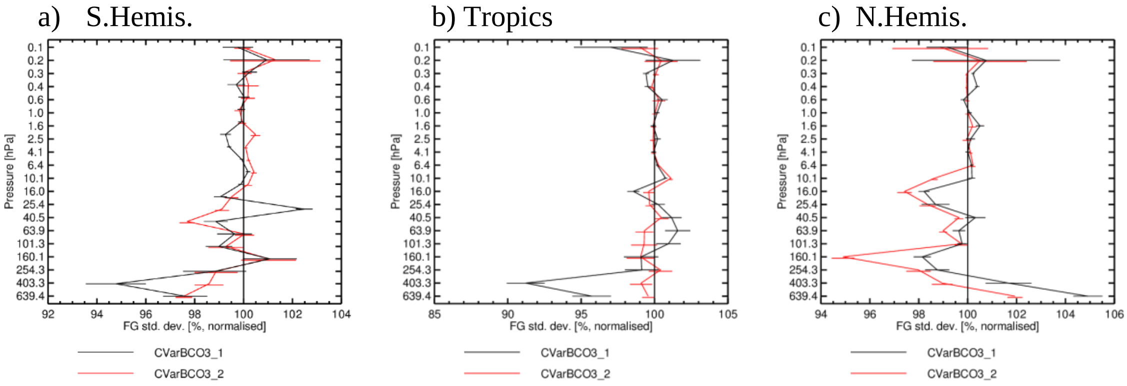

Figure 19: Normalised standard deviation of FG-departures [%] for assimilated SBUV retrievals from NOAA-19. The values have been normalised by equivalent values of the Control. Black lines indicate results from the CVarBCO3_1 experiment, red lines indicate results for the CVarBCO3_2 experiment. Horizontal bars indicate significance intervals at the 95 % level. The three panels show, respectively, a) the Southern Hemisphere, b) the Tropics, and c) the Northern Hemisphere., for the period June to August 2015.

The ozone analyses of the experiments discussed here have also been compared to MLS retrievals and ozone sondes, to further evaluate the changes introduced through the bias correction changes. Mostly, the changes to the biases in the ozone analysis are small compared to the mean differences between the MLS retrievals and the ozone analyses (*Figure 20*). In some regions, the bias against MLS is closer to zero (e.g., at high southern latitudes around 20-40hPa), but some stronger biases can also be found (e.g., over the northern tropics around 10-30 hPa). Over the Northern Hemisphere, where a reasonable sample of ozone sondes is available, comparisons to ozone sondes suggest some improvements in the vertical structure of the biases in the 20-200 hPa range (*Figure 21*). Even though the sample size is small, this is an encouraging result, as it gives some support for the changes introduced through CVarBC.

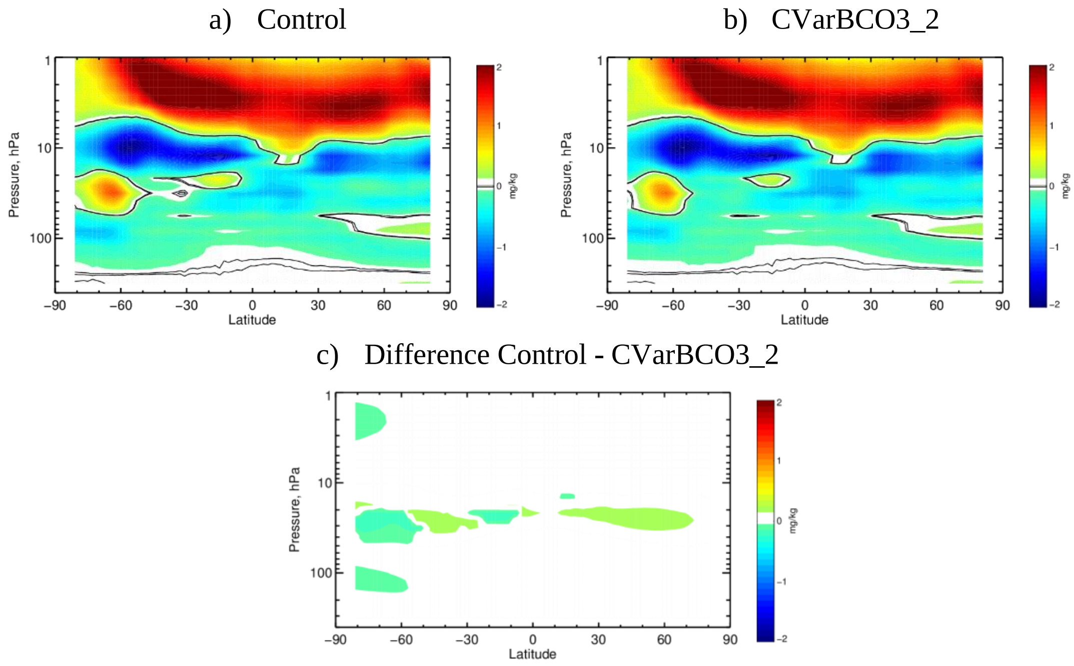

Figure 20: Zonal bias of the ozone analyses [mg/kg] from the Control (a) and the CVarBCO3_2 (b) experiment against MLS retrievals (MLS minus analysis) for the period June to August 2015. c) Difference in ozone analyses between the two experiments.

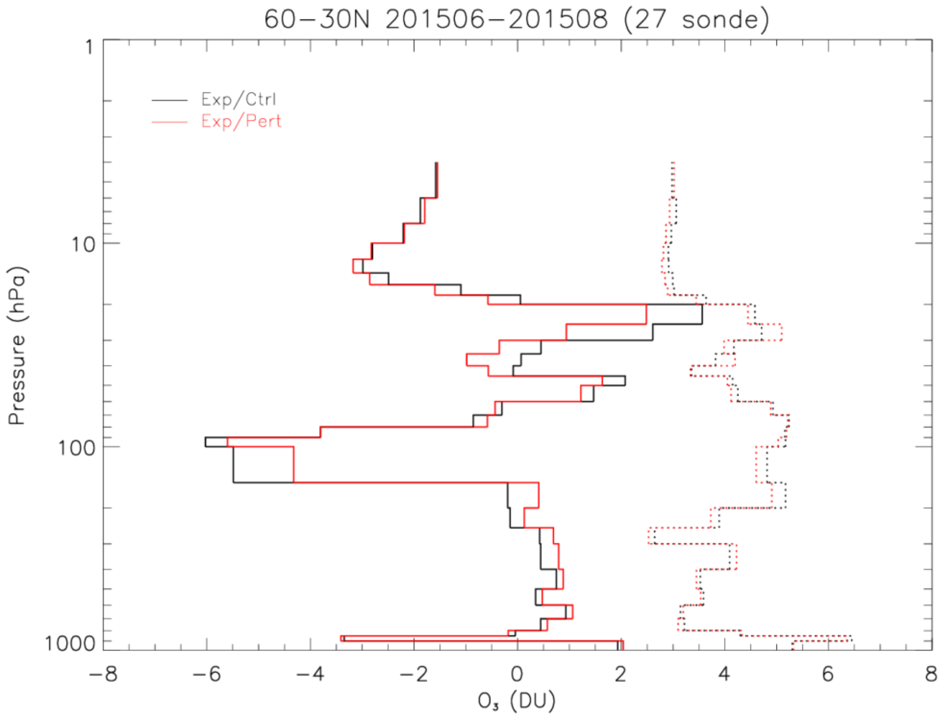

Figure 21: Mean (solid) and standard deviation (dotted) of the differences between ozone observations from sondes and the analyses over the Northern Hemisphere. Black indicates results from the Control, whereas red indicates results from the CVarBCO3_2 experiment. Results are based on 27 sonde ascends.

Lastly, the forecast impact of the above changes is neutral over the period considered, in line with expectations given the relatively small changes to the ozone analysis (not shown).

4.3 Discussion

In this section we have investigated the use of CVarBC for all ozone channels from hyperspectral infrared instruments, in comparison to using VarBC and assimilating a single ozone channel per instrument without bias correction. The main findings are:

- Applying a constraint on the size of the bias correction to all ozone channels for hyperspectral infrared instruments is a viable alternative to anchoring the variational bias correction for ozone channels and the resulting ozone analysis, compared to the ad-hoc selection of a single channel assimilated without bias correction.
- CVarBC applies sizeable bias corrections to the channels previously used as anchor channels for CrIS and AIRS. This puts into question whether these channels indeed can be assimilated without bias correction. Bias corrections for other ozone channels are relatively unchanged.
- The two approaches lead to a very similar performance in terms of biases in the ozone analysis, with some benefits for the CVarBC experiment with a relatively weak constraint in terms of the fit to ozone radiances and SBUV retrievals.
- The performance of the CVarBC scheme is sensitive to the strength of the constraint placed on the size of the bias correction, and too strong a constraint can lead to inappropriate dampening of spectral structures in the applied bias corrections.

The findings presented here should be viewed in the context of the results of Bormann et al. (2015) who found very significant benefits from updating the choice of ozone anchor channel for IASI when more weight was placed on the IASI ozone channels. Our results suggest that the introduction of CVarBC would have resulted in a similarly significant benefit compared to using the old anchor, without the need for an ad-hoc choice of anchor channel. So while the benefits of CVarBC shown here appear relatively small, they are only small because the anchor channel for IASI has recently been revised. Similarly, further experimentation in the context of the old observation errors for IASI shows much stronger benefits from CVarBC when used instead of the old anchor channel (not shown). This provides further evidence that the use of CVarBC indeed makes the bias correction more robust against changes in the radiative transfer biases in single channels, provided the overall bias of the assimilated ozone channels is indeed small.

5 Conclusions

The present memorandum explores the use of a modified version of VarBC in which the size of the bias correction is controlled through an additional constraint ("Constrained VarBC, CVarBC"). We applied this new methodology to two areas where currently ad-hoc decisions of assimilating data without any bias corrections have been made in the ECMWF system, namely the assimilation of upper stratospheric temperature observations from AMSU-A and ozone observations from hyperspectral infrared sounders. In both cases, our results show that the new method is able to constrain bias corrections successfully, while at the same time being able to allow for some observation-related bias structures to be corrected. In both cases, the overall bias characteristics of the temperature or ozone analysis are similar when CVarBC is applied compared to current practice, while showing some benefits in terms of consistency with other observations.

An additional benefit of applying CVarBC is that it results in a bias correction treatment that is relatively easy to maintain. Of course, some benefits of CVarBC found in the present experimentation could be achieved through other approaches. For instance, a static bias correction that addresses only inter-satellite or scan-position dependent biases could be applied in the case of AMSU-A channel 14. However, this would require updates whenever a new instrument is introduced or these structures change. This is particularly cumbersome in reanalysis applications, and it is here that we see the clearest benefits in this regard.

The present experimentation has examined the performance of CVarBC in the context of strong-constraint 4-dVar and in the presence of considerable model bias. At least in the case of the treatment of the stratospheric temperature analysis, there are clear links between this work and developments of estimating the model bias in 4-dVar as performed in weak-constraint 4d-Var (e.g., Fisher et al 2011, Goddard 2016). The use of weak-constraint 4d-Var is expected to be re-activated for the stratosphere with cycle 43r1. Although the two methods are addressing different aspects of the problem, their interaction should be studied. Weak-constraint 4d-Var relies on observational constraints to estimate the model bias (such as assimilating AMSU-A channel 14 without a bias correction), and the ability of CVarBC to provide such a constraint should be confirmed. The model biases in the stratosphere are also expected to change considerably with cycle 43r1, due to the change in the ozone climatology. While this should not affect the ability of CVarBC to provide a useful constraint, the performance needs to be re-evaluated. In addition, our current experimentation covers relatively short periods of several months, whereas drifts in the bias corrections have previously been observed over longer time-scales such as at least one year. Longer experimentation with CVarBC are hence advised.

There are also some general open questions regarding the application of CVarBC not addressed here and opening opportunities for further work. As seen in the CVarBC experiments with ozone, the performance of CVarBC is sensitive to the specification of the bias uncertainty (parameters $\mathbf{R}_b$ or α). More work would be beneficial to determine better ways to specify these parameters (together with the value of the "expected bias" $\mathbf{b}_0$), including their physical and statistical interpretation. This most likely requires a better understanding of the sources of the biases, for instance the calibration uncertainty in the case of the stratospheric AMSU-A channels or the magnitude of radiative transfer biases in the case of the ozone experimentation. This may also lead to a re-formulation of the additional cost-function term introduced for CVarBC to better reflect which characteristics can be best constrained.

The present memorandum considered two very different areas of applying CVarBC, and there are other areas for which CVarBC could be considered. For instance, previous experience has highlighted problems with interaction between VarBC and quality control in cases of skewed departure distributions, resulting in the choice to constrain the bias correction by not allowing for an airmass-dependent correction (e.g., Auligné and McNally, 2007). CVarBC may also offer benefits in this area, possibly allowing the correction of a part of the airmass bias that is currently neglected. Studies in this direction are left for future work.

Acknowledgements

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