TECHNICAL MEMORANDUM

584

Toward a consistent reanalysis of the upper stratosphere based on radiance measurements from SSU and AMSU-A

Shinya Kobayashi[1,2],
Marco Matricardi[1], Dick Dee[1]
and Sakari Uppala[1]

[1]European Centre for Medium-Range Weather
Forecasts, Reading, UK

[2]Japan Meteorological Agency, Tokyo, Japan

Research Department

February 2009

Submitted to Quart.J. Roy.Meteor.Soc.

European Centre for Medium-Range Weather Forecasts
Europäisches Zentrum für mittelfristige Wettervorhersage
Centre européen pour les prévisions météorologiques à moyen

Series: ECMWF Technical Memoranda
A full list of ECMWF Publications can be found on our web site under:
http://www.ecmwf.int/publications/

Contact: library@ecmwf.int

European Centre for Medium Range Weather Forecasts
Shinfield Park, Reading, Berkshire RG2 9AX, England

ABSTRACT

Radiance measurements from the Stratospheric Sounding Unit (SSU) and the Advanced Microwave Sounding Unit (AMSU-A) are the primary source of information for stratospheric temperature in reanalyses of the satellite era. To improve the time consistency of the reanalyses, radiance biases need to be properly understood and accounted for in the assimilation system. The investigation of inter-satellite differences between SSU and AMSU-A radiance observations shows that these differences are not accurately reproduced by the operational version of the radiative transfer model for TOVS (RTTOV-8). We found that this deficiency in RTTOV was mainly due to the treatment of the Zeeman effect (splitting of the Oxygen absorption lines at 60 GHz) and to changes in the spectral response function of the SSU instrument that are not represented in RTTOV. On this basis we present a revised version of RTTOV which can reproduce SSU and AMSU-A inter-satellite radiance differences more accurately.

Assimilation experiments performed with the revised version of RTTOV in a four-dimensional variational analysis system (4D-Var) show some improvements in the stratospheric temperature analysis. However, significant jumps in the stratospheric temperature analysis still occur when switching satellites, which is due to the fact that systematic errors in the forecast model are only partially constrained by observations. Using a one-dimensional retrieval equation, we show that both the extent and vertical structure of the partial bias corrections must inevitably change when the nature of the radiance measurement changes with the transition from SSU to AMSU-A.

1. Introduction

Stratospheric temperature reanalyses, dominated by radiance data from the Stratospheric Sounding Unit (SSU) and the Advanced Microwave Sounding Unit (AMSU-A), are strongly affected by instrument biases for these sounders. Changing bias characteristics in stratospheric channels are often reflected as jumps in stratospheric temperature analyses due to satellite transitions or as drifts due to slower changes in biases. These features can mask the true climate signals and make it difficult to reliably estimate long-term temperature trends. Thus biases in observations must be accounted for to produce a consistent atmospheric dataset suitable for climate research.

Using satellite data in an assimilation system requires a fast radiative transfer model (RTM) for predicting radiances from first-guess model fields. Several different RTMs are in use at NWP centres, e.g. the radiative transfer model for TOVS (RTTOV) (Saunders et al., 1999) and the Community Radiative Transfer Model (CRTM) (Kleespies et al., 2004). Especially for early satellite instruments, systematic errors in the interpretation of the measured radiances can result from an improper characterization of the spectral response functions or from changes in the concentration of radiatively active constituents that are unaccounted for in the RTMs. These types of error in the RTMs will generate biases in the data assimilation, and must therefore be addressed as well when using satellite observations for reanalysis.

Stratospheric temperatures have been retrieved from radiance observations made by the NOAA polar orbiting satellites since 1978. Data from infrared SSU channels on the TIROS-N to NOAA-14 satellites have been used to retrieve stratospheric temperature information. From NOAA-15 onward SSU was replaced by AMSU-A, which is a higher vertical resolution microwave instrument. Raw SSU radiances were first assimilated in ECMWF's 45-year ERA-40 reanalysis and more recently in the Japanese 25-year Reanalysis (JRA-25). Both reanalyses encountered difficulties to fully utilize the SSU radiance data. Particularly problematic periods are the early 1980s, when SSUs had large inter-satellite biases, and the late 1990s, when AMSU-A data first became available. These problems are exacerbated by the presence of large systematic errors in the background temperatures combined with inadequate data coverage for most of the period.

As pointed out by Nash and Forrester (1986), one possible explanation for the large SSU biases is the variation of the SSU spectral response function over time and between different satellites. This is not taken into account in the RTTOV radiative transfer model used for ERA-40 and JRA-25. The quality of the RTTOV simulations for the stratospheric channels of AMSU-A has also been questioned. Garand et al. (2001) found that radiances computed by RTTOV differ significantly from those computed by other forward models, possibly due to the treatment of the Zeeman effect in RTTOV.

In section 2 of this paper, we use co-located observations produced by the Simultaneous Nadir Overpass (SNO) technique (Cao et al., 2005) to evaluate inter-satellite SSU radiance differences and inter-satellite radiance differences between SSU and AMSU-A. In section 3 we present a revision of the RTTOV model that more accurately reproduces the observed SSU and AMSU-A inter-satellite radiance differences. Section 4 presents results of assimilation experiments performed with this revised version of the RTTOV model. In section 5 we use a one-dimensional retrieval equation to explain the impact on stratospheric temperature analyses of changes in radiative transfer characteristics when transitioning from SSU to AMSU-A. Conclusions are summarized in section 6.

2. Evaluation of inter-satellite biases

We use the SNO technique (Cao et al., 2005) to estimate inter-satellite biases between SSU instruments, This technique compares nadir observations made by different satellite instruments at the same time and location. Since both instruments view identical atmospheric profiles, this comparison produces reliable estimates of the inter-satellite biases that can be attributed to differences in the radiometric and spectroscopic performance of the instruments. Figure 1a shows time series of measured inter-satellite radiance differences between NOAA-6 and NOAA-7 for SSU channel 3 over the Antarctic. The seasonal dependence of the relative bias evident in Figure 1a can be correlated with the lapse rate in the upper stratosphere, indicating that the weighting functions corresponding to the two instruments are not identical. Figure 1b shows inter-satellite radiance differences between SSU channel 3 and AMSU-A channel 14 , both measured by the SNO technique and simulated using RTTOV. The discrepancies, which are especially significant in spring and winter, cannot be explained by instrument errors alone, which suggests that the RTTOV radiance simulations themselves may be inaccurate.

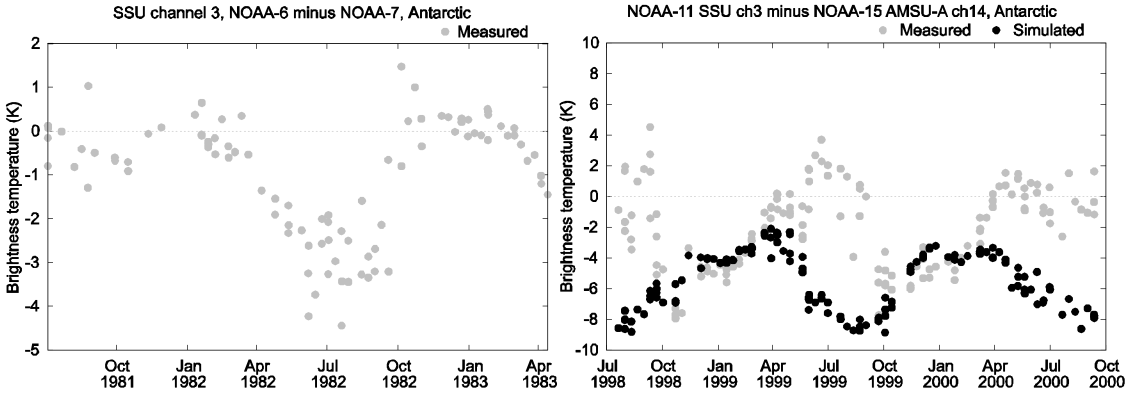


Figure 1. Inter-satellite differences between (a) radiance measurements from SSU channel 3 on NOAA-6 and NOAA-7 and (b) radiance measurements from SSU channel 3 on NOAA-11 and AMSU-A channel 14 on NOAA-15 over the Antarctic, obtained with the SNO technique (gray) and the corresponding simulated differences using RTTOV (black). Simulated differences are not shown for (a) since they are always zero.

3. Revision of radiative transfer models

3.1. SSU

SSU is a three-channel infrared radiometer designed to measure radiances in the 15 µm carbon dioxide absorption band. The SSU uses a pressure modulation technique where the pressure in a cell of carbon dioxide gas in the instrument's optical path is varied in a cyclic manner. The spectral performance of the instrument depends on the mean cell pressure, whose long-term stability is crucial for obtaining time-consistent observations. As it turned out, a sealing problem caused cell pressures to increase during storage on the ground and then to decrease after launch. The Met Office, which produced the instrument, has routinely monitored and recorded the mean cell pressure at six-month intervals subsequent to the launch of each spacecraft. Figure 2 shows daily values of the mean cell pressures estimated from these records.

The gradual reduction of cell pressure affects the level of peak energy for the SSU channels. Figure 3 shows typical changes to the weighting functions, computed for a U.S. Standard Atmosphere 1976 using the LBLRTM line-by-line radiative transfer model (Clough et al., 2004) and the HITRAN line parameter database (Rothman et al., 2005). Channels 2 and 3, which both peak in the upper stratosphere, are most affected by cell-pressure loss.

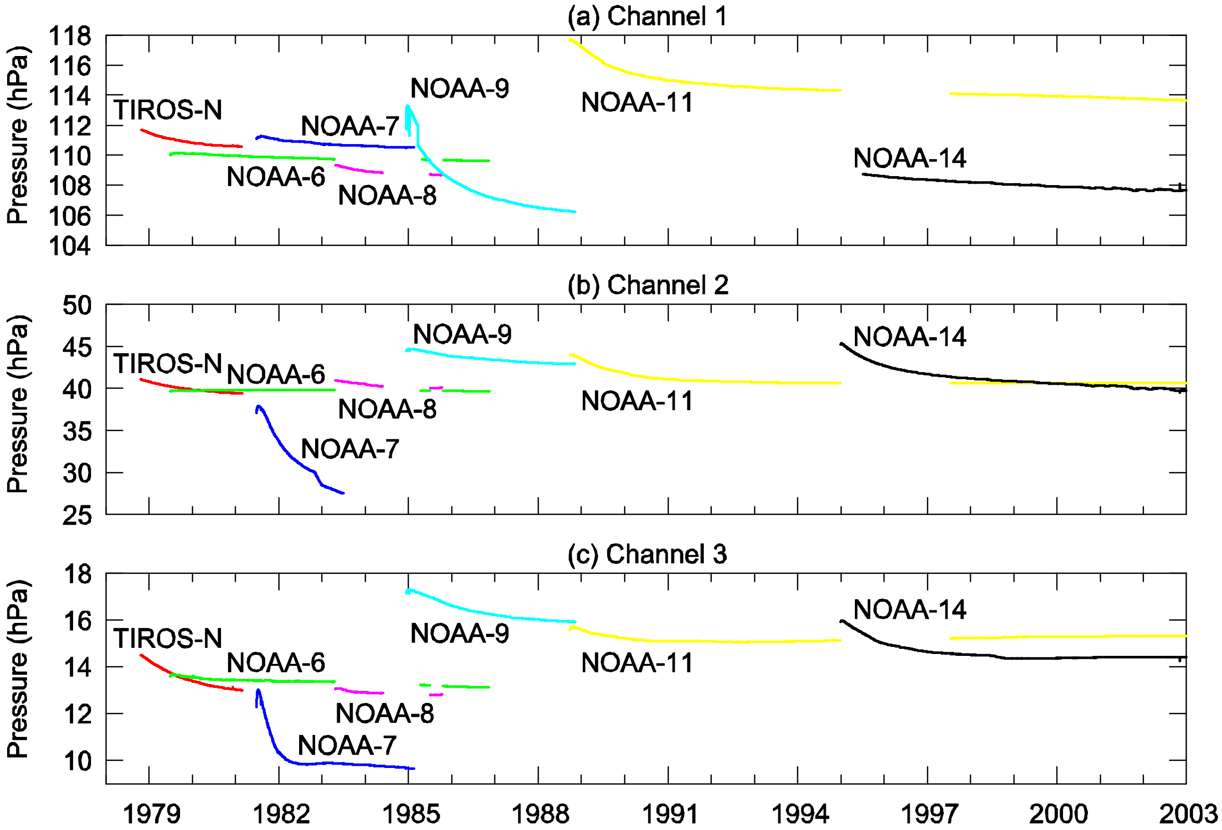


Figure 2: Daily values of mean cell pressures for channels 1, 2 and 3 of all SSU instruments as a function of time. These values were interpolated from the Met Office's six-monthly estimates using a linear relationship between mean cell pressure and modulation frequency.

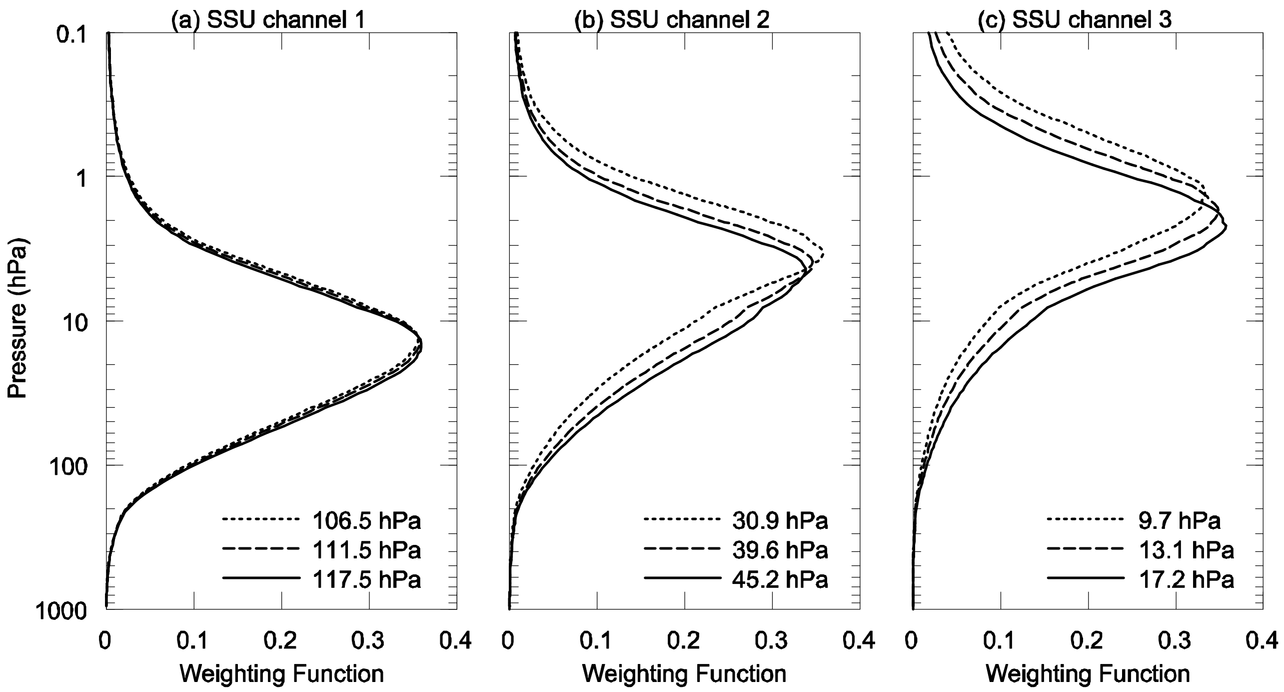


Figure 3: Impact of changes in mean cell pressure on the weighting functions for (a) channel 1, (b) channel 2 and (c) channel 3 of SSU for a U.S. Standard Atmosphere 1976, with carbon dioxide at 330 ppmv (parts per million by volume).

We studied the impact of recorded SSU cell pressure changes by accurately modelling their effect on the radiance measurements using the LBLRTM line-by-line model (Clough et al., 2004). Changes in the atmospheric CO2 concentration were also taken into account in the line-by-line calculations. Figure 4 shows time series of line-by-line simulated inter-satellite differences for the same pair of satellites shown in Figure 1a, together with the actual differences obtained with the SNO technique. The figures for the other SSU channels and other pairs of overlapping satellites are shown in the Appendix. While discrepancies between the observed and simulated inter-satellite differences still exist (possibly due to uncertainties in the band-pass filter and the calibration algorithm), the seasonal cycle is much better captured in the line-by-line calculations for channels 2 (see appendix) and 3 (see Figure 4). This indicates that cell pressure changes are the main cause for the observed inter-satellite biases in these channels. Cell pressure changes have little impact on the computed radiances for channel 1 (see appendix) and therefore the biases in this channel must be dominated by other causes, such as uncertainties in the band-pass filter and the calibration algorithm.

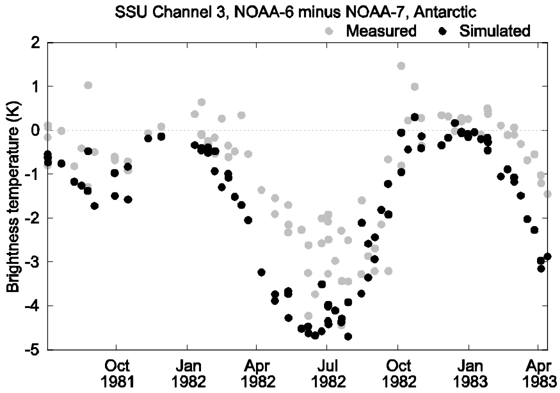


Figure 4: Inter-satellite differences between radiance measurements from SSU channel 3 on NOAA-6 and NOAA-7 over the Antarctic, obtained with the SNO technique (gray, as shown in Figure 1a) and the corresponding simulated differences using the LBLRTM model to account for the pressure loss in the carbon dioxide cell (black).

Based on these results we expect that the inclusion of effects of cell pressure changes in RTTOV will reduce biases in the radiative transfer computations. Accordingly, new RTTOV coefficients have been generated for SSU that properly take into account the variation of the mean pressure in the carbon dioxide cell in each of the instruments.

3.2. AMSU-A

AMSU-A is a multi-channel microwave radiometer designed to retrieve vertical profiles of temperature from about 3 hPa (45 km) to the surface. The AMSU-A stratospheric channels measure the radiance originating from the 60-Ghz oxygen absorption lines. These magnetic-dipole absorption lines are split by the terrestrial magnetic field. This splitting is due to the Zeeman effect which is particularly important at low pressures when the magnitude of the line splitting is comparable to or smaller than the line width (Rosenkranz and Staelin, 1988) and can thus affect the high-peaking stratospheric channels of AMSU-A.

RTTOV represents the Zeeman effect by a scalar approximation described in Liebe et al. (1993), which models the effect simply by increasing the line-broadening parameter for the oxygen absorption lines. This approximation was introduced in RTTOV-5 and has been used in subsequent versions. We compared attenuation rates at frequencies that include the pass bands of AMSU-A channel 14, using alternative representations of the Zeeman effect: the RTTOV scalar approximation; an explicit treatment of the line splitting; and omission of the Zeeman effect. All results were obtained using the line-by-line model by Rayer (2001) that utilizes the Millimeter-wave Propagation Model (MPM) 89 (Liebe, 1989) for the water vapour lines and the MPM92 (Liebe et al., 1992) for the oxygen lines. Figure 5a shows that the scalar approximation is accurate at frequencies near the centre of the oxygen absorption line, but overestimates attenuation rates within the pass bands of AMSU-A channel 14. As shown in Figure 5b, this results in an anomalous upward shift of the weighting function for this channel.

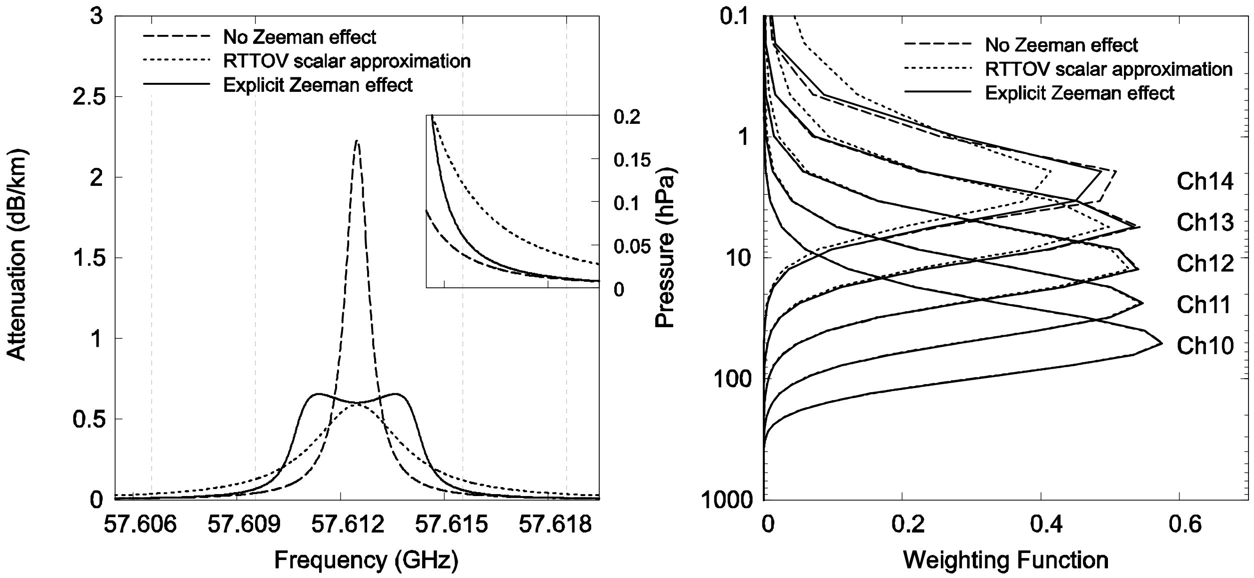


Figure 5 (a) Simulation of attenuation rates at frequencies near the pass bands of AMSU-A channel 14 at 0.29 hPa and (b) weighting functions for AMSU-A stratospheric channels based on a U.S. Standard Atmosphere 1976, using no Zeeman effect (dash), the RTTOV scalar approximation (dot), and an explicit representation of the Zeeman effect (solid) in the presence of a magnetic field of 60 μT in the propagation direction.

Figure 5b also shows that for AMSU-A channel 14 the RTTOV weighting function computed without the Zeeman effect is much closer to that obtained with an explicit treatment of the line splitting. Therefore the scalar approximation of the Zeeman effect results in radiance simulations that are less accurate than those obtained by omitting it completely. While a better solution could be obtained by including an explicit model for Zeeman splitting in RTTOV, this requires a long-term development effort that is outside the scope of this paper. As a practical short-term solution to improve the RTTOV simulation of AMSU-A stratospheric radiances, we have trained RTTOV by performing new line-by-line computations that exclude Zeeman splitting.

Figure 6 shows time series of inter-satellite radiance differences calculated with the new line-by-line model for the same pair of satellites shown in Figure 1b, together with the actual inter-satellite radiance differences obtained with the SNO technique. The remarkable agreement between the measured and the computed radiance differences indicates a significant improvement of the accuracy of the revised RTTOV radiative transfer simulations.

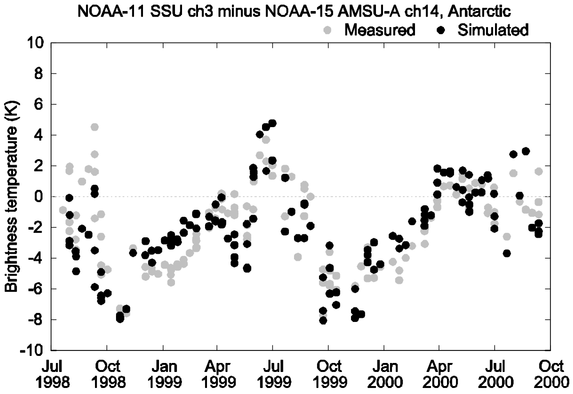


Figure 6: Inter-satellite differences between radiance measurements from SSU channel 3 on NOAA-11 and AMSU-A channel 14 on NOAA-15 over the Antarctic, obtained with the SNO technique (gray; as shown in Figure 1b) and the corresponding simulated differences using the revised line-by-line model for AMSU-A and the current version of RTTOV for SSU (black).

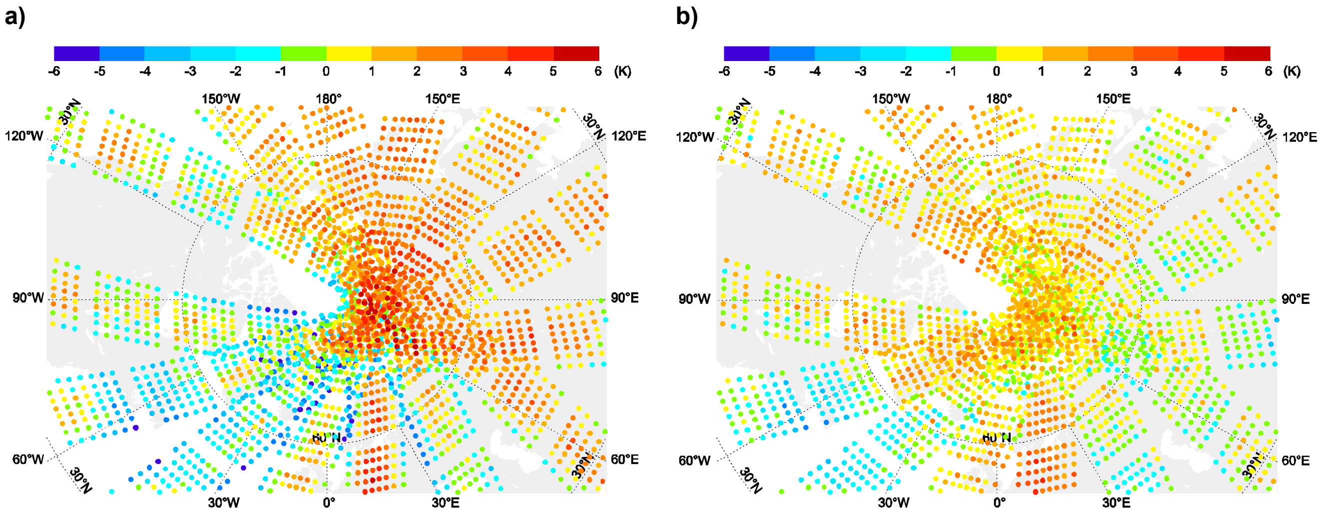
4. Assimilation experiments

4.1. Experiment 1: RTTOV using new SSU coefficients

To assess the impact of the new SSU coefficients in RTTOV on the reanalysis of upper-stratospheric temperatures, several data assimilation experiments were performed using ECMWF’s ERA-Interim system . This assimilation system was developed for the purpose of producing a reanalysis of the satellite-rich era 1989-present. Simmons et al. (2007) provide a description of the configuration of ERA-Interim and discuss key elements of its performance. An important feature of ERA-Interim is the use of a variational bias correction method (Auligné et al., 2007) for the adaptive estimation and correction of biases in satellite radiance data. Dee and Uppala (2008) have evaluated the performance of this method in the reanalysis context, and include a detailed discussion of the special difficulties associated with the use of data from SSU and AMSU-A for constraining the upper-stratospheric model biases.

Our experiment covers the month of January 1983, during which SSU observations were available from NOAA-6 and NOAA-7. For the purpose of the assessment, SSU data from NOAA-6 were not assimilated but used instead as independent observations for verification. As our control experiment we used the configuration of the ERA-Interim production system (T255L60 with the top level at 0.1 hPa) which includes the operational RTTOV coefficients. For the new RT experiment the system configuration was identical except for the inclusion of new RTTOV coefficients for SSU. In both experiments all satellite radiance data were subject to variational bias correction. In order to constrain the upper-stratospheric temperature analysis in the presence of a large, warm, forecast model bias, the SSU channel 3 radiances were corrected for scan biases only.

Figure 7 shows analysis departures from the uncorrected NOAA-6 SSU channel 3 radiances over the Arctic, for the control (panel a) and for the new RT experiment (panel b). Also shown is the corresponding 2 hPa temperature analysis field for the new RT experiment (panel c). Departures for the new RT experiment are generally smaller than in the control experiment, and vary less with viewing angle. Given the inverse lapse rate in the stratosphere, the operational SSU coefficients presumably overestimate the optical depth for the slant path. The improved fit to the passively monitored observations in the new RT experiment is also reflected in the reduced standard deviations of departures shown in Figure 8.



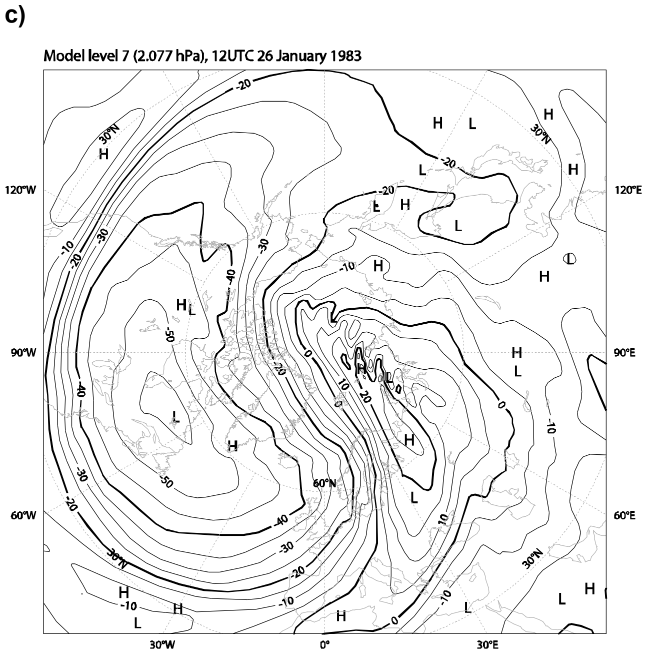


Figure 7: Uncorrected observation minus analysis departure values for the passively monitored NOAA -6 SSU channel 3 observations from 03 to 15UTC on 26 January 1983 for (a) the control and (b) the new RT experiment, and (c) the corresponding 2 hPa temperature analysis of the new RT experiment at 12UTC on 26 January 1983.

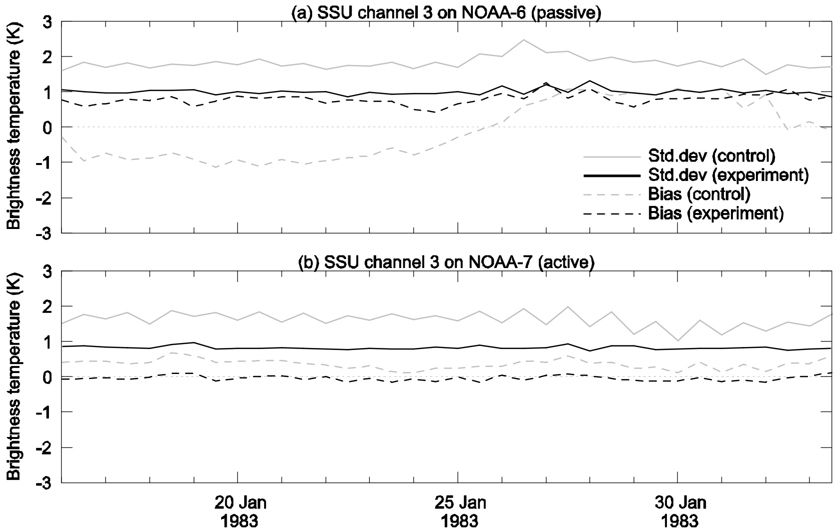


Figure 8: Time series of means and standard deviations for analysis departures from uncorrected SSU channel 3 observations over the Arctic.

4.2. Experiment 2: RTTOV using new coefficients for AMSU-A

Similar assimilation experiments with the ERA-Interim system have been performed to test the impact of the revised AMSU-A coefficients on the reanalysis of upper-stratospheric temperatures. These experiments cover a one-year period starting in August 1998 when AMSU-A became operational. The control assimilation used the operational AMSU-A coefficients while revised AMSU-A coefficients were used for the new RT experiment. All satellite radiance data were subject to VarBC. In order to constrain the upper-stratospheric temperature biases in the forecast model radiance data from AMSU-A channel 14 were corrected for scan biases only,.

Figure 9 shows the evolution of the vertical temperature structures in polar regions for the two assimilations. The control assimilation tends to create spurious features near model levels 6 and 10 (2 and 5 hPa respectively) when the strong polar vortex develops in winter. This is because the weighting function for AMSU-A channel 14 in the operational RTTOV peaks too high, resulting in radiance simulations that are too warm when the mesosphere is warmer than the stratosphere, as tends to be the case in polar regions during winter. In the new RT experiment, these spurious features have been reduced and the vertical temperature structure varies more smoothly with the season. Monthly averaged zonal mean temperatures also show a significant reduction of the spurious features in the polar regions (not shown).

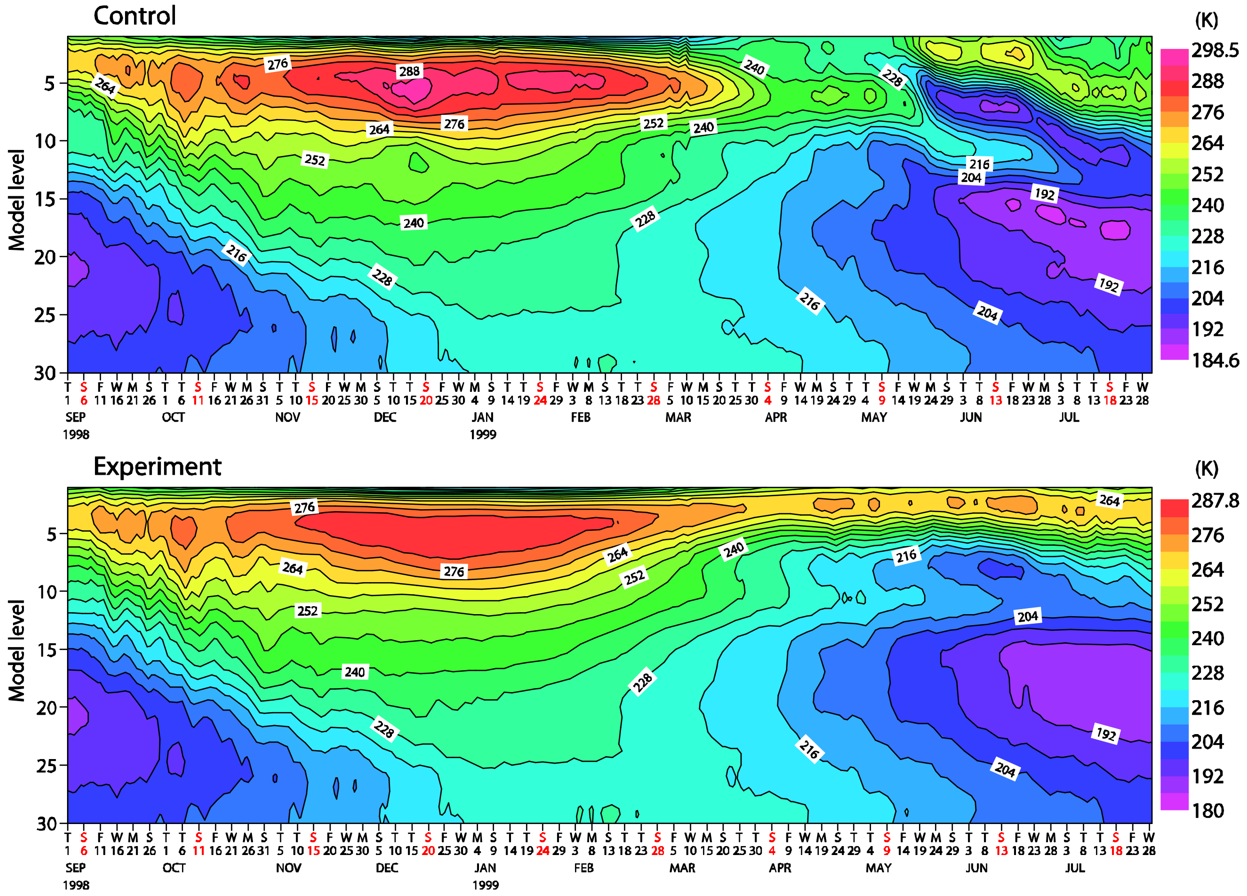


Figure 9:.Evolution of the vertical temperature structures over the Antarctic (60 to 90S) from September 1998 to July 1999 for assimilations using (a) the current RTTOV coefficients for AMSU-A and (b) the new RTTOV coefficients for AMSU-A.

4.3. Experiment 3: use of SSU radiances from NOAA-6 and NOAA-7 platforms

To produce a consistent multi-decadal stratospheric temperature dataset, an assimilation system should be able to produce analyses whose quality is not significantly affected by a change of the observing system. In this section we have investigated this aspect of the assimilation system by performing observing system experiments (OSE) using SSU observations from different platforms, in order to ascertain whether the use of revised SSU coefficients results in more consistent analysed temperature fields. The experiments cover January 1983 when SSU observations were available from both NOAA-6 and NOAA-7. Two pairs of experiments were carried out: the first pair using operational RTTOV coefficients for SSU, and the second pair using revised coefficients. In each pair, one experiment used SSU data from NOAA-6 only while the other experiment used SSU data from NOAA-7 only. We would like to see improved consistency in the pair of assimilations that uses the revised coefficients. As before, all satellite radiances were subject to VarBC, with SSU channel 3 radiances corrected for scan bias only.

Figure 10 shows monthly averaged height-latitude cross sections of zonal mean differences between temperature analyses obtained from the first pair (using operational coefficients) in panel a, and from the second pair (using revised coefficients) in panel b. Each of these plots shows the analysed inter-satellite

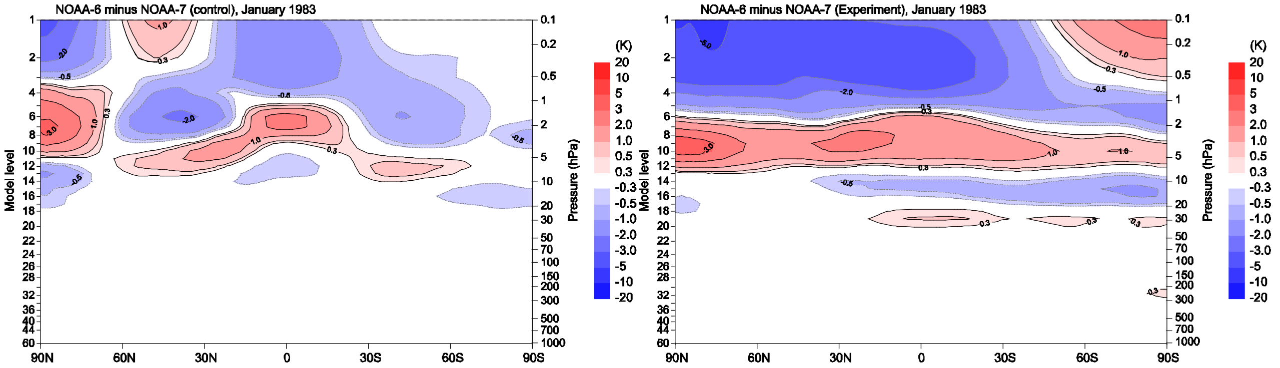


Figure 10: Height-latitude cross sections of zonally averaged differences, averaged over January 1983, between temperature analyses from an assimilation using SSU observations from NOAA-6 only and an assimilation using SSU observations from NOAA-7 only, for (a) the control assimilations and (b) the new RT experiments.

differences for the two SSU instruments given a fixed set of RTTOV coefficients. Even though, as discussed previously, SSU inter-satellite differences are much better reproduced by the revised version of RTTOV, the differences between the temperature analyses obtained with the revised coefficients are larger in some places than those obtained with the operational coefficients. To interpret this result we note that the response of the assimilation system to biases in the background depends on the RTM used, as well as on the background constraint used for the analysis. The constraint imposed on the upper stratospheric temperatures by the uncorrected SSU channel 3 observations may play a role in generating the oscillating patterns in the analysis differences shown in Figure 10b. We will return to this issue in Section 5.

4.4. Experiment 4: Transition from SSU channel 3 to AMSU-A channel-14

In order to estimate the most likely state of the atmosphere during periods when multiple observing systems overlap, all available observations should be utilized. However, in the presence of model bias the accuracy of the analysis strongly depends on the nature of the constraints implied by the observations. In the ERA-Interim reanalysis prior to the introduction of AMSU-A in 1998, the model warm bias in the upper layers was constrained by radiance data from SSU channel 3. These data were corrected only for scan bias in order to maintain a fixed constraint (or anchor) for the upper-stratospheric temperature fields. Starting in August 1998 data from AMSU-A channel 14 were used instead to anchor the top levels in ERA-Interim, in anticipation of the termination of the SSU data record in 2006. In this section we describe the impact of this change on the stratospheric temperatures based on a parallel experiment identical to ERA-Interim except that the upper stratosphere continued to be anchored by SSU rather than AMSU-A. The experiment was started in July 1998, just before the anchoring was switched from SSU channel 3 to AMSU-A channel 14 in ERA-Interim (August 1998), using initial conditions from ERA-interim. The system configuration for the parallel experiment is identical to ERA-Interim except for the anchoring. While the AMSU-A observations are assimilated using the new RTTOV coefficients, the SSU observations are assimilated using the operational RTTOV coefficients since the revision of SSU coefficients was not available in time for the production of ERA-Interim. Nevertheless, since the characteristics of the SSU instruments in operation during this period are very close to those assumed in the operational RTTOV, the SSU radiances simulated by RTTOV are believed to be reasonably accurate.

Figure 11 shows height-latitude cross section of zonally averaged differences between the temperature analyses from ERA-Interim and the parallel experiment, averaged for September 1998. The use of a different anchoring channel clearly has a significant impact on the upper-stratospheric temperatures over polar regions, with different vertical structures reaching down into the lower stratosphere. These structures reflect the different instrument characteristics for SSU and AMSU-A and their implied constraints on the analysis. This result, together with those of Experiment 3, suggests that the influence of instrument characteristics on analysis error structures needs to be better understood in order to improve the consistency in time of stratospheric reanalyses. Toward this end we present an error analysis based on a one-dimensional simplification of the analysis equation.

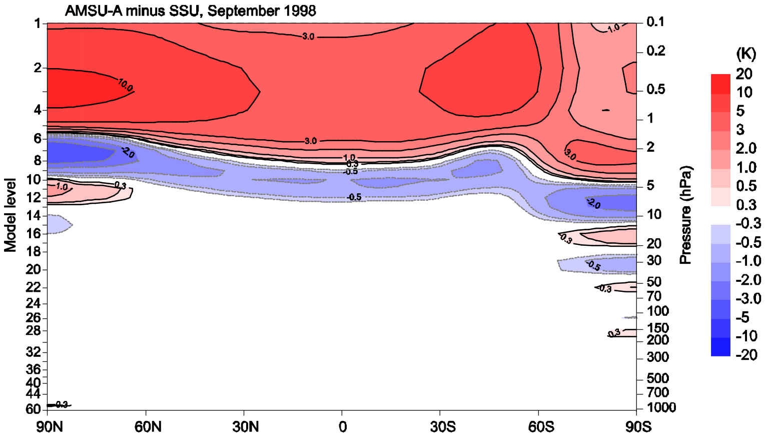


Figure 11: Height-latitude cross section of zonally averaged differences between temperature analyses anchored by AMSU-A channel 14 and SSU channel 3, averaged for September 1998.

5. One-dimensional error analysis

In sections 4.3 and 4.4 we found that significant shifts in the reanalysis of stratospheric temperatures can still occur when switching observing systems, even when the RTM is able to accurately represent the differences between overlapping observations from the two systems. To investigate further, we consider the impact of a single observation on the temperature analysis in a vertical column, following Rodgers (2000).

Suppose the vector x represents the true state of the atmosphere in a vertical column. Given a measurement vector y with errors ε and an a-priori (background) state estimate xb, the optimal linear analysis xa is given by

$$\begin{aligned} x_a - x_b &= K\left[y - Hx_b\right] \\ &= K\left[H(x - x_b)\right] + \varepsilon \\ &= KH(x - x_b) + K\varepsilon \end{aligned} \tag{1}$$

where the matrix H is the Jacobian of the radiative transfer model. The optimal matrix of analysis weights K (the gain) is

$$K = BH^T\left[HBH^T + R\right]^{-1} \tag{2}$$

where B and R are the background and observation error covariance matrices, respectively. In order to simulate the behaviour of the ERA-Interim system, we used a diagonal R as in ERA-Interim and specified B as in the ECMWF NWP-SAF 1D-Var package (Chevalier, 2004). Figure 12 shows vertical correlations of temperature background errors represented in B. Figure 13 shows the elements of the Jacobians for the observing systems used in Experiments 3 and 4 of the previous sections. These were first constructed using the 43 RTTOV layers and then interpolated to the 60-layer ERA-Interim model levels, taking the layer thicknesses into account.

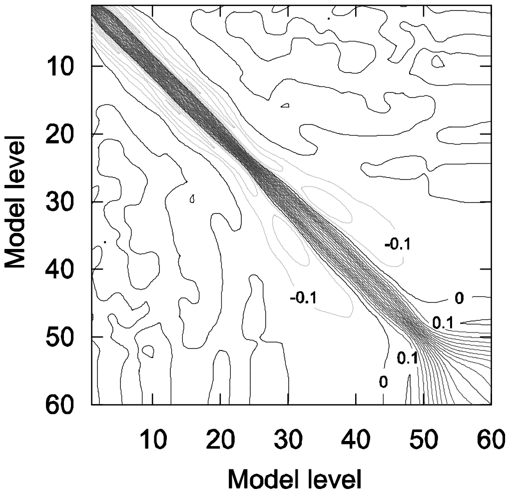


Figure 12: Vertical correlations of temperature background errors assumed in the ECMWF NWP-SAF 1D-Var package.

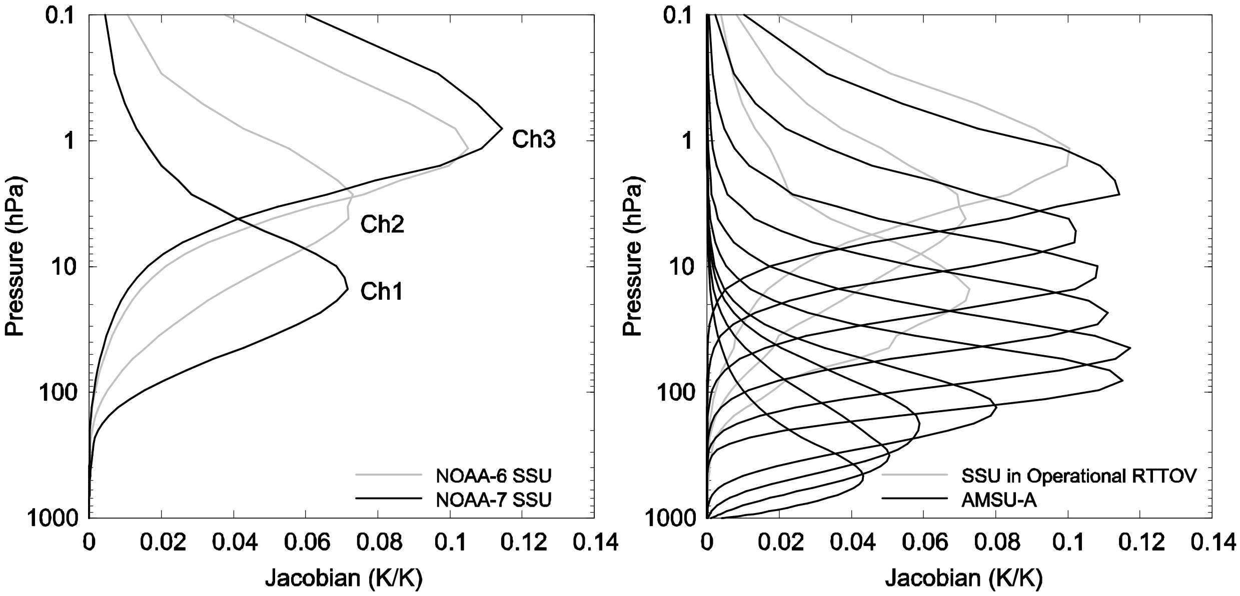


Figure 13: Temperature Jacobians for (a) SSU channels used in Experiment 3 and (b) SSU and AMSU-A channels used in Experiment 4, based on the U.S. Standard Atmosphere 1976. Note that SSU channel 2 on NOAA-7 was not used in Experiment 3 due to the drift of its spectroscopic characteristics.

We first consider the impact on the analysis of a single channel only. We take the highest-peaking channel since it is used to anchor the reanalysis and therefore has a dominant impact on the mean state. In the case of a single observation, the Jacobian H reduces to a row vector representing the error pattern that can be measured by the channel, while the gain K reduces to a column vector representing the corresponding increment pattern.

Figure 14 shows the Jacobian and gain vectors for SSU channel 3 on NOAA-6 and NOAA-7 used in Experiment 3, and for SSU channel 3 and AMSU-A channel 14 used in Experiment 4. For ease of interpretation, the Jacobian vectors are normalised, and the gain vectors are scaled by the normalisation coefficients used for the corresponding Jacobian vector. As seen in Figure 12, the background errors used in ERA-Interim are characterised by narrow vertical correlations and anti-correlation layers below and above the main peak. This characteristic is reflected in the gain vectors associated with each of the sounding systems shown in Figure 14. The plots also show considerable differences in the height of the main peaks as well as in the amplitude of the anti-correlations for these sounding systems. When the observations are used to correct large, systematic errors in the background, the gain patterns determine the shape and extent of this correction. Therefore, even if observations are unbiased and radiative transfer calculations are accurate, the residual bias in the analysis will be affected by characteristics of the observing system. Any systematic change in the observing system will then result in a shift in the reanalysis.

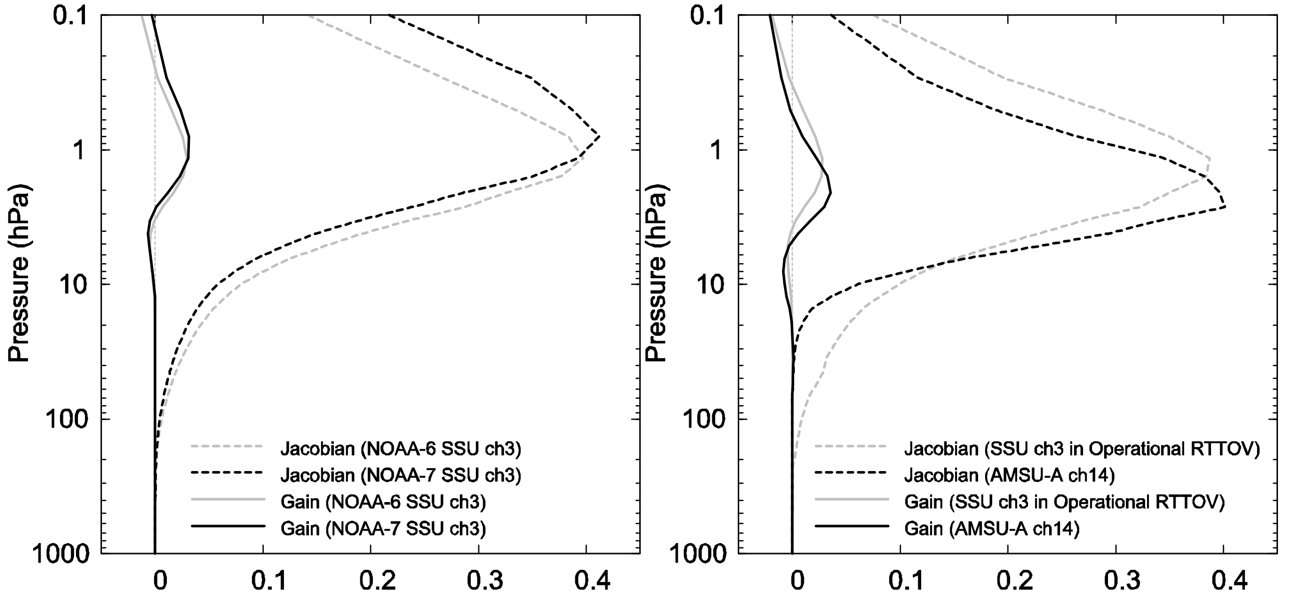


Figure 14: Jacobian and gain vectors for (a) SSU channel 3 on NOAA-6 and NOAA-7 used in Experiment 3 and (b) SSU channel 3 and AMSU-A channel 14 used in Experiment 4.

We next consider the impact of observations from multiple channels. Using a singular value decomposition (SVD) of the averaging kernel KH, the analysis equation (1) can be expressed as

$$x_a - x_b = U\Lambda V^T (x - x_b) + K\varepsilon \tag{3}$$

where the matrices U and V contain the left and right hand singular vectors, and Λ is a diagonal matrix with singular values. The columns of V form an orthonormal basis for the a priori errors that can be measured with the sounding system, while the columns of U form an orthonormal basis for the corresponding increment patterns, which have a sensitivity given by the magnitude of the singular value. Since KH is generally asymmetric, U and V are not identical, which implies that the increment patterns differ from the background error patterns. An advantage in using SVD over an eigenvalue decomposition is its orthogonality, which makes it easier to transform the variables between the real space and the singular vector space.

Figure 15 shows the left and right hand singular vectors associated with SSU and AMSU-A as used in Experiments 3 and 4. Since AMSU-A has more channels with a higher vertical resolution, it is sensitive to error patterns with shallower vertical structures and the corresponding increment patterns are in better agreement with these structures. In the upper stratosphere, however, vertical error structures are deeper than in the lower atmosphere, and the corresponding increment patterns are less consistent with these. In fact, increments in the upper stratosphere can have the opposite sign from the corresponding error pattern. These anti-correlated increments may have detrimental effects on the stratospheric temperature analysis and even amplify biases in the upper stratosphere.

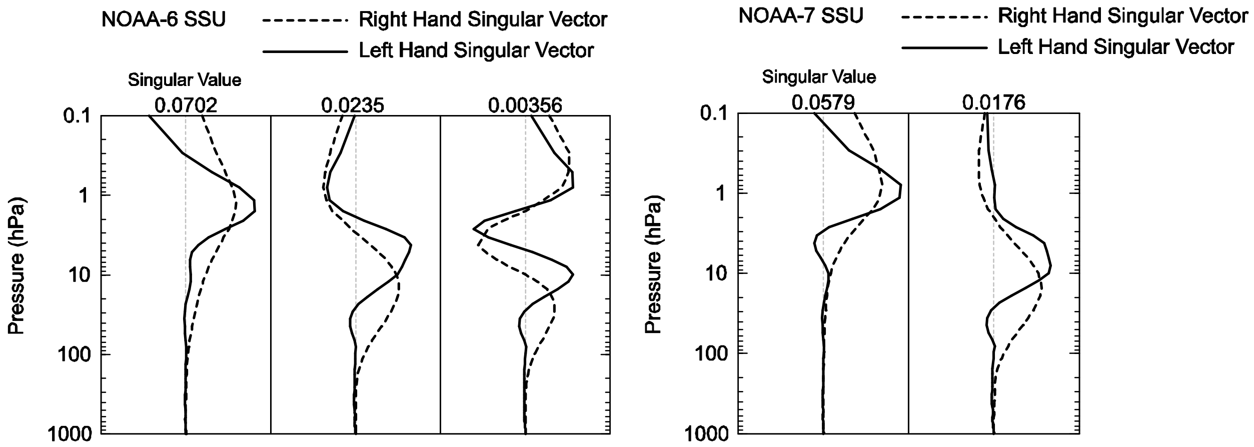
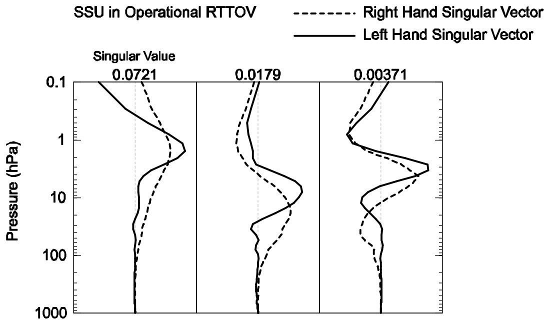


Figure 15: Normalised right (dash) and left (solid) hand singular vectors and singular values (printed at the top of each frame) for averaging kernels associated with SSU channels on (a) NOAA-6 and (b) NOAA-7 used in Experiment 3. Each pair of singular vectors represents an error pattern (dash) that can be measured by the sounding system (dash) and the corresponding increment pattern (solid) with a sensitivity given by the magnitude of the singular value. The actual increment is the product of the singular value and left hand singular vector. Note that only two pairs of singular vectors exist for SSU channels on NOAA-7 since channel 2 was blacklisted.



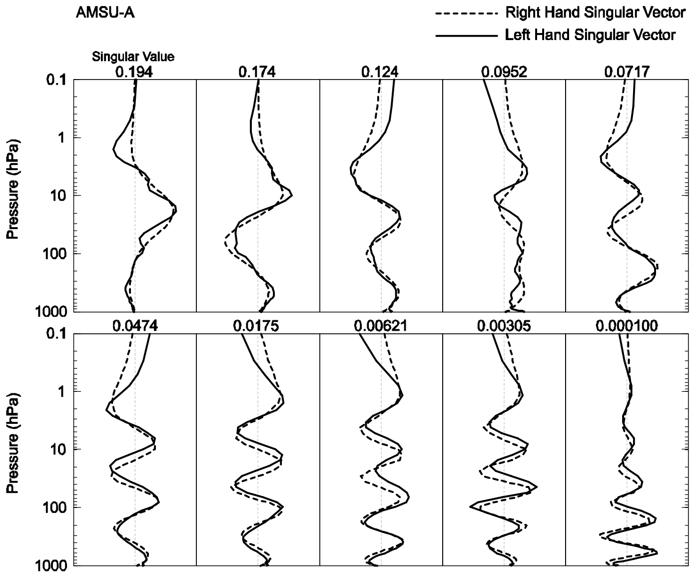


Figure 16: As Figure 15, but for the (a) SSU and (b) AMSU-A sounding systems used in Experiment 4.

The singular values associated with the highest-level increments are generally small, implying that the observations have only small impact on the analysis in this 1D system, and consequently, that the analysis is dominated by the background. The impact of the observations on the analysis depends on the background errors as well as on measurement sensitivities, as expressed in equation (2). Replacing the background error covariance matrix B in this equation by its eigendecomposition shows that the correlation between Jacobians and leading eigenvectors of the B matrix needs to be large in order for observations to have a large impact. However, Figures 12 and 13 show that vertical length scales associated with the B matrix are much smaller than those associated with the SSU and AMSU-A Jacobians, resulting in small correlations between them.

From this discussion it is clear that further examination of ECMWF's background error covariance modelling for the upper stratosphere is needed, but this is beyond the scope of this paper.

6. Conclusion

This study addresses several aspects of the use of SSU and AMSU-A data that are important for obtaining a consistent multi-decadal reanalysis of mid- and upper-stratospheric temperatures. In the context of the RTTOV package, radiative transfer modelling for both instruments was improved in order to reduce inter-satellite biases and inconsistencies between the handling of the two sensors. Radiative transfer coefficients for SSU were updated based on more appropriate spectral response functions and by allowing variable CO2 input profiles in RTTOV. For AMSU-A, inaccurate treatment of the Zeeman splitting effect in RTTOV was found to result in an overestimation of optical depths. To address this, the radiative transfer coefficients for AMSU-A were revised by omitting the Zeeman splitting effect altogether. The updated RTTOV was validated by simulating inter-satellite radiance differences for co-located observations and comparing them with observed differences obtained with the SNO technique. Results of this exercise showed a substantial reduction of biases and inconsistencies.

Assimilation experiments with the ERA-Interim system, incorporating the updated RTTOV package, demonstrated some clear improvements in the stratospheric temperature reanalysis. Nevertheless, systematic discrepancies between analyses produced with observations from different satellite instruments still remain. This is due to the fact that the available observations can only partly correct the model bias in the upper stratosphere, while the vertical structure as well as the extent of the corrections change when the instrument changes. We performed a linear error analysis of the impact of a single observation in a vertical column to clarify this in detail. Our error analysis showed that the vertical structures represented by the background error covariances used in ERA-Interim are very shallow, which may have a detrimental effect on the upper stratospheric temperature analysis. These results illuminate a difficult aspect of the inversion of remotely sensed observations. Further research on background covariance modelling for the upper stratospheric temperature reanalysis is needed to fully benefit from the improvements in radiative transfer modelling presented here.

These improvements in the interpretation of stratospheric measurements from SSU and AMSU-A will, hopefully, also lead to improvements in the forecast models used for reanalysis. Ultimately it is the presence of large biases in the assimilating model that causes spurious shifts and other artefacts when significant changes occur in the observing system, even if all assimilated observations are unbiased and correctly represented by the assimilation system. In sparsely observed regions such as the upper stratosphere, these shifts can be significant relative to the observed climate signal. Further progress on this problem requires a significant reduction of systematic errors in the forecast model used for assimilation.

Acknowledgements

The authors wish to thank H. Brindley (Imperial College), A. Geer (ECMWF) and J. Nash (Met Office) for providing us with valuable information on the SSU instrument, and A. McNally for his helpful suggestion on how to analyse the results of experiments. The authors also wish to thank R. Saunders (Met Office) for his generous support on this study. Shinya Kobayashi is very thankful to ECMWF and JMA for supporting and arranging his secondment to ECMWF.

References

Auglinė, T., A.P. McNally, D.P. Dee, 2007: Adaptive bias correction for satellite data in a numerical weather prediction system. *Q. J. R. Meteorol. Soc.* **133**: 631-642.

Cao, C., H. Xu, J. Sullivan, L. McMillin, P. Ciren, Y.T. Hou, 2005: Intersatellite Radiance Biases for the High-Resolution Infrared Radiation Sounders (HIRS) on board NOAA-15, -16, and -17 from Simultaneous Nadir Observations. *J. Atmos. Oceanic Technol.* **22**: 381-395.

Chevalier P. 2004: A one-dimensional variational analysis package. [Online] Available:
http://www.metoffice.gov.uk/research/interproj/nwpsaf/ecmwf_1dvar/nwpsaf-ec-ud-001.pdf

Clough, S.A., M.W. Shephard, E.J. Mlawer, J.S. Delamere, M.J. Iacono, K. Cady-Pereira, S. Boukabara, P.D. Brown, 2004: Atmospheric radiative transfer modeling: a summary of the AER codes. *J Quant. Spectrosc. and Radiat Transfer* **91**: 233-244.

Dee, D., and S. Uppala, 2008: Variational bias correction in ERA-Interim. *ECMWF Technical Memorandum*, No. 575. European Centre for Medium-Range Weather Forecasts, Shinfield, Reading, UK [Online] Available: http://www.ecmwf.int/publications/

Garand L., D.S. Turner, M. Larocque, J. Bates, S. Boukabara, P. Brunel, F. Chevallier, G. Deblonde, R. Engelen, M. Hollingshead, D. Jackson, G. Jedlovec, J. Joiner, T. Kleespies, D.S. McKague, L. McMillin, J.-L. Moncet, J.R. Pardo, P.J. Rayer, E. Salathe, R. Saunders, N.A. Scott, P. Van Delst, H. Woolf, 2001: Radiance and Jacobian intercomparison of radiative transfer models applied to HIRS and AMSU channels. *J. Geophys. Res.* **106**: 24,017-24,031.

Liebe, H.J., 1989: MPM - an atmospheric millimeter-wave propagation model. *Int. J. Infrared Milli.* **10**: 631-650.

Liebe, H.J., P.W. Rosenkranz and G.A. Hufford, 1992: Atmospheric 60-GHz oxygen spectrum: new laboratory measurements and line parameters. *J. Quant. Spectrosc. Radiat. Transfer* **48**: 629-643.

Liebe, H.J., G.A. Hufford and M.G. Cotton, 1993: Propagation modeling of moist air and suspended water/ice particles at frequencies below 1000 GHz. in *Proc. NATO/AGARD Wave Propagation Panel*, 52nd Meeting, Paper No. 3/1-10, Mallorca, Spain, May 1993.

Nash J, Forrester G.F., 1986: Long-term monitoring of stratospheric temperature trends using radiance measurements obtained by the TIROS-N series of NOAA spacecraft. *Adv. Space Res.* **6**: 37-44.

Onogi K., J. Tsutsui, H. Koide, M. Sakamoto, S. Kobayashi, H. Hatsushika, T. Matsumoto, N. Yamazaki, H. Kamahori, K. Takahashi, S. Kadokura, K. Wada, K. Kato, R. Oyama, T. Ose, N. Mannoji, R. Taira. 2007. The JRA-25 Reanalysis. *J. Meteor. Soc. Japan* **85**: 369-432.

Rayer, P.J., 2001: Microwave transmittance models for RTTOV. [Online] Available: http://www.metoffice.gov.uk/research/interproj/nwpsaf/rtm/rtm_reports.html

Rodgers, C.D., 2000: Inverse methods for atmospheric sounding, theory and practice, *Series on atmospheric, oceanic and planetary physics*, Vol. 2, World scientific, 238pp.

Rosenkranz, P.W. and Staelin, D.H., 1988: Polarised thermal microwave emission from oxygen in the mesosphere. *Radio Sci*. **23**: 721-729.

Rothman, L.S., D. Jacquemart, A. Barbe, D. Chris Benner, M. Birk, L.R. Brown, M.R. Carleer, C. Chackerian Jr, K. Chance, L.H. Couderth, V. Danai, V.M. Devic, J.-M. Flaud, R.R. Gamache, A. Goldman, J.-M. Hartmann, K.W. Jucks, A.G. Maki, J.-Y. Mandin, S.T. Massie, J. Orphal, A. Perrin, C.P. Rinsland, M.A.H. Smith, J. Tennyson, R.N. Tolchenov, R.A. Toth, J. Vander Auwera, P. Varanasi, G. Wagner, 2005: The HITRAN 2004 molecular spectroscopic database. *J Quant. Spectrosc. and Radiat Transfer* **96**: 139-204.

Saunders R., M. Matricardi, and P. Brunel. 1999. An improved fast radiative transfer model for assimilation of satellite radiance observations. *Q. J. R. Meteorol. Soc*. **125**: 1407-1425

Simmons, A., S. Uppala, D. Dee and S. Kobayashi. 2007. ERA-Interim: New ECMWF reanalysis products from 1989 onwards. *ECMWF Newsletter*, No. 110. [Online] Available: http://www.ecmwf.int/publications/

Uppala, S. M., P. W. Kållberg, A. J. Simmons, U. Andrae, V. da Costa Bechtold, M. Fiorino, J. K. Gibson, J. Haseler, A. Hernandez, G. A. Kelly, X. Li, K. Onogi, S. Saarinen, N. Sokka, R. P. Allan, E. Andersson, K. Arpe, M. A. Balmaseda, A. C. M. Beljaars, L. van de Berg, J. Bidlot, N. Bormann, S. Caires, F. Chevallier, A. Dethof, M. Dragosavac, M. Fisher, M. Fuentes, S. Hagemann, E. Holm, B. J. Hoskins, L. Isaksen, P. A. E. M. Janssen, R. Jenne, A. P. McNally, J.-F. Mahfouf, J.-J. Morcrette, N. A. Rayner, R. W. Saunders, P. Simon, A. Sterl, K. E. Trenberth, A. Untch, D. Vasiljevic, P. Viterbo, and J. Woollen, 2005. The ERA-40 re-analysis. *Q. J. R. Meteorol. Soc*. **131**: 2961-3012.

Appendix: Time series of the inter-satellite biases in the SSU observations

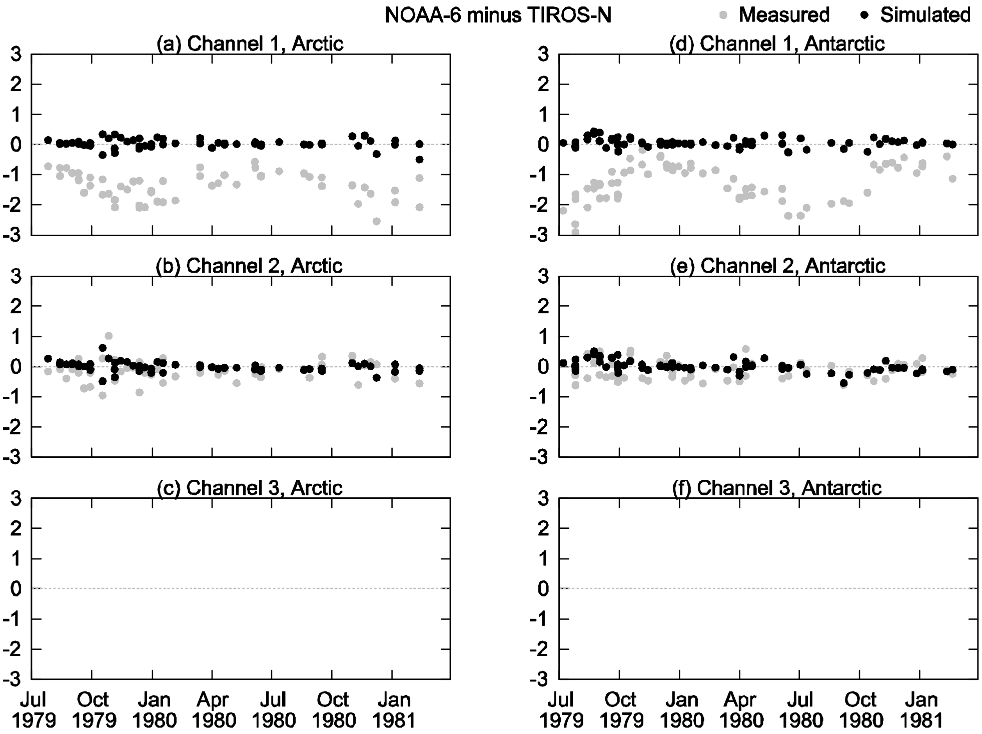


Figure 17 Inter-satellite differences between radiance measurements from SSUs on NOAA-6 and TIROS-N over the Arctic (left) and Antarctic (right), obtained with the SNO technique (gray) and the corresponding simulated differences using the revised version of RTTOV (black). Differences in channel 3 are not shown since SSU channel 3 on TIROS-N malfunctioned soon after the launch.

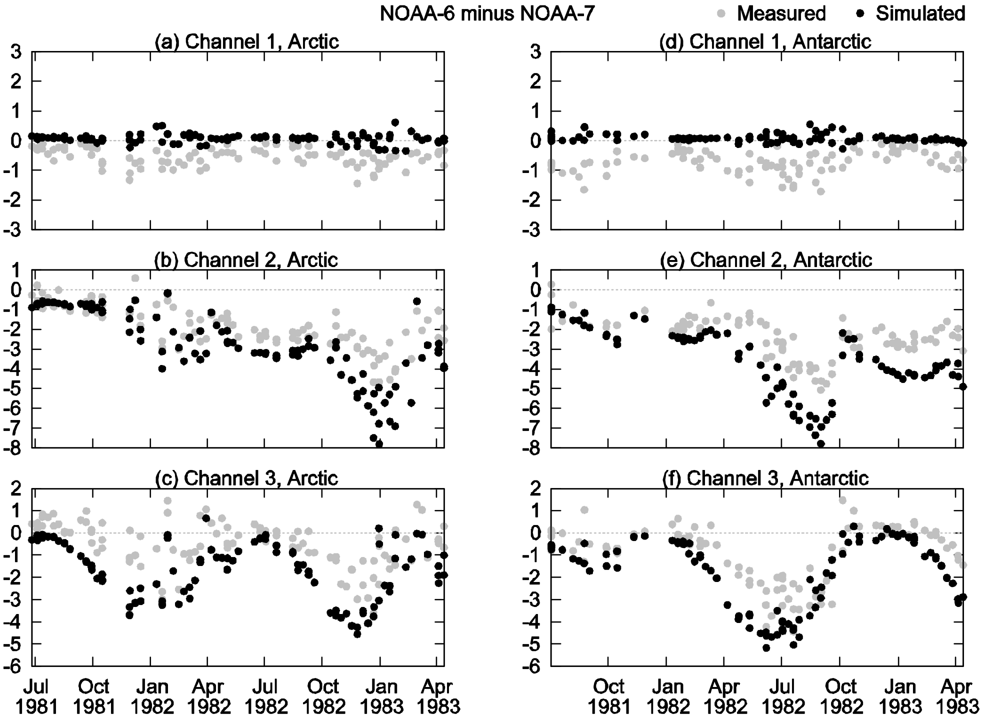


Figure 18. Same as Figure 17, but for radiance measurements from SSUs on NOAA-6 and NOAA-7

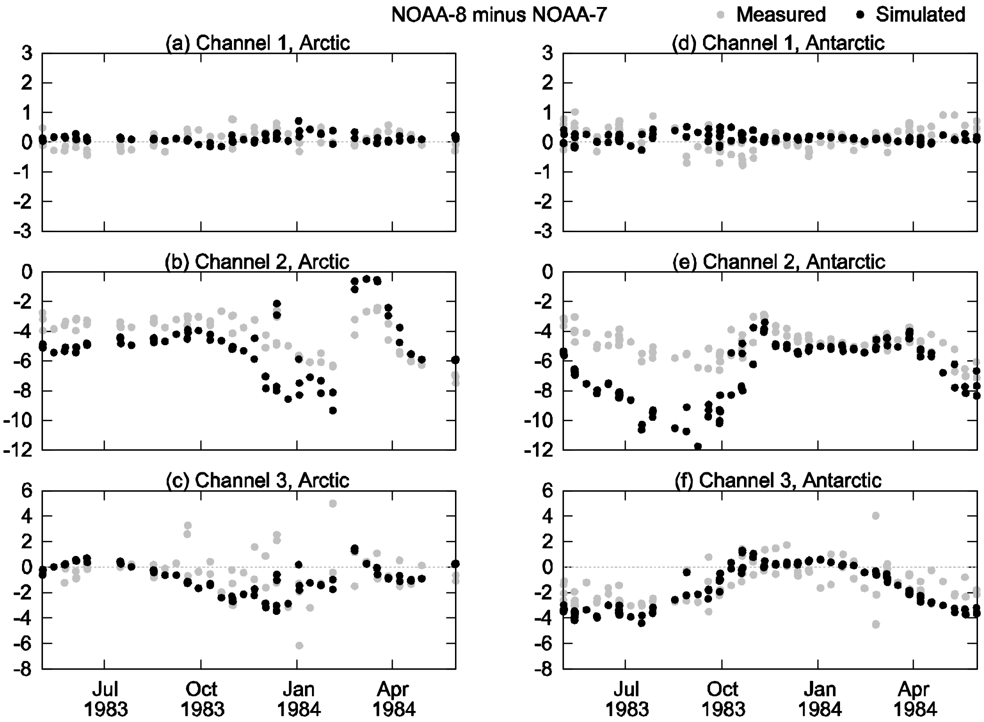


Figure 19. Same as Figure 17, but for radiance measurements from SSUs on NOAA-8 and NOAA-7.

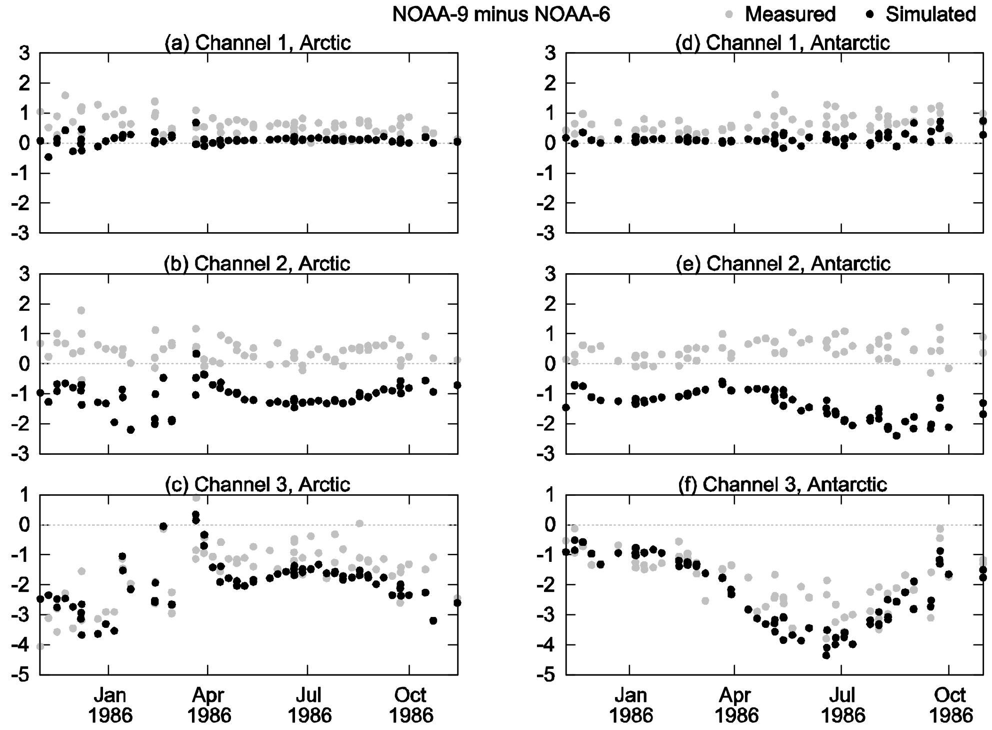


Figure 20. Same as Figure 17, but for radiance measurements from SSUs on NOAA-9 and NOAA-6.

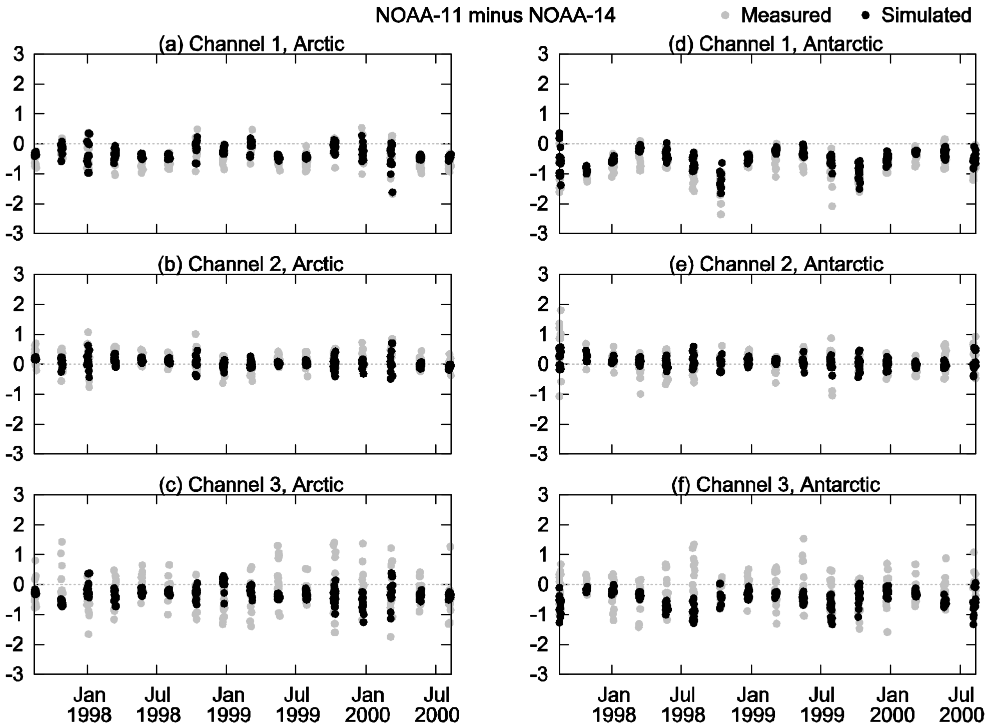


Figure 21. Same as Figure 17, but for radiance measurements from SSUs on NOAA-11 and NOAA-14.