NWP SAF

Satellite Application Facility
for Numerical Weather Prediction

Associate Scientist Report NWPSAF-MO-VS-013

Version 1.1

15 April 2005

Extended studies with the IASI 1DVar code to characterise the impact of AIRS fast model errors on AIRS retrieval accuracy

V. Sherlock

NIWA

Eumetsat Satellite Applications Facility

Associate Scientist Mission

Extended studies with the IASI_1DVar code to characterise the impact of AIRS fast model errors on AIRS retrieval accuracy

Vanessa Sherlock

15 April 2005 revision

NIWA
295-301 Evans Bay Parade
Kilbirne 6003
Wellington
New Zealand
v.sherlock@niwa.co.nz

Contents

1 Context of the extended studies

The extended studies proposed and undertaken in this NWP SAF Associate Scientist mission focus on two relatively distinct aspects or methods for improving channel selection strategies and data use for AIRS.

The first of these studies concerns the validation the predictions of suboptimal linear theory as to the impact of fast model errors on retrieval accuracy. These predictions have been proposed as useful guide to determine robust channel selections (and associated requirements for the specification of the observation error covariance matrix) for operational data assimilation, but have never been explicitly tested using full nonlinear iterative retrievals. The method, results and conclusions of this study are detailed in Section 2.

The second of these studies uses fast model differences as a proxy for fast model errors, and quantifies the impact of these errors on retrieval accuracy in and operational context, with bias correction. We then examine the use of simple fast model error threshhold criteria to identify spectral intervals where model errors compromise retrieval accuracy. The method, results and conclusions of this study are detailed in Section 3. An overall summary and conclusions is given in Section 5.

2 Verifying linear predictions of suboptimal retrieval accuracy

2.1 Introduction

In a previous study [Sherlock et al., 2003] we used linear retrieval theory to characterise retrieval accuracy in the presence of forward model and Jacobian errors for the Gastropod model. These studies predicted that accurate description of forward model error correlations is important where forward model errors make a significant contribution to the observation error covariance matrix $\mathbf{R}$ – neglecting forward model error correlations was shown to affect retrieval accuracy through the propagation of both observation errors and associated, correlated Jacobian errors into the retrieved atmospheric state.

While linear theory provides useful predictions of expected model performance (in optimal and suboptimal retrieval scenarios), true model performance can only be determined by actually performing ensembles of retrievals.

In this study we used the IASI_1DVar code to characterise retrieval errors for ensembles of retrievals performed using the NESDIS channel set, and the complete AIRS channel set. We performed retrievals with the full specification of, and a diagonal approximation to the observation error covariance matrix to characterise the effect of neglecting forward model and Jacobian error correlations.

2.2 Method

Spectra were simulated and retrievals were performed with the AIRS prelaunch instrument spectral response function, and assumed unit surface emissivity. The instrumental noise and forward model error covariance (of Gastropod transmittance prediction errors) described in Sherlock et al. [2003] were also used in this study. Relevant error characteristics are reproduced in Figures 7 and 8 for the entire AIRS spectrum.

Retrievals were performed for temperature on 43 pressure levels between 0.1 and 1013.25 hPa, humidity (ln(q)) on 26 pressure levels between 122.0 and 1013.25 hPa, surface air temperature and humidity, and skin temperature. The background error covariance $\mathbf{B}$ of Collard and Healy [2003] was assumed for these retrieval variables.

Profiles from the ECMWF 50-level diverse profile set [Chevallier, 1999] were perturbed in accordance with the background error covariance. Specifically, an eigenvector decomposition of $\mathbf{B}$ was performed, and a given perturbation of the state vector was generated from the sum over eigenvectors $\mathbf{e}$:

$$\mathbf{dx} = \sum_i \sigma_i . rG_i . \mathbf{e}_i, \tag{1}$$

where the rG_i are random Gaussian numbers and σ_i is the standard deviation of the mode i. To ensure consistency with subsequent IASI_1DVar processing, perturbed profiles were checked to ensure that the humidity profile was not supersaturated (or reset to the saturated mixing ratio) and perturbed profile variables did not lie outside the fastmodel regression bounds[1] (or reset to the IASI_1DVar soft limits). These checked perturbed profiles constituted the ensemble of true atmospheric states to be retrieved (the unperturbed state was the background profile for the retrieval).

Realisations of instrumental noise and forward model error were generated from the instrumental noise and forward model error covariances (using the eigenvector decomposition method described above) for each perturbed state. These noise realisations were added to the fast model radiance calculation for the perturbed atmospheric state to generate the observed brightness temperature spectra for retrievals.

Two series of retrievals were undertaken: retrievals for an ensemble of 100 perturbations to the tropical profile P012 and retrievals for an ensemble of 2 perturbations to each of a set of 69 tropical, midlatitude and high latitude profiles (138 realisations in total).

2.2.1 Retrieval error characterisation

Background and retrieval errors (background – truth, retrieval – truth) were estimated for each realisation of the IASI_1DVar ensembles. Where retrievals did not converge in 10 iterations, or failed for some other reason, the retrieval error was set to the background error for that realisation. These errors were then used to estimate the bias and the error covariance matrices for the ensembles (background and retrieval).

Linear retrieval error covariances were calculated using optimal linear theory for full specification of $\mathbf{R}$ [Rodgers, 1990], and suboptimal linear theory for a diagonal approximation to the full $\mathbf{R}$ matrix [Watts and McNally, 1988]:

$$\mathbf{A}_{subopt} = \mathbf{A}_{opt} + \mathbf{W}(\mathbf{R} - \mathbf{R}_{diag})\mathbf{W}^{\mathrm{T}}, \tag{2}$$

where $\mathbf{W}$ is the Kalman gain matrix. As such, the suboptimal retrieval error covariance estimate includes the propogation of unmodelled correlated forward model errors into the retrieved atmospheric state, but does not attempt to include the effects of Jacobian errors[2], even though fast model Jacobian errors (which are always present, even if small) will be propogated into the

[1] In the IASI_1DVar code, the retrieved profile is checked (and reset) at each iteration to ensure variables do not lie outside the the fastmodel regression bounds. If the true profile lies outside these bounds convergence (and hence retrieval error characteristics) can be affected by these resets.

[2] Estimation of the effects of Jacobian errors is beyond the scope of this study (and indeed most fast model error characterisation studies) due to the computational cost of generating reference Jacobians using line-by-line models. The estimate of suboptimal retrieval accuracy due to forward model error propogation alone is readily implemented, and it is useful to explore the limitations of this approach for practical applications.

IASI_1DVar ensemble retrieval errors. The linear retrieval error covariances for the set of 69 diverse atmospheres were estimated (assuming independent errors) from the sum of the individual covariance matrices for the N atmospheric states $\mathbf{A}_i$:

$$\mathbf{A} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{A}_i. \tag{3}$$

Direct comparison with prediction from linear theory for optimal (or suboptimal) retrievals is complicated by the relatively low number or realisations (a compromise, to enable a large range of retrieval scenarios to be explored), and hence somewhat noisy estimates of ensemble background and retrieval error covariances. The diagonal elements of the covariance matrices are generally well determined, but the full correlation structure is not well estimated. Consequently, measures derived from the full error covariance matrices (degrees of freedom for signal (DFS) and information content) are often affected by noisy signals in the trailing eigenmodes.

Direct comparison with linear theory is also complicated by the fact that profile checks and resets can modify the distribution of applied perturbations and hence the ensemble background error covariance.

To account for these problems when characterising retrieval accuracy we projected covariance matrices (ensemble background and retrieval, linear retrieval) onto the eigenvectors of the IASI_1DVar background error covariance matrix. In this case, the projection coefficient is the variance associated with the mode. The fractional reduction of variance is examined eigenmode by eigenmode, by comparing the variance associated with the mode before and after retrieval. These projection coefficients and fractional reduction of variance can be used further, to provide a quantitative measure of measurement information, which we denote pseudo DFS:

$$\text{pseudo DFS}_M = \sum_{i=1}^{M} \left(1 - \frac{\mathbf{e}_i^{\mathrm{T}} \mathbf{A} \mathbf{e}_i}{\mathbf{e}_i^{\mathrm{T}} \mathbf{B} \mathbf{e}_i} \right), \tag{4}$$

where $\mathbf{A}$ and $\mathbf{B}$ are the retrieval and background error covariance matrices, and $M \leq N_{state}$, the dimension of the state vector (note when $M = N_{state}$ and $\mathbf{B}$ and $\mathbf{A}$ are the linear retrieval error covariances the pseudo DFS is equal to the DFS of linear theory). Diagonal elements of the background and retrieval error covariance matrices are also compared graphically.

2.2.2 Treatment of ozone

Ozone profiles are neither perturbed or retrieved in the studies detailed in sections 2.3 and 3, implying the ozone profile is known perfectly. Retrieval error characterisations therefore do not include errors in stratospheric temperature and ozone retrievals due to uncertainties in the a priori estimate of ozone. This is not a major limitation in the context of the current verification of the predictions of suboptimal linear theory, but does restrict some of the conclusions for operational data assimilation which are drawn in the fast model cross retrieval studies in Section 3. These limitations are addressed in Section 4.

Ozone profiles in the ECMWF 50 level profile set are drawn from climatology, and are therefore not necessarily consistent with the thermodynamic structure (and hence dynamics) of the associated model state (P,T,q). Large increases in fast model errors in the ozone bands have been observed when fast model validation has been performed using the ECMWF 50 level profile set [Sherlock et al., 2003, Matricardi et al., 2001], and attributed to differences in the physical correlations between stratospheric temperature and ozone in the ECMWF 50 level profile set and fast model regression profile sets. These errors will potentially affect retrieval error characterisations derived in these studies.

2.3 Results

2.3.1 Retrievals for atmosphere 012 with the NESDIS channel set

Background and retrieval error characteristics for the atmosphere 012 (P012) are illustrated in Figure 1. The background error distributions for the IASI_1DVar ensemble are modified by the profile checks for temperature at pressures less than 1 hPa, and for humidity at pressures greater than 900 hPa or less than 200 hPa. The distribution of background temperature perturbations is slightly skewed at pressures less the 10 hPa (as indicated by the bias in the ensemble of background errors), but this is a relatively small contribution to the total error. The distribution of humidity perturbations below 900 hPa presents similar characteristics.

The standard deviations of temperature and humidity retrieval errors for the ensemble of 100 IASI_1DVar retrievals (denoted monte carlo in the Figure legends) with full specification of $\mathbf{R}$ are generally in very good agreement with the predictions from optimal linear theory. Differences are observed in boundary layer and upper tropospheric humidity, where profile checks modify background error characteristics significantly. In the upper troposphere, the relative reduction in variance is lower in the ensemble of IASI_1DVar humidity retrievals.

Bias is reduced to low levels for retrieved tropospheric (P $<$ 200 hPa) and upper stratospheric (10 – 0.3 hPa) temperatures. There is a apparant increase in bias in humidity retrievals in the upper troposphere (P $<$ 200 hPa) and in the lower troposphere (700 – 900 hPa), due to a slight skew in the distribution retrieval errors. All biases are small compared to the standard deviation of retrieval errors.

The principal impact of neglecting forward model error correlations on the ensemble of IASI_1DVar retrievals is the reduction in retrieval accuracy for upper tropospheric humidity (P $<$ 300 hPa). There are small reductions in accuracy in humidity retrievals throughout the remainder of the troposphere, and a small reduction in temperature retrieval accuracy in the mid and upper troposphere (600 – 100 hPa), but they do not affect the benefit of the data assimilation significantly. Neglecting forward model error correlations also has a modest effect on convergence. An additional iteration was required in 10% of retrievals with a diagonal approximation to $\mathbf{R}$. The number of iterations was doubled in a further 5% of retrievals and 2% of retrievals failed to converge after 10 iterations (as compared with 0% for retrievals with full specification of $\mathbf{R}$).

The suboptimal linear error covariance estimate does not predict the observed tropospheric temperature and humidity error inflation, probably due to the fact that the effects of Jacobian errors are neglected. Previous studies [Sherlock et al., 2003] which estimated the impact of a diagonal approximation to $\mathbf{R}$ in the presence of correlated forward model and Jacobian errors did predict comparable increases in tropospheric temperature and humidity retrieval errors, albeit for different atmospheric states and reduced (130 channel) channel subsets.

The standard deviation of surface air humidity retrieval errors is greater than the ensemble background error. This is a feature of all the IASI_1DVar retrievals performed, including retrievals with the RTTOV model. This arises because the distributions of surface humidity errors (background and retrieval) are skewed and the standard deviation estimate is sensitive to small differences in the largest errors. Robust estimates of the spread of the error distributions based on the interquartile range indicate surface humidity retrieval errors are less than or equal to background errors in at least 50% of the data set.

2.3.2 Retrievals for the set of 69 atmospheres with the NESDIS channel set

Background and retrieval error characteristics for the set of 69 diverse atmospheres (AS69) are illustrated in Figure 2. The humidity background error distributions for the IASI_1DVar ensemble are substantially modified (standard deviations reduced, small biases introduced) by the profile checks. Background error distributions for stratospheric temperatures are also affected.

The standard deviations of temperature and humidity retrieval errors for the ensemble of 138 IASI_1DVar retrievals with full specification of **R** are generally in good agreement with the predictions from optimal linear theory. Again, differences are observed in boundary layer and upper tropospheric humidity, where profile checks modify background error characteristics significantly. The IASI_1DVar temperature retrieval errors are also slightly larger (0.1 K) at pressures less than 10 hPa.

Neglecting forward model error correlations leads to small reductions in retrieval accuracy at all levels for both temperature and humidity for the ensemble of IASI_1DVar retrievals, however, their impact on upper tropospheric humidity retrievals is reduced, as compared to the P012 retrievals.

As previously, neglecting forward model error correlations had a modest effect on convergence. Additional iterations were required in 13% of retrievals with a diagonal approximation to **R** and 3% of retrievals failed to converge after 10 iterations (as compared with 0% for retrievals with full specification of **R**).

The suboptimal linear retrieval error covariance estimate provides a reasonable qualitative prediction of error inflation in stratospheric temperature and upper tropospheric humidity retrievals, but underestimates the actual levels of error inflation derived from the IASI_1DVar ensembles (which again we attribute to the unmodelled effects of Jaobian errors).

Overall, the IASI_1DVar retrievals confirm the results of the P012 ensemble, and predictions from linear theory: suboptimal retrievals, neglecting fast model error correlations, do not significantly reduce retrieval accuracy when using the NESDIS channel selection or similar channel subsets with the Gastropod model.

The temperature error characteristics at pressures less than 10 hPa, and their sensitivity to the specification of the observation error covariance, do differ from the predictions of linear theory. This may be due to differences in physical correlations between stratospheric temperature and ozone in the fast model regression set and in the ECMWF 50 level profile set [Sherlock et al., 2003] and more extensive use of the ozone ν_1 and ν_3 bands in the NESDIS channel set.

2.3.3 Projection onto the eigenvectors of B

The variances associated with each eigenvector of **B** are illustrated in Figure 3 for the background error covariance matrix **B** and for the background and retrieval error covariance matrices of the IASI_1DVar P012 and AS69 ensembles (left and right hand panels respectively).

For the P012 and AS69 IASI_1DVar background errors the variances associated with each of these eigenmodes are generally comparable with the variances of **B**. However, in the leading temperature modes (stratospheric temperature modes) of the P012 ensemble, and in many of the humidity modes of the P012 and AS69 ensembles the variance is lower, due to the profile checks described above. The variance is significantly higher in the trailing humidity eigenmodes (modes 66–72) of the P012 and AS69 ensembles.

The ensemble retrieval errors generally show substantial reductions in variance in the leading temperature and humidity modes. However, there are increases in variance in the trailing temperature (40-45) and humidity (72) modes.

Figure 4 illustrates the fractional reduction of variance in each mode, $\frac{\mathbf{e}_i^{\mathrm{T}}\mathbf{A}\mathbf{e}_i}{\mathbf{e}_i^{\mathrm{T}}\mathbf{B}\mathbf{e}_i}$, for the ensemble retrievals and from linear theory. The error inflation described becomes more apparant in this representation, corresponding to fractional reduction of variances greater than one.

The significance the error inflation in modes 45, 71 and 72, which have very small associated variances (also indicating **B** is poorly conditioned), and indeed the modes 40–44, which all present high frequency oscillations between 20 and 150 hPa and between 500 and 900 hPa, is less clear. Their contribution to the total retrieval error covariance is small, and the eigenvectors do not appear to represent error modes of physical significance. Additionally, the projection coefficients in these modes do not appear to be sensitive to the details of the specification of **R**.

For these reasons we exclude these modes from the pseudo DFS calculation, and focus this measure on the fractional reduction of variance in the leading temperature (1–34) and humidity (46-63) modes, and how it is influenced by the specification of the observation error covariance matrix.

The pseudo DFS (pDFS) for the ensemble of 100 retrievals for atmosphere P012 with the NESDIS channel set (324) are reported in the fourth major column of the first row of Table 1. A diagonal approximation to **R** leads to a loss of 1.9 pDFS. Returning to Figures 1 and 4, we see this is due to increased error in retrieved humidity modes when a diagonal approximation to **R** is assumed.

The pseudo DFS (pDFS) for the ensemble of 138 retrievals for the 69 atmospheres with the NESDIS channel set (324) are reported in third row of Table 1. In this case a diagonal approximation to **R** leads to a loss of 1.8 pDFS, and is associated with increased errors in both temperature and humidity modes.

The difference between the ensemble pseudo DFS and the DFS predictions from optimal linear theory result from the overall reduction in background error covariance in the IASI_1DVar retrievals (thus reducing the potential information content of the measurements) and the inflation of errors in the coupled surface air – lower tropospheric temperature modes (additionally, reductions in bias on retrieval and the associated information content are not taken into account in this analysis of the ensemble error covariance matrices). The reductions in pDFS associated with the diagonal approximation to **R** are larger than estimates based on the suboptimal linear DFS calculations presented here (0.5–0.9 DFS), but are comparable with previous predictions from linear theory, including the effects of Jacobian errors (1.9–2.2 DFS) [Sherlock et al., 2003].

2.3.4 P012 retrievals using all AIRS channels

Background and retrieval error characteristics of retrievals using all AIRS channels[3] for atmosphere P012 are illustrated in Figure 5. Again, there is good agreement between the ensemble retrieval errors and optimal linear theory when foward model and Jacobian error correlations are taken into account (full specification of **R**).

Neglecting fast model error correlations has a significant impact on retrieval accuracy for the IASI_1DVar ensemble. There is a substantial increase in humidity errors when retrievals are performed with a diagonal approximation to **R**. This is particularly true of the upper troposphere ($P < 300$ hPa), where retrieval and background errors are comparable, and in the lower troposphere ($P > 800$ hPa), where neglecting fast model error correlations leads to retrieval errors which exceed background errors. Neglecting fast model error correlations also has a significant impact on temperature retrievals in the troposphere and stratosphere (both bias and standard

[3]Strictly speaking, retrievals are performed with 2317 of the 2378 channels, as the "popcorn" channels are excluded from the retrieval channel selection (and in linear error covariance estimates).

deviation).

Neglecting forward model error correlations also has a marked impact on convergence, with the number of iterations increased by 1 or more in 90% of retrievals using a diagonal approximation to **R**, and with retrievals failing to converge in 42% of cases.

The pseudo DFS for retrievals using the full set of AIRS channels and a diagonal approximation to **R** is just 4.2, compared with 21.1 when retrievals are performed with the full specification of **R**. Thus, in this case, neglecting fast model error correlations almost completely compromises the benefit of data assimilation.

Qualitatively, suboptimal linear theory gives reasonable predictions of the effect of neglecting forward model error correlations: substantial error inflation at all levels, and potential degradation of a priori humidity information in the upper and lower troposphere. Quantitatively, suboptimal linear retrieval error covariance estimates underestimate the extent of error inflation derived from the IASI_1DVar ensembles, with the exception of upper (P $<$ 300 hPa) and lower (P $>$ 900 hPa) tropospheric humidity retrievals, where errors are overestimated (however these are two regions where profile checks modify the distribution of IASI_1DVar ensemble profile perturbations significantly, and this may mitigate suboptimal retrieval errors for the ensemble).

Conversely, previous linear retrieval studies [Sherlock et al., 2003] predicted that Jacobian errors would result in degraded retrieval accuracy (for retrievals with the full AIRS channel set) even when a full specification of **R** is used in retrievals. This is not borne out by the IASI_1DVar retrievals, where retrieval accuracy approaches the optimal linear retrieval accuracy with full specification of **R**. There are two possible reasons for these differences. Firstly, the suboptimal linear error covariance estimate effectively assumes the same Jacobian error for all realisations, whereas Jacobian errors may 'average out' from realisation to realisation. Secondly, extreme profiles (with the worst error characteristics) were considered in the previous linear retrieval studies to characterise the effects of Jacobian error. Thus Jacobian errors, and hence their impact on retrieval accuracy, could be significantly smaller in the current case.

2.3.5 AS69 retrievals using all AIRS channels

Background and retrieval error characteristics of retrievals using all AIRS channels for the AS69 atmospheres are illustrated in Figure 6. As previously, there is good agreement between the IASI_1DVar retrievals with full specification of **R** and optimal linear theory, but there is significant degradation in retrieval accuracy at all levels when a diagonal approximation is made to **R**, and the benefit of data assimilation is almost completely compromised.

The pseudo DFS for the IASI_1DVar ensemble of retrievals with a diagonal approximation to **R** is 1.7, compared with 19.9 for retrievals with full specification of **R**. Retrieval accuracy is significantly reduced in all modes (not shown), and retrieval errors exceed background errors for upper tropospheric humidity. When compared with the results of the tropical P012 atmosphere above, these results suggest that the sensitivity of retrieval accuracy to specification of fast model error correlations is greater in drier atmospheres, consistent with previous predictions from suboptimal linear theory.

As in the case of retrievals for the P012 atmosphere with the full set of AIRS channels, convergence rates are also strongly affected by the diagonal approximation to **R**, with one or more additional iterations required for 85% of retrievals, and 64% of retrievals failing to converge.

As previously, suboptimal linear theory gives reasonable qualitative predictions of the effect of neglecting forward model error correlations: substantial error inflation at all levels, and loss of all potential humidity information in the upper troposphere (P $<$ 300 hPa), but underestimates the extent of error inflation derived from the IASI_1DVar ensembles, with the exception of upper tropospheric humidity.

2.4 Conclusions

Despite difficulties with direct comparison of the statistics derived from ensembles of IASI_1DVar retrievals and the predictions of linear theory, the results obtained provide a qualitative confirmation of the conclusions of previous studies using linear theory, namely:

- For typical AIRS channel subsets used in operational data assimilation, Gastropod model errors do not have a significant impact on retrieval accuracy. A diagonal approximation to **R** leads to small decreases in retrieval accuracy, but the information loss is insignificant for practical purposes.

- For retrievals with the full AIRS channel set, neglecting Gastropod model error correlations has a significant impact on retrieval accuracy, and can completely compromise the benefit of data assimilation in some circumstances. However – in contrast to the predictions of suboptimal linear theory – with full specification of model error correlations retrieval accuracy approaches that of optimal linear theory.

- Linear error covariance estimates including suboptimal forward model error propogation give reasonable qualitative predictions of the impact of neglecting forward model error correlations, but generally underestimate the errors derived from the IASI_1DVar retrievals, suggesting the effects of Jacobian errors must be taken into account when characterising suboptimal retrieval accuracy. As this represents a significant computational overhead for estimates based on linear theory, monte carlo approaches, like the one presented here, are probably the more direct and practical means to assess the impact of model errors on retrieval accuracy. Furthermore, monte carlo approaches can be readily extended to encorporate other aspects (e.g. bias correction) of an operational data assimilation system (see Section 3).

The diagonal approximation to **R** has also been shown to have a measurable impact on convergence rates, and again, this is particularly important for retrievals using the all AIRS channels.

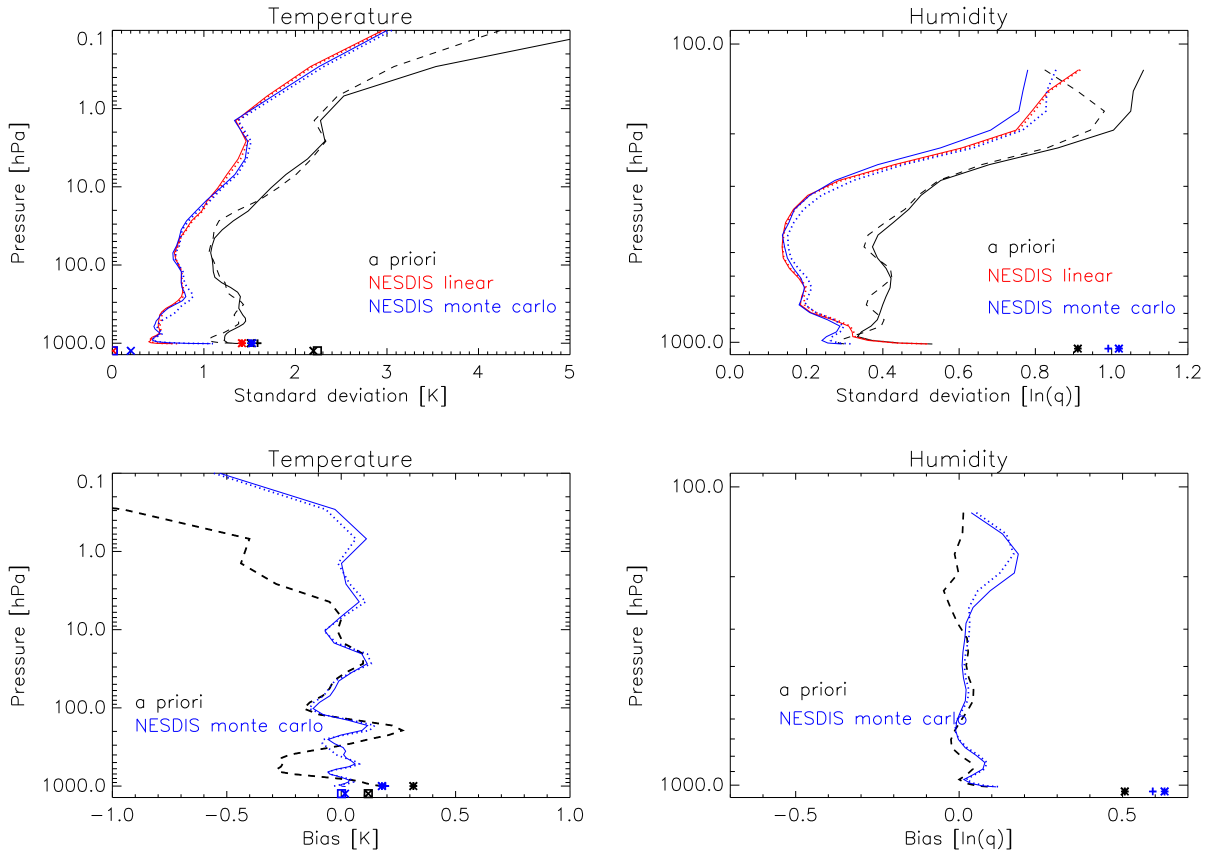

Figure 1: Error characteristics (bias and standard deviation) of retrievals performed using the NESDIS channel set for atmosphere P012. Background errors are traced in black. The dashed black line illustrates the bias and standard deviation of the ensemble of background states used in retrievals. The corresponding standard deviations of the background error covariance matrix **B** are illustrated by the solid black line. Retrieval errors are illustrated for the ensemble of IASI_1DVar retrievals (monte carlo) in the blue curves. Corresponding errors predicted by optimal and suboptimal linear theory are illustrated in red. In each case, solid lines indicate retrievals using a full specification of the observation error covariance matrix **R** (i.e. full specification of forward model error correlation), and dotted lines indicate retrievals performed with a diagonal approximation to **R**. The errors in background surface air variables are illustrated using a black plus (**B**) and asterisk (ensemble). Errors for retrieved surface air variables are illustrated with the same symbols (plus = full **R**, asterisk = diag **R**), in the colour code of the relevant series. The background, optimal and suboptimal linear retrieval errors for surface humidity are 1.45, 1.42 and 1.43 respectively and do not appear on the humidity standard deviation plot. Skin temperature errors are illustrated below air temperature errors in temperature bias and standard deviation plots. The errors in background skin temperature are illustrated using a black square (**B**) and cross (ensemble). Errors for retrieved skin temperature are illustrated with the same symbols (square = full **R**, cross = diag **R**), in the colour code of the relevant series. Skin temperature retrieval errors are of the order of 0.01 K for the linear and full **R** IASI_1DVar retrieval cases.

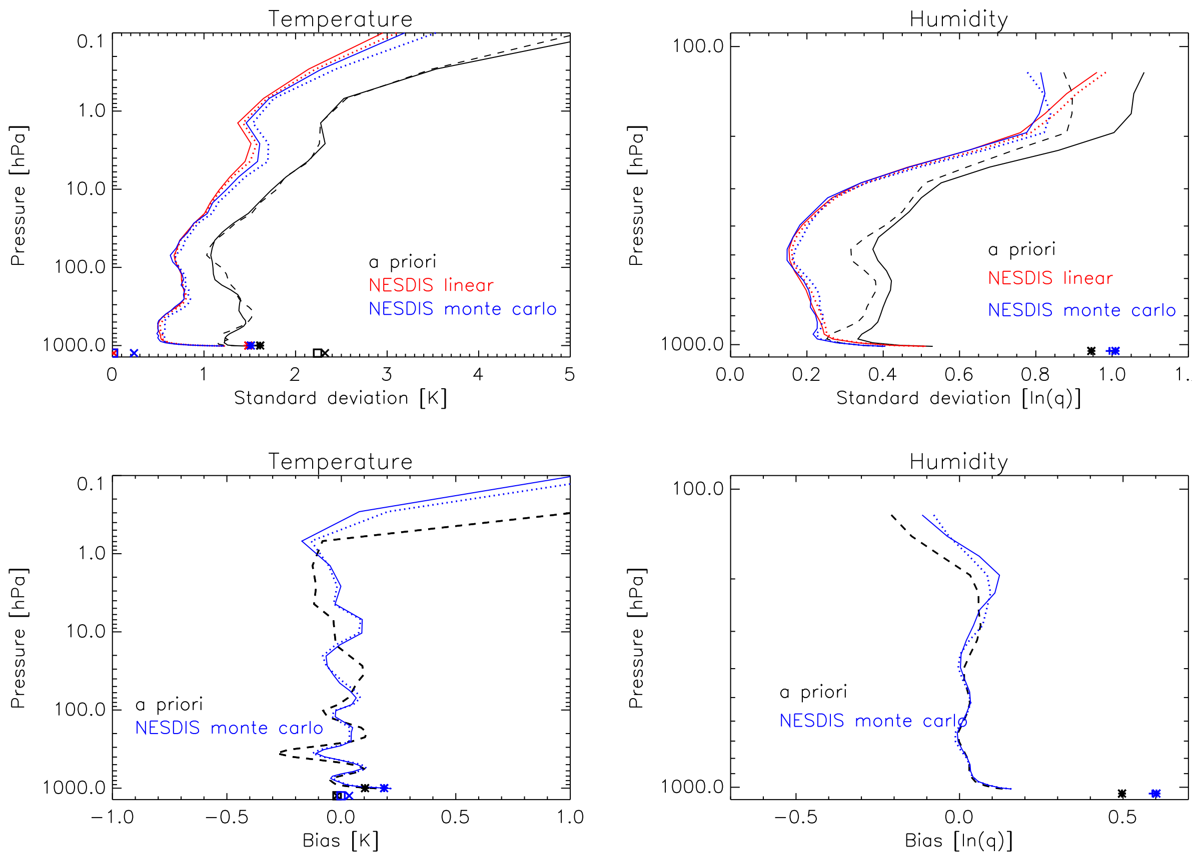

Figure 2: Error characteristics of retrievals performed using the NESDIS channel selection for the set of 69 diverse atmospheric states. Background, optimal and suboptimal linear retrieval errors for surface humidity are 1.45, 1.40 and 1.41 respectively and do not appear on the humidity standard deviation plot. All line styles and symbols are as defined in Figure 1.

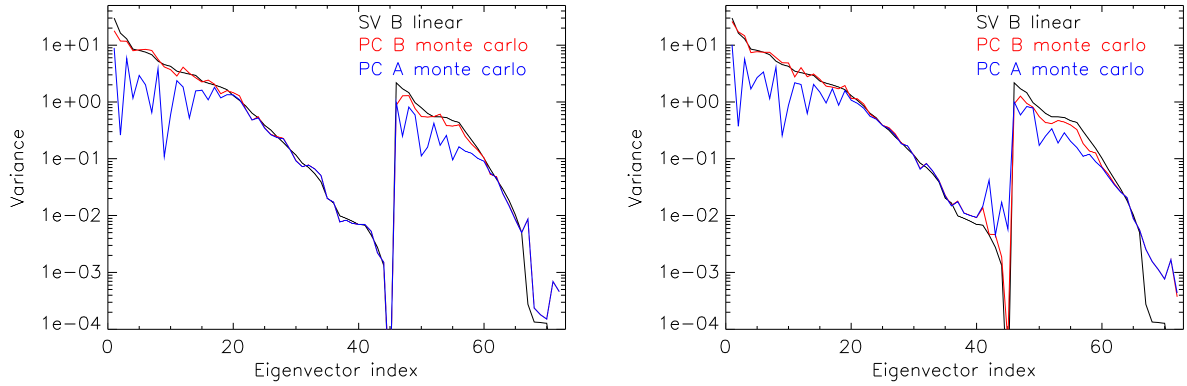

Figure 3: Characterisation of the full error covariance matrices by projection onto the eigenvectors of the background error covariance **B**. Left hand panel: background and retrieval error characteristics for the P012 ensemble. Right hand panel: background and retrieval error characteristics for the ensemble of 69 diverse atmospheres. Indices 1–45 correspond to temperature error modes, indices 46-72 correspond to humidity error modes. The variance of each mode of **B** is illustrated with the black curve. The variance associated with each mode in the ensemble background error covariance is illustrated with the red curve, and the variance associated with each mode in the ensemble of retrievals (using the NESDIS channel set and a full specification of **R**) is illustrated in blue.

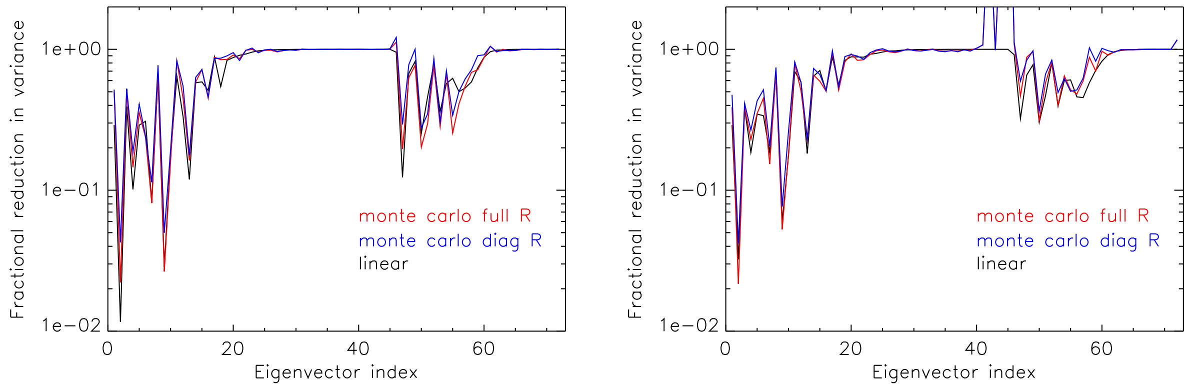

Figure 4: Fractional reduction of variance for atmosphere P012 (left panel) and the set of 69 atmospheric states (right panel), for retrievals using the NESDIS channel set. Optimal linear fractional reduction of variance is traced for reference.

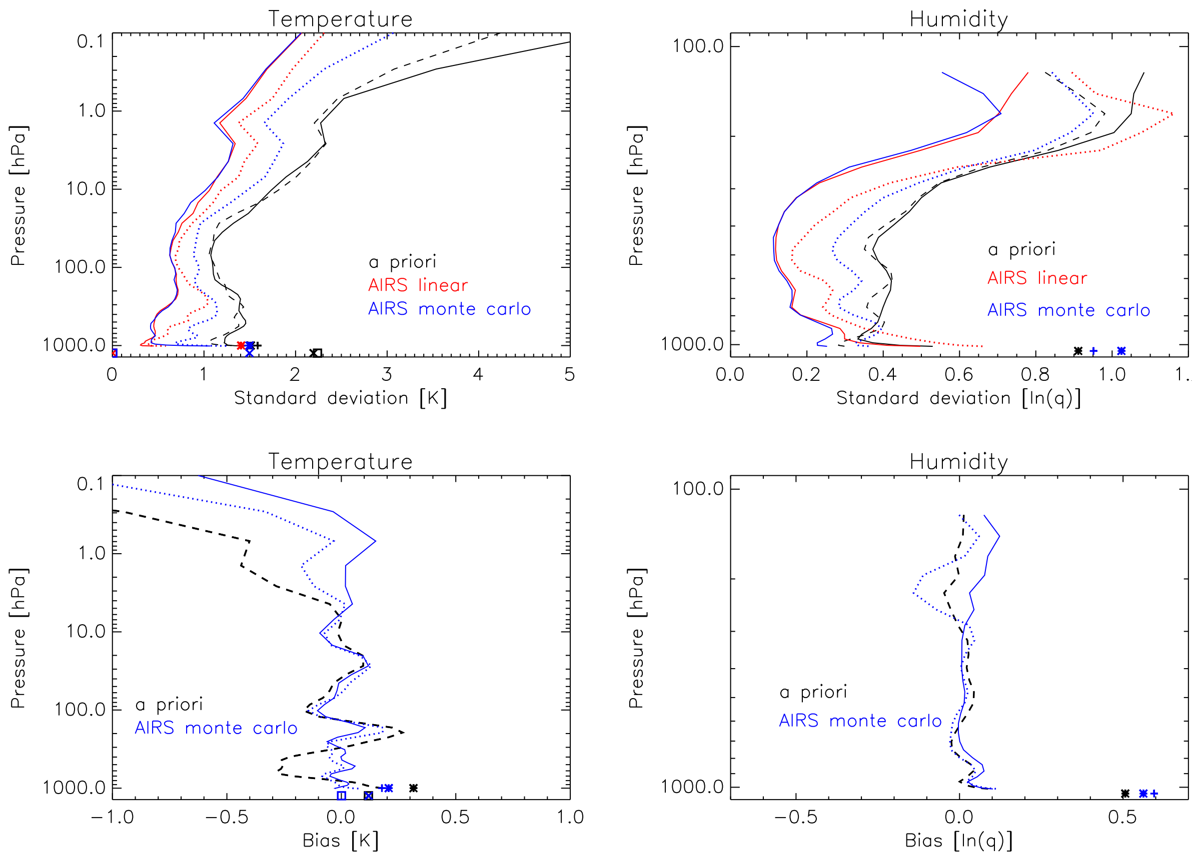

Figure 5: Error characteristics of retrievals performed using the entire AIRS channel set for atmosphere P012. Background, optimal and suboptimal linear retrieval errors for surface humidity are 1.45, 1.40 and 1.58 respectively and do not appear on the humidity standard deviation plot. All line styles and symbols are as defined in Figure 1.

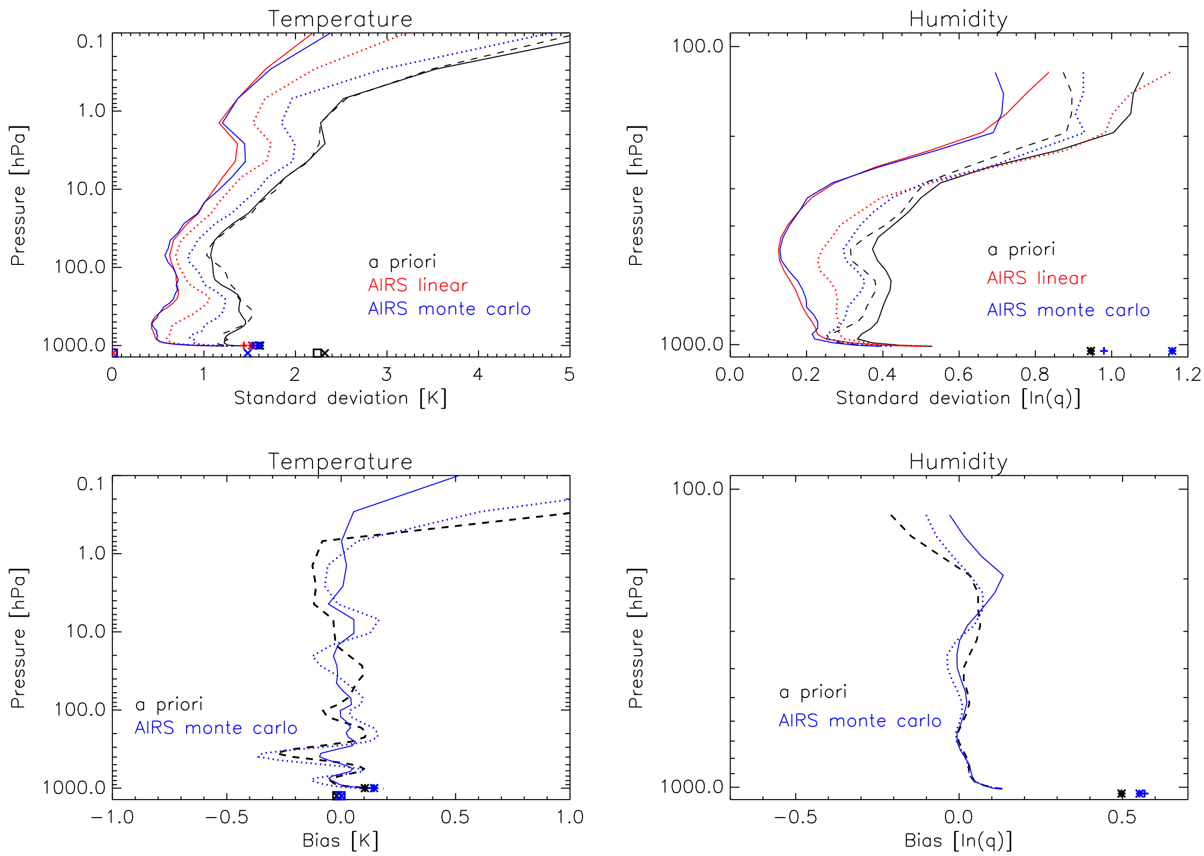

Figure 6: Error characteristics of retrievals performed using the entire AIRS channel set for the set of 69 diverse atmospheres. Background, optimal and suboptimal linear retrieval errors for surface humidity are 1.45, 1.39 and 1.44 respectively and do not appear on the humidity standard deviation plot. All line styles and symbols are as defined in Figure 1.

Series	ret	ref	bias	chan	N_{real}	N_{ret} full **R**	N_{ret} diag **R**	pDFS Monte-C full **R**	pDFS Monte-C diag **R**	DFS Linear full **R**	DFS Linear diag **R**
P012	G	G	-	324	100	100	98	17.5	15.6	18.2	17.7
P012	G	G	-	2378	100	100	58	21.1	4.2	21.7	6.0
AS69	G	G	-	324	138	138	134	16.1	14.3	17.6	16.7
AS69	G	G	-	2378	138	137	88	19.9	1.7	21.3	6.9

Table 1: Summary of retrieval characteristics for experiments to verify the predictions of linear theory. Results are tabulated with identifiers for the series (P012, AS69), fast model used to perform the retrievals (ret) and generate the observations (ref), the number of channels used in retrievals (324=NESDIS, 2378=AIRS), the number of realisations in experiment, the number of sucessful retrievals, the pseudo DFS for the ensemble of retrievals, and the DFS predicted from optimal and suboptimal linear theory for retrievals with full specification of **R** and with a diagonal approximation to **R** respectively. G denotes Gastropod, R denotes RTTOV in subsequent Tables.

3 Retrieval error characterisation using fastmodel differences as a proxy for fast model errors

3.1 Introduction

AIRS fast model differences are now generally of the order of 0.1 – 1.0 K, comparable with current AIRS O – B statistics. This suggests fast model errors may be a significant source of error in some channels or spectral intervals. It is therefore of interest to use fast model differences as a proxy for the true errors in fast model representions of atmospheric radiative transfer, and to characterise the potential impact of these errors on retrieval accuracy.

A preliminary study was undertaken in the course of an ISAT funded visit to the Met Office in October 2003, where observed spectra were simulated using one fast model, and retrievals were performed using a second fast model. We will refer to this as 'cross-retrieval' hereafter. These studies showed that differences in spectroscopy in the CO_2 ν_3 band head could result in significant degradation of tropospheric temperature and humidity retrievals.

However, radiances were not bias corrected in these studies, so results were not representative of potential operational analysis errors, and retrievals were only performed for single cases, and were therefore not statistically representative of an ensemble of retrievals for a given atmospheric state, or the range of atmospheric states encountered in practice.

In this study we addressed these limitations. We estimated a flat bias correction and forward model error covariance matrix from fast model differences for the AS69 set of atmospheres. We then performed cross-retrievals for the P012 and AS69 ensembles considered previously. Retrievals were performed both with and without bias correction (the latter representing an extreme case of inadequate bias correction) and with full and diagonal approximations to the observation error covariance matrix $\mathbf{R}$. Retrievals were performed with the NESDIS channel selection – as this is the most relevant for current operational applications. However we also performed retrievals with a 266 channel subset of the NESDIS channel set, which excludes any channels where the fast model differences show either high bias or high standard deviation, and assessed the use of such criteria for defining robust channel selections for operational data assimilation.

3.2 Method

Spectra were simulated, and retrievals were performed with the AIRS postlaunch instrument spectral response function (version 2) and assumed unit spectral emissivity. The background error covariance of Collard and Healy [2003] and the AIRS instrumental noise of Sherlock et al. [2003] are used in these studies.

RTTOV and Gastropod forward calculations for the unperturbed profiles of the AS69 profile set were used to derive a flat bias correction (the mean brightness temperature difference in each channel) and estimate the forward model error covariance matrix.

As previously, spectra were simulated for each perturbed profile of the P012 and AS69 ensembles. A realisation of the instrumental noise was generated for each of these simulations, and added to the fast model spectrum to generate the observed brightness temperature spectrum for retrievals. The fast model used to generate the observed spectrum is referred to as the reference model.

Retrievals are characterised with the measures used previously (graphical comparison of the background and retrieval error biases and standard deviations, pseudo DFS (and DFS from linear theory)). Cross retrievals, performed with and without bias correction, are compared with retrievals using the reference model (without bias correction). Retrieval information content and convergence characteristics for all experiments described below are summarised in Tables 2 and 3.

3.3 Results

3.3.1 Characterisation of fast model errors

The bias and standard deviations of the RTTOV–Gastropod fast model differences are illustrated in Figure 7. Gastropod forward model error (strictly, transmittance prediction error) characteristics are traced for reference.

Significant biases (of the order of 0.5 – 1.0 K) are found in the CO_2 ν_2 and ν_3 bands, and are as large as 2 K in the CO_2 ν_2 Q branch and the CO_2 ν_3 band head. Biases of 0.5 – 1.0 K are also found in isolated water vapour lines in the longwave window region and some (but not all) channels in the H_2O ν_2 band.

Standard deviations are comparable or greater than instrumental noise levels in the O_3 ν_1 and ν_3 bands, the CO_2 ν_3 band, the shortwave window region, the H_2O ν_2 band and water vapour line centres in longwave window region.

The origin of these most significant differences is, at least in part, due to differences in spectroscopy. Gastropod is based on HITRAN98, which includes revised H_2O line parameters[4] [Toth, 2000], assumes the CKD2.4 water vapour continuum model and includes revised line mixing in the CO_2 bands [Strow et al., 2003]. RTTOV, on the other hand, is based on HITRAN96 and CKD2.1.

Additional error sources may also play a role e.g. differences in stratospheric extrapolation assumptions may affect high peaking channels in the CO_2 bands; fast model transmittance prediction errors may make a significant contribution to observed differences in some channels in the H_2O ν_2 band.

The observed errors in the ozone bands may not be representative of true model errors. Large increases in forward model errors have observed in these bands when independent fast model validation has been performed using the ECMWF 50 level profile set [Sherlock et al., 2003, Matricardi et al., 2001]. As described previously, these increases have been attributed to differences in the physical correlations between stratospheric temperature and ozone in the ECMWF 50 level profile set and in fast model regression profile sets.

Figure 8 illustrates the correlation structure of the observation error covariance matrices **R** with **F** derived from Gastropod forward model errors and with **F** derived from RTTOV–Gastropod fast model differences.

In the case where **F** is derived from Gastropod forward model errors the off-diagonal elements of **R** are generally small, with the exception of correlated errors in channels on water vapour line centres within the window regions, within the H_2O ν_2 band, and between such channels in the window regions and the 1200–1400 cm^{-1} interval of the H_2O ν_2 band. There is also a significant contribution from correlated errors within the O_3 ν_1 and ν_3 bands, and negative error correlations between channels in the O_3 band and channels on water vapour line centres.

In the case where **F** is derived from RTTOV–Gastropod fast model differences, off-diagonal contributions to **R** are larger across most of the spectrum because fast model differences are comparable with or greater than instrumental noise levels in many spectral intervals, and these

[4]Simulations for the U.S. Standard atmosphere [Sherlock, 2000] indicate these spectroscopic differences can give rise to brightness temperature differences of 0.5 – 1.0 K, however large variability in atmospheric water vapour abundances may mean these spectroscopic differences manifest themselves as large standard deviations, rather than large biases in brightness temperature statistics c.f. fast model bias and standard deviations in the H_2O ν_2 band.

differences exhibit strong inter-channel correlations. Correlation structure is more complex and can differ significantly from the Gastropod forward model error correlation structure. For example, there are negative correlations between errors in the 1200-1400 and 1400-1600 cm^{-1} intervals of the H_2O ν_2 band; there are significant error correlations within the CO_2 ν_3 band; there is a negative correlation between errors in channels between and centred on water vapour lines in the longwave window region; and there is a positive correlation between errors in channels on water vapour line centres in the longwave window region, channels in the ozone bands and channels in the 1400–1600 cm^{-1} interval of the H_2O ν_2 band.

3.3.2 P012 case studies: comparison of reference model retrievals

The error characteristics of reference retrievals (each model retrieving from its own spectra, plus a realisation of the instrumental noise) are illustrated in Figure 9 for atmosphere P012. The retrieval error characteristics are essentially the same for the two models. RTTOV gives slightly better retrievals of stratospheric temperatures at pressures less than 1 hPa, while Gastropod gives slightly better retrievals of upper tropospheric humidity (P < 200 hPa), and skin temperature (IASI_1DVar fails one retrieval when using RTTOV). Note also the same error inflation and bias in retrievals of surface air temperature with the two models. Characteristics for the surface humidity retrievals are similar.

As these differences are minor, the pseudo DFS for retrievals with the two models is essentially the same (see Table 2). The pseudo DFS is relatively insensitive to the specification of $\mathbf{R}$, as might be expected, as reference retrievals do not contain the propogation of the correlated fast model error (model difference) component of the observation error[5].

Comparing the linear DFS (Table 3) with results where $\mathbf{F}$ is based on Gastropod forward model error estimates (Table 1), fast model differences result in a small loss of 0.3 – 0.4 DFS for atmosphere P012 and the AS69 ensemble, with full specification of $\mathbf{R}$. This is due to a small increase in stratospheric temperature retrieval errors (P < 10 hPa) which presumably results from increased observation errors (and hence reduced weight given to observations) in the CO_2 ν_3 head (errors in the ozone bands may also play a role). Neglecting fast model error correlations leads to more significant losses (1.6 – 2.2 DFS), as compared with suboptimal retrievals with Gastropod forward model error estimates. This result is as expected, given the high inter-channel error correlations of the $\mathbf{R}$ matrix derived from fast model differences decribed above.

Comparison of reference retrieval accuracy and the predictions from linear theory yield essentially equivalent results (for both models) to results of Figures 1 and 2 and discussion thereof, and will not be detailed further here.

3.3.3 P012 case studies: cross-retrieval with and without bias correction

Retrieval error characterisations for cross-retrievals using RTTOV and Gastropod are illustrated for atmosphere P012 in Figures 10 and 11. Retrieval error characteristics generally share common features which we detail here, noting model-specific differences where relevant.

When retrievals are performed without bias correction retrieved temperatures show large biases, of the order of 1 K in the troposphere and greater than 1 K in the upper stratosphere (P < 1 hPa). It is difficult to make a similar general statement about humidity bias characteristics.

[5] It is therefore not valid to compare the reference pDFS for a diagonal approximation to $\mathbf{R}$ with the predictions from suboptimal linear theory in Table 3. This comparison is valid for the cross-retrievals, which do include the propogated fast model error (model difference) component of the observation error.

The standard deviation of upper stratospheric temperature and boundary layer humidity ($P > 900$ hPa) are increased relative to the bias corrected cases (as is the RTTOV upper tropospheric humidity retrieval), and exceed the background errors in the first two instances. Increased retrieval errors (due to the propogation of fast model errors into the retrieved state) result in the loss of 4–5 pDFS relative to reference retrievals, with full specification of $\mathbf{R}$.

A diagonal approximation to $\mathbf{R}$ increases errors in tropospheric temperature and humidity retrievals (but improves RTTOV retrievals of stratospheric temperatures). It also modifies the structure and tends to amplify the bias in retrievals. The diagonal approximation to $\mathbf{R}$ also modifies convergence, with 33% of retrievals with Gastropod and 25% of retrievals with RTTOV requiring one or more additional iterations, and 5% of retrievals failing to converge with a diagonal approximation to $\mathbf{R}$ (as compared to 0 or 1% in reference retrievals). A diagonal approximation to $\mathbf{R}$ results in the loss of 6–9 pDFS relative to reference retrievals.

Bias correction reduces retrieval errors (standard deviation and bias). The impact of a diagonal approximation to $\mathbf{R}$ on retrieval error standard deviations is reduced, except for lower tropospheric humidity retrievals (Gastropod bias corrected humidity retrieval errors still exceed background errors when retrievals are performed with a diagonal approximation to $\mathbf{R}$). The diagonal approximation to $\mathbf{R}$ also results in increased amplitude bias structures and modifies the structure of bias in tropospheric temperature retrievals.

3.3.4 P012 case studies: comparison of bias-corrected cross-retrievals and reference retrievals

Retrieval error characterisations for bias corrected cross-retrievals are compared with reference retrieval errors for atmosphere P012 in Figures 12 and 13.

With bias correction the standard deviation of temperature retrievals is comparable with reference retrieval errors, and the temperature biases for bias-corrected retrievals with full specification of $\mathbf{R}$ are comparable with reference retrieval biases (bias correction actually improves the bias in the RTTOV retrievals of temperature at 0.1 hPa). As noted above, a diagonal approximation to $\mathbf{R}$ increases the amplitude of the retrieval biases.

Even with bias correction, humidity retrieval accuracy is decreased in the mid and upper troposphere relative to reference retrievals. Full specification of $\mathbf{R}$ is essential for the accuracy of the bias-corrected lower tropospheric humidity retrievals. With full specification of $\mathbf{R}$ bias-corrected and reference humidity retrieval biases are comparable. A diagonal approximation to $\mathbf{R}$ increases this bias for the bias-corrected retrievals.

Propogation of fast model errors leads to a reduction of 2 pDFS with full specification of $\mathbf{R}$, and a reduction of 3 pDFS with a diagonal approximation to $\mathbf{R}$.

Propogation of fast model errors also modifies convergence characteristics. With full specification of $\mathbf{R}$ 7% of bias-corrected retrievals with RTTOV required one or more extra iteration, as compared with reference retrievals. When a diagonal approximation to $\mathbf{R}$ is assumed, 15% of RTTOV retrievals required one or more extra iterations, and 1% of retrievals failed (compared with 0% in reference retrievals). Similarly, with full specification of $\mathbf{R}$ 9% of bias-corrected retrievals with Gastropod required one or more extra iterations and 1% of retrievals failed (c.f. 0% in reference retrievals). With a diagonal approximation to $\mathbf{R}$ 17% of Gastropod retrievals required one or more extra iterations, and 3% of retrievals failed (c.f. 0% in reference retrievals).

3.3.5 AS69 case studies: comparison of reference model retrievals

The error characteristics of reference retrievals for the AS69 set of atmospheres are illustrated in Figure 14. As for atmosphere P012 previously, the retrieval error characteristics are essentially the same for the two models. Gastropod gives slightly better tropospheric temperature retrievals, RTTOV gives slightly better upper tropospheric humidity retrievals, but these differences are not significant in practice.

3.3.6 AS69 case studies: cross-retrieval with and without bias correction

Retrieval error characterisations for RTTOV and Gastropod cross-retrievals for the AS69 set of atmospheres are illustrated in Figures 15 and 16.

As in the case of atmosphere P012, when retrievals are performed without bias correction retrieved temperatures are biased by ~ 1 K in the troposphere and > 1 K in the upper stratosphere (P $<$ 1 hPa). The temperature biases for each model show similar structure to the P012 biases illustrated previously (checked explicitly but not shown).

With full specification of $\mathbf{R}$ retrievals without bias correction have larger standard deviations in upper stratospheric temperature retrievals (and throughout the entire stratosphere for RTTOV temperature retrievals) compared with bias corrected retrievals. The same is true of mid troposphere humidity retrievals. In the upper troposphere humidity retrievals with and without bias correction show similar errors (standard deviation), and Gastropod retrieval accuracy is worse that that for RTTOV. These errors result in a loss of of ~7–8 pDFS.

A diagonal approximation to $\mathbf{R}$ results in increased errors in lower tropospheric temperature retrievals. Gastropod stratospheric temperature retrieval errors (100 – 1 hPa) and also increased to levels comparable with RTTOV errors (full and diagonal $\mathbf{R}$). Humidity errors are also increased throughout the troposphere, and lower tropospheric humidity retrieval errors exceed backgound errors. RTTOV upper tropospheric humidity retrieval errors increase with a diagonal approximation to $\mathbf{R}$ (but remain better than Gastropod retrieval errors with full or diagonal $\mathbf{R}$). As previously, the diagonal approximation to $\mathbf{R}$ also modifies the structure and tends to increase amplitude of bias in retrievals. Pseudo-DFS of 0–2 suggests there is little or no benefit from data assimilation under these conditions.

The diagonal approximation to $\mathbf{R}$ modifies convergence characteristics, with 40% of Gastropod retrievals and 20% of RTTOV retrievals requiring one or more additional iterations. 10% of RTTOV and 25% of Gastropod retrievals fail to converge with a diagonal approximation to $\mathbf{R}$.

As previously, bias correction reduces retrieval errors (standard deviation and bias) and the diagonal approximation to $\mathbf{R}$ has a reduced impact on retrieval errors.

3.3.7 AS69 case studies: comparison of bias-corrected cross-retrieval and reference retrievals

Retrieval error characterisations for bias corrected cross-retrievals are compared with reference retrieval errors for the AS69 set of atmospheres in Figures 17 and 18.

With bias correction, the standard deviation of temperature retrievals at pressures greater than 10 hPa is comparable with reference retrieval accuracy. Bias-corrected retrieval accuracy is slightly worse for upper stratospheric temperatures (P $<$ 10 hPa). Temperature bias for retrievals performed with full specification of $\mathbf{R}$ is in close agreement with the bias of reference retrievals (and similarly for humidity) [6].

[6]This reduction in bias in bias corrected retrievals, as compared to the P012 series, may be due to summation

Even with bias correction, the accuracy of humidity retrievals is decreased in the mid and upper troposphere. Full specification of **R** does not appear as critical as previously for lower tropospheric humidity retrievals.

Fast model errors lead to a reduction of 2.5–3.5 pDFS with full specification of **R** (4.5–5.5 pDFS with a diagonal approximation **R**). They also modify convergence characteristics, with 10% of RTTOV retrievals and 8% of Gastropod retrievals requiring one or more additional iterations, as compared with reference retrievals.

As previously, the diagonal approximation to **R** also modifies convergence characteristics. 10% of RTTOV and 16% of Gastropod bias-corrected retrievals required one or more additional iterations when a diagonal approximation was made to **R**.

3.3.8 Retrievals with a 266 channel subset of the NESDIS channel set

The experiments described above do not allow one to determine whether the degradation of the humidity retrievals is due to bias correction errors, or whether it reflects fast model errors in modelled H_2O absorption (or both).

To pursue this issue further, and explicitly examine the effect of the large bias corrections applied in the CO_2 bands on humidity retrievals, we performed a set of reference and cross-retrievals for the P012 atmosphere and AS69 ensemble with the Gastropod model using a subset of the NESDIS channel set, where 51 channels with biases greater than 0.5 K or less than -0.5 K and further 7 channels with standard deviations in excess of 0.3 K were excluded from the channel selection. This channel selection is referred to as the 266 channel subset. The spectral intervals where channels are excluded should be readily identifiable in Figure 7.

Comparison of linear DFS for the 324 and 266 channel selections in Table 2 indicates the exclusion of the 58 channels leads to a loss of 1.5–1.7 DFS. As illustrated in Figure 19, this information loss is associated with decreased accuracy in stratospheric temperature retrievals ($P < 50$ hPa).

Reference retrievals are compared with linear theory for the 266 channel selection in Figure 20, and can be compared directly with the equivalent plots for the NESDIS channel set in Figure 2. Retrieval accuracy with the 266 channel set is essentially equivalent to the retrieval accuracy for the NESDIS channel selection, with the exception of the increased errors (bias and standard deviation) stratospheric temperature retrievals at pressures less than 50 hPa, due to the channel exclusion described above. Although Figures 19 and 20 only present results for the AS69 ensemble of atmospheres, equivalent results are obtained for the P012 atmosphere.

Figure 21 compares the retrieval accuracy of the 324 and 266 channel selections for P012 Gastropod cross-retrievals without bias correction. With full specification of **R**, temperature retrieval standard deviations for the 266 channel selection are better than or comparable with errors for the 324 channel selection, except in the 50–0.5 hPa interval. However the accuracy of temperature retrievals using the 266 channel selection is more sensitive to a diagonal approximation to **R** in the lower troposphere and the 50–0.5 hPa region. The bias in temperature retrievals using the 266 channel selection is reduced in the troposphere, and biases tend to be positive (compared with a quasi-symmetric bias structure for retrievals with the 324 channel selection).

Humidity retrieval errors are essentially the same for the two channel selections for both full and diagonal specifications of **R**. The small improvement in boundary layer humidity retrievals using the 266 channel set (and full specification of **R**) is of note, as this channel selection

over an ensemble of atmopsheric states: if retrieval biases differ from state to state, this will result in lower bias, but higher standard deviations for the ensemble.

excludes two channels with large errors (bias and standard deviation) centred on water vapour lines in the longwave window region. Humidity retrieval biases are modified for the 266 channel selection, but strong sensitivity to the specification of **R** makes it difficult to make any further generalisations.

Figure 22 illustrates an equivalent comparison for the AS69 ensemble of atmospheric states. In this case, temperature retrieval errors for the 266 channel set are slightly better than those for the 324 channel selection in the troposphere (P $>$ 100 hPa) and the upper stratosphere (P $<$ 1.0 hPa), but remain poorer than the 324 channel selection in the 50–1 hPa interval. Temperature retrieval errors with the 266 channel set show less sensitivity to specification of **R** in the troposphere, but greater sensitivity to the specification of **R** in the upper stratosphere. The bias in temperature retrievals is reduced at pressures greater than 10 hPa for the 266 channel selection.

Humidity retrieval errors for the 266 channel set are better than or comparable with errors for the 324 channel selection throughout the troposphere. Improvements for retrieval errors with full specification of **R** are minor, but mid-tropospheric humidity retrievals with a diagonal approximation to **R** are markedly improved. Humidity retrieval biases are also generally reduced for retrievals using the 266 channel subset.

Note finally, with reference to Table 2, the 266 channel selection gives marked improvements in pDFS (compared to reference retrievals, and in absolute terms), and generally improves the convergence characteristics of cross retrievals without bias correction.

Figures 23 and 24 compare the retrieval accuracy of the 324 and 266 channel selections for Gastropod cross-retrievals with bias correction. With the exception of stratospheric temperature retrievals (due to information loss associated with the exclusion of 58 channels in the 266 channel selection), and some minor differences in sensitivity to a diagonal approximation to **R** (P012 lower tropospheric temperature and boundary layer humidity, and AS69 stratospheric temperature retrievals) retrieval accuracy with the two channel sets is essentially identical. Similarly, comparison of bias corrected and reference retrievals for the 266 channel selections gives essentially the same picture as Figures 13 and 18 for the 324 channel set.

These results lead us to conclude that large model errors in high peaking channels of the CO_2 bands could have an impact on the accuracy of stratospheric and tropospheric temperature and tropospheric humidity retrievals, due to the nonlinearity of atmospheric radiative transfer and fast model error correlations. However, the experiments undertaken suggest that the observations are sufficiently independent to ensure that retrieval accuracy in the troposphere is not compromised, provided bias correction can be performed accurately. Section 4 addresses whether these conclusions are affected by retrieval errors due to uncertainty in the background ozone profile (assumed to be perfectly known here).

These results also suggest the reduced accuracy of water vapour cross-retrievals is principally due to fast model differences in modelling H_2O absorption (including differences in spectroscopic parameters and (potentially) transmittance prediction errors), rather than errors associated with bias correction in screened channels of the CO_2 bands. Channel selection in spectral intervals where H_2O is a principal absorber are not significantly affected by the gross screening threshholds used here. Detailed examination of which specific channels or spectral intervals are most important must await further study.

Finally, the results of the simple screening procedure highlight how the impact of channel selection on retrieval accuracy cannot be assessed in isolation, but rather, depends critically on other aspects of the assimilation system (bias correction, specification of the observation error covariance matrix)[7]. Thus the effects of suboptimal data assimilation are not easy to predict, and arguably can only be assessed by monte-carlo style experiments of the sort undertaken here.

3.4 Conclusions

The results of the experiments undertaken for a representative ensemble of atmospheric states with bias correction suggest that if current fast model differences are representative of real fast model errors, and if bias correction can be performed accurately, the accuracy of temperature retrievals using the NESDIS channel selection should not significantly compromised by model errors. Some small losses in the accuracy of stratospheric temperature retrievals are predicted, but are probably not significant in practice. However, larger losses in tropospheric humidity retrieval accuracy are predicted, and measurement information on upper tropospheric humidity may be completely compromised.

Full specification of the observation error covariance matrix **R** is important for lower tropospheric humidity retrievals in some atmospheric conditions (e.g. P012). Full specification of **R** also minimizes retrieval biases and improves convergence rates.

Bias correction may be an effective solution for temperature retrievals in the cases considered here because the largest biases (in fast model differences) principally occur in the CO_2 absorption bands, where the radiative transfer operator is quasi-linear. These results may not be generally applicable to cases where large biases need to be corrected in spectral intervals with variable absorbers. Further study also is needed to characterise the impact of errors in background and retrieved ozone profiles on the accuracy of bias corrected retrievals (and is addressed in Section 4).

Specific experiments to determine the reason for degradation of the humidity retrievals suggest this is principally due to fast model differences in modelling H_2O absorption, rather than errors associated with bias correction in screened channels of the CO_2 bands. Further study is required to identify the specific channels or spectral intervals which most affect water vapour retrieval accuracy.

Finally, the results of the simple screening procedure for channel subset selection clearly illustrate how the accuracy of retrievals with a given channel selection depends critically on other aspects of the assimilation system (bias correction, specification of the observation error covariance matrix), and suggest that monte-carlo simulation studies of the type undertaken here have an important role to play in estimating and minimizing the impact of suboptimal retrieval choices in operational data assimilation systems.

[7]For example, in the case in question, an operational centre may choose to use a diagonal approximation to **R** (for computational efficiency) and exclude the 58 screened channels (or use alternative, independent (microwave) observations to constrain stratospheric temperature retrievals), tolerating a loss in stratospheric temperature retrieval accuracy in order to minimize the effects of imperfect bias correction and model error correlations on the accuracy of tropospheric temperature and humidity retrievals.

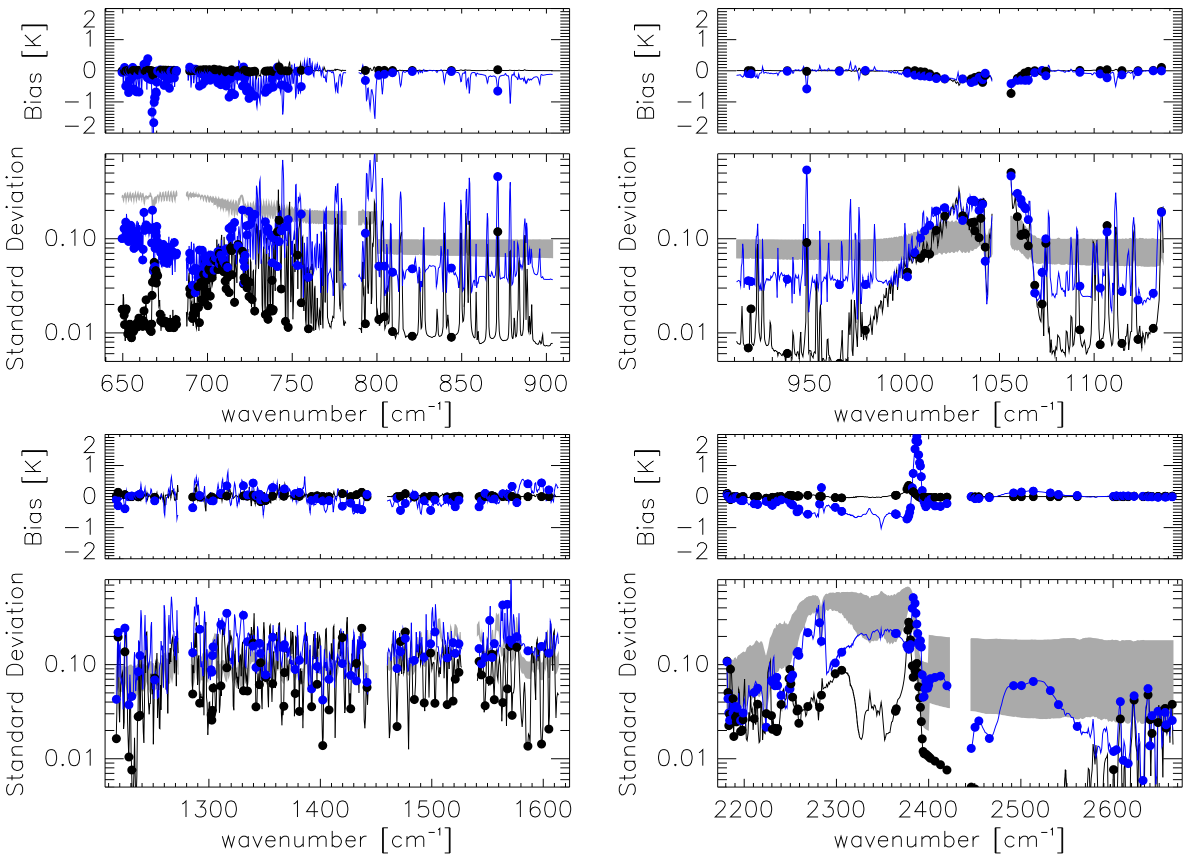

Figure 7: Bias and standard deviation of Gastropod forward model errors (black) and Gastropod–RTTOV differences (blue) for the AIRS instrument. Lower bound estimates of AIRS instrumental noise levels for a representative range of scene temperatures are illustrated with grey shading. Channels in the NESDIS channel set are indicated with filled circles.

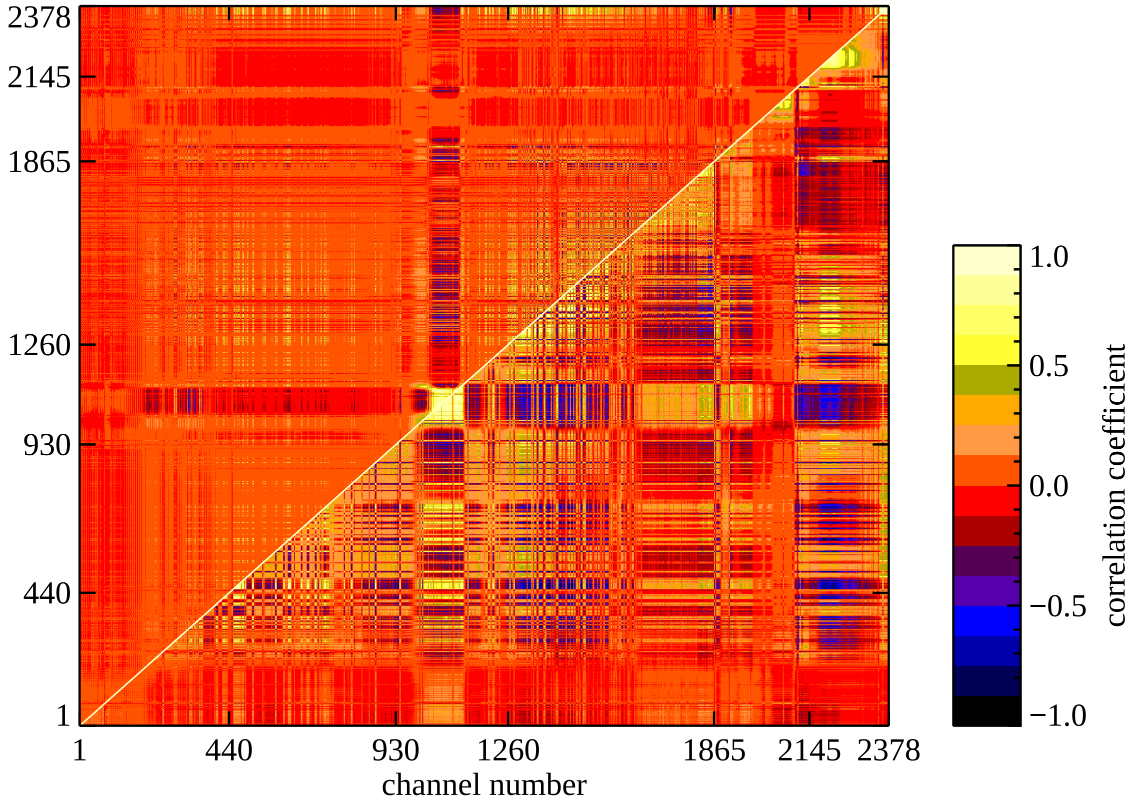

Figure 8: Correlation coefficients for the observation error covariance matrix $\mathbf{R} = \mathbf{E} + \mathbf{F}$. Upper triangle, correlations for the case where $\mathbf{F}$ is the Gastropod forward model error covariance matrix. Lower triangle, correlations for the case where $\mathbf{F}$ is the forward model error covariance matrix derived for the RTTOV–Gastropod differences.

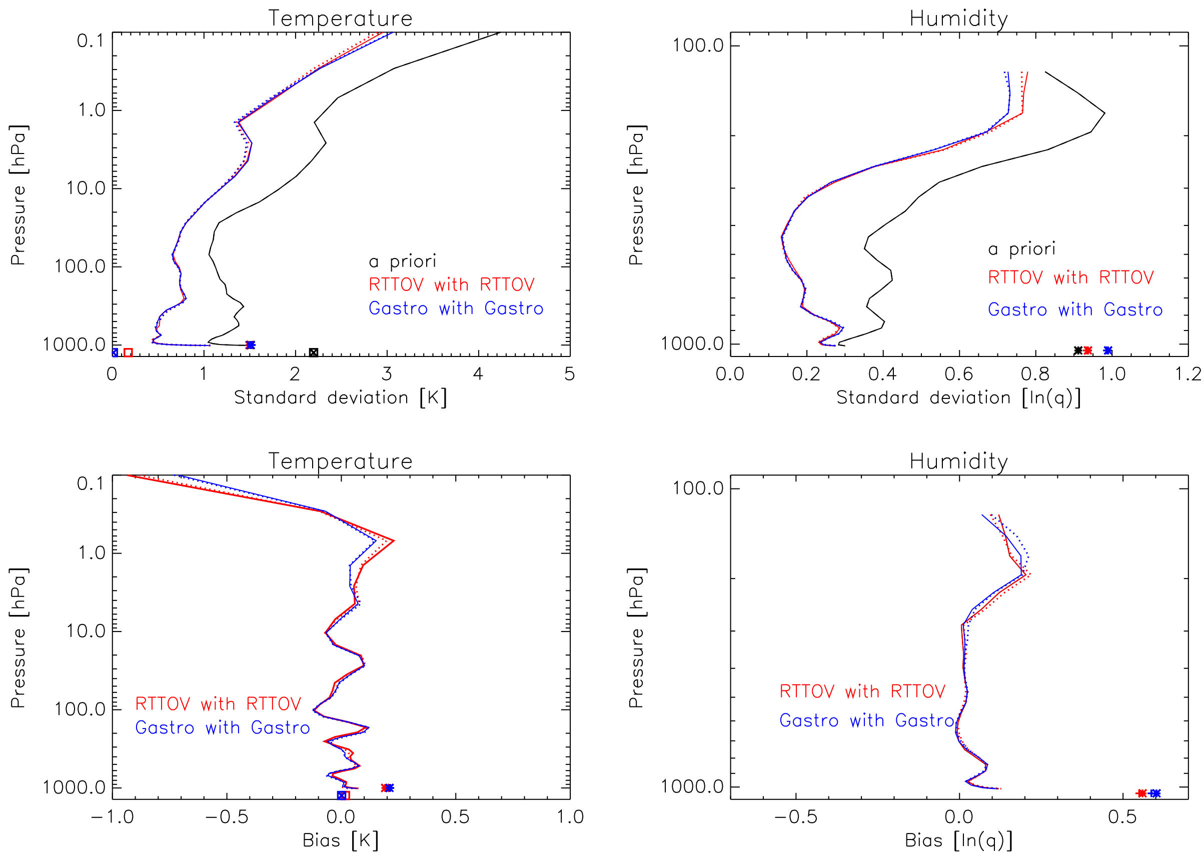

Figure 9: Error characteristics of reference retrievals using the NESDIS channel selection for profile P012. The solid black line illustrates the standard deviation of the background errors for the ensemble of states used in retrievals. The red curves illustrate the retrieval errors for the ensemble of states for retrievals using the RTTOV model from reference spectra simulated with RTTOV. The blue curves illustrate the equivalent information for retrievals using the Gastropod model from reference spectra simulated with Gastropod. With the exception of the solid black line, all line and symbol styles are as defined previously in Figure 1.

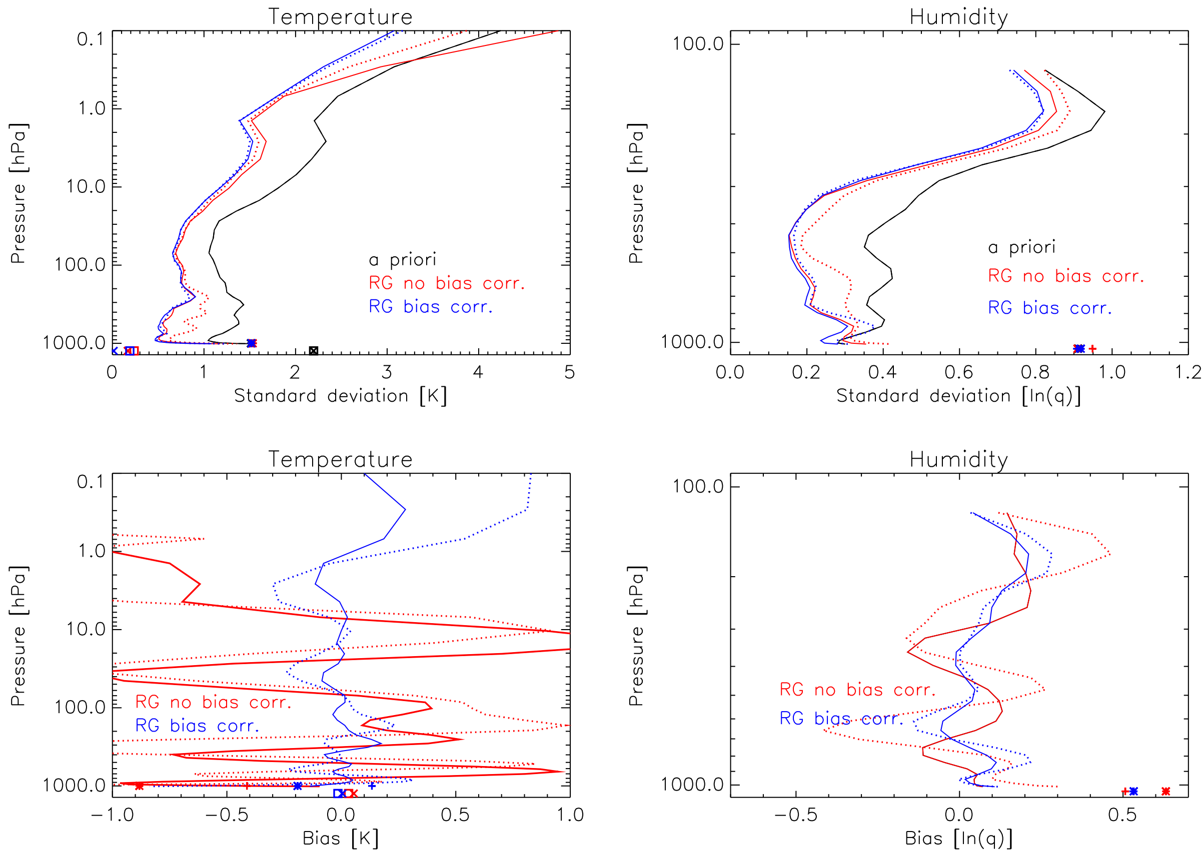

Figure 10: Error characteristics of cross retrievals with and without bias correction for retrievals using RTTOV from spectra simulated with Gastropod (atmosphere P012, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

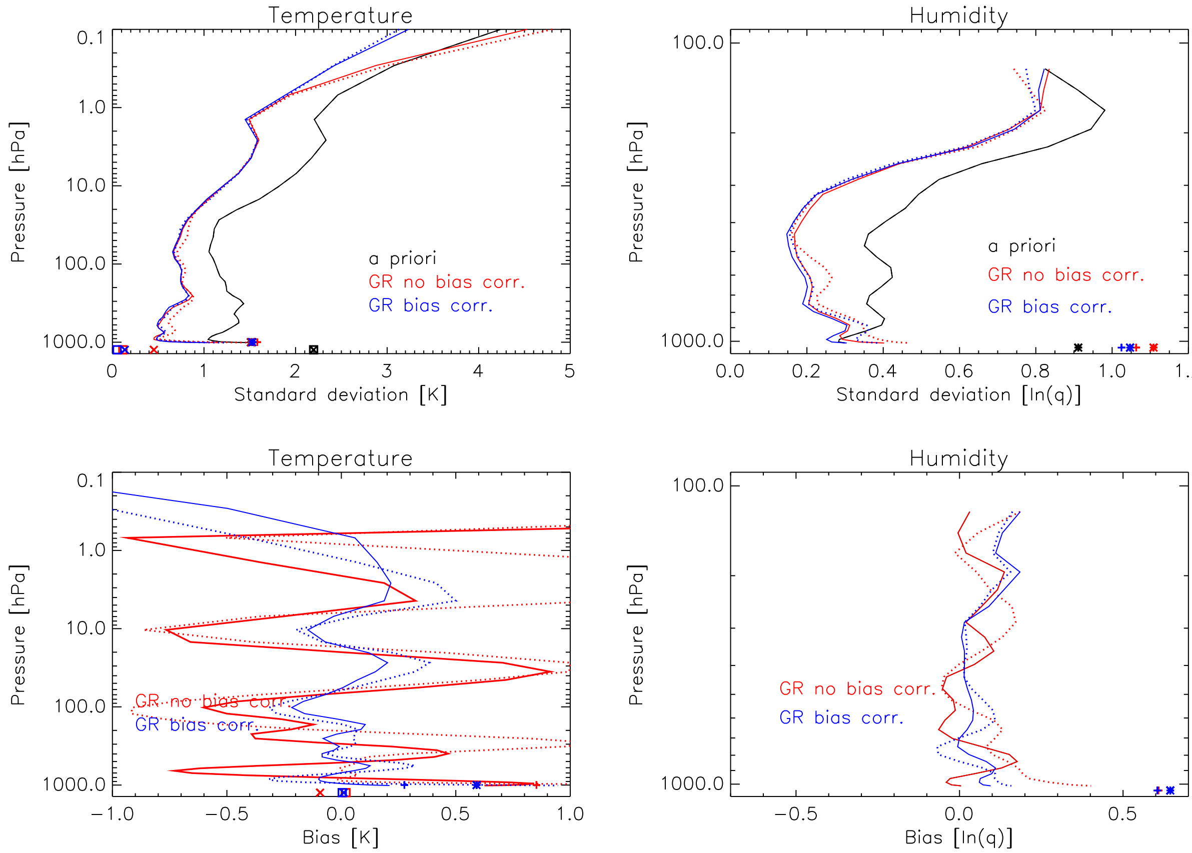

Figure 11: Error characteristics of cross retrievals with and without bias correction for retrievals using Gastropod from spectra simulated with RTTOV (atmosphere P012, NESDIS channel selection). The bias in surface humidity retrievals with a diagonal approximation to **R** is 1.16, and does not appear in the humidity bias plot. All line styles and symbols are as defined in Figure 9.

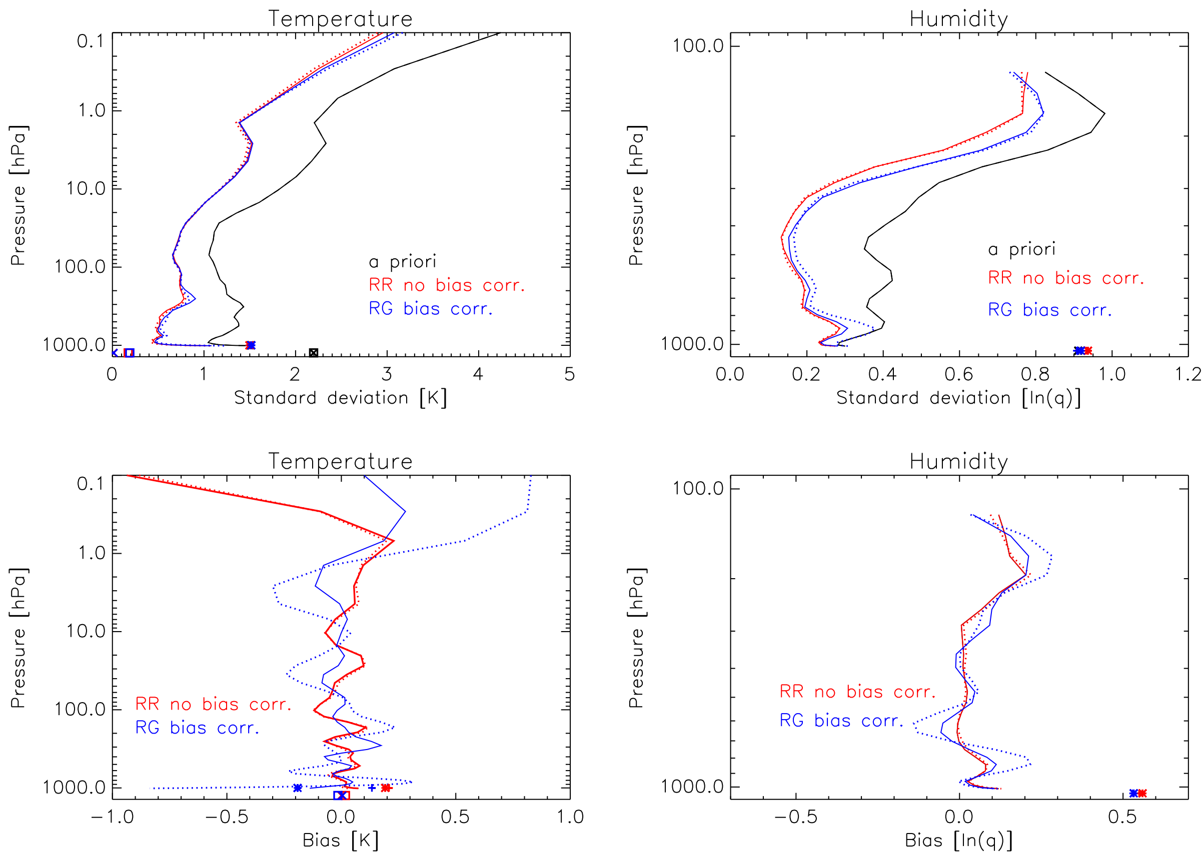

Figure 12: Comparison of the error characteristics of RTTOV bias corrected cross retrievals (from spectra simulated with Gastropod) and RTTOV reference retrievals (atmosphere P012, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

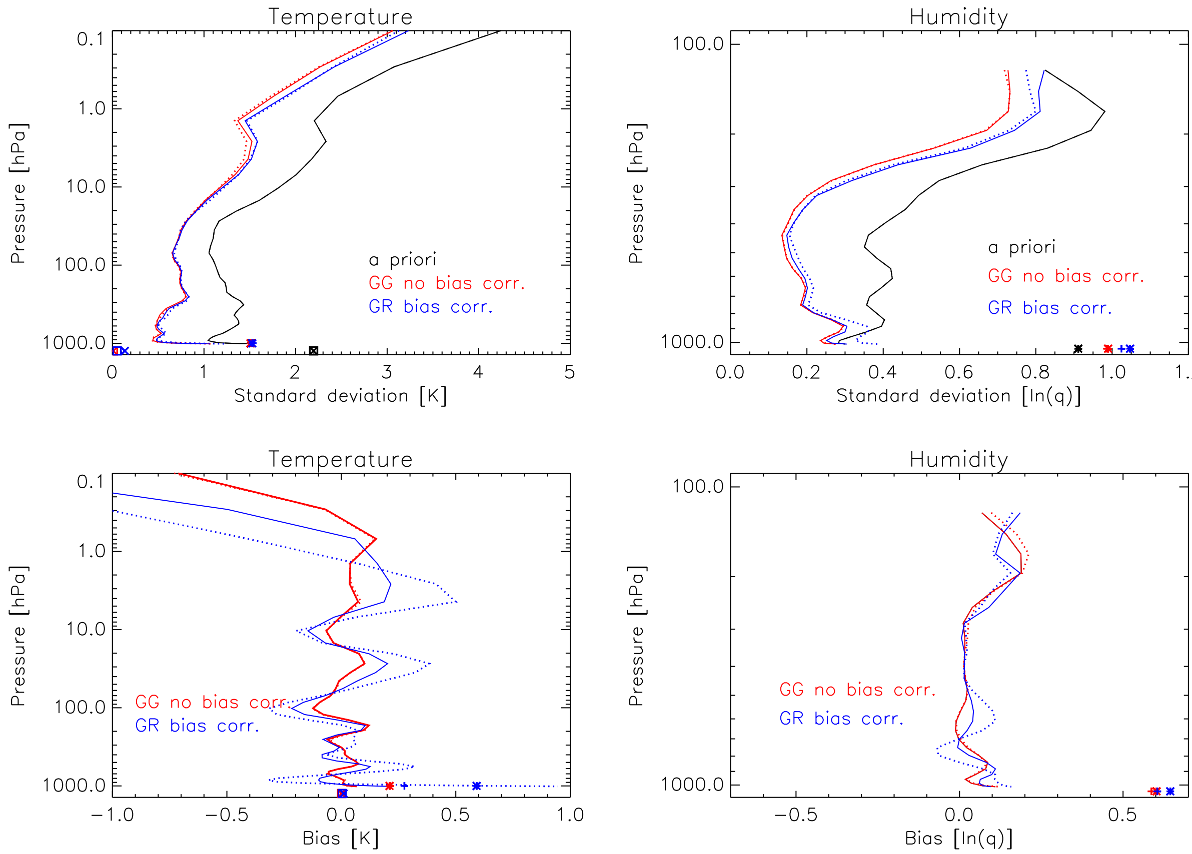

Figure 13: Comparison of the error characteristics of Gastropod bias corrected cross retrievals (from spectra simulated with RTTOV) and Gastropod reference retrievals (atmosphere P012, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

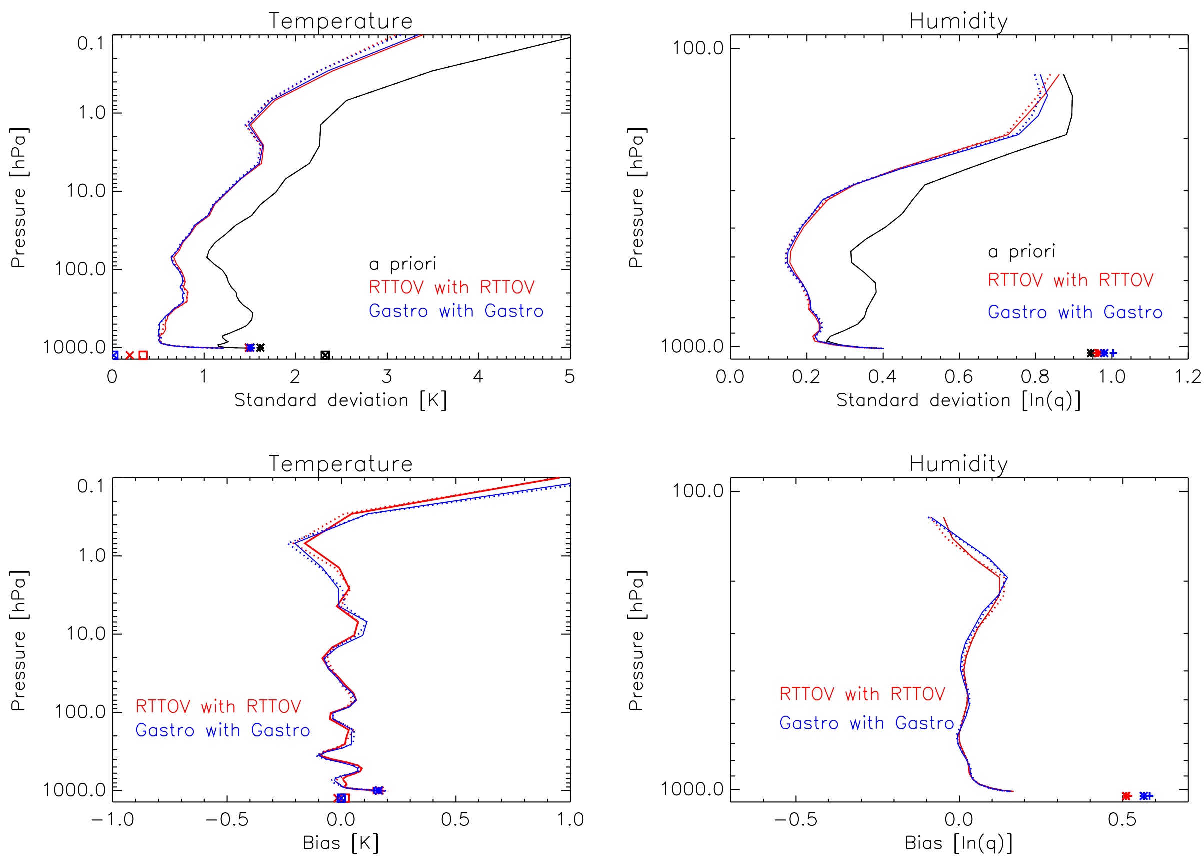

Figure 14: Error characteristics of reference retrievals using the NESDIS channel selection for the AS69 profiles. All line styles and symbols are as defined in Figure 9.

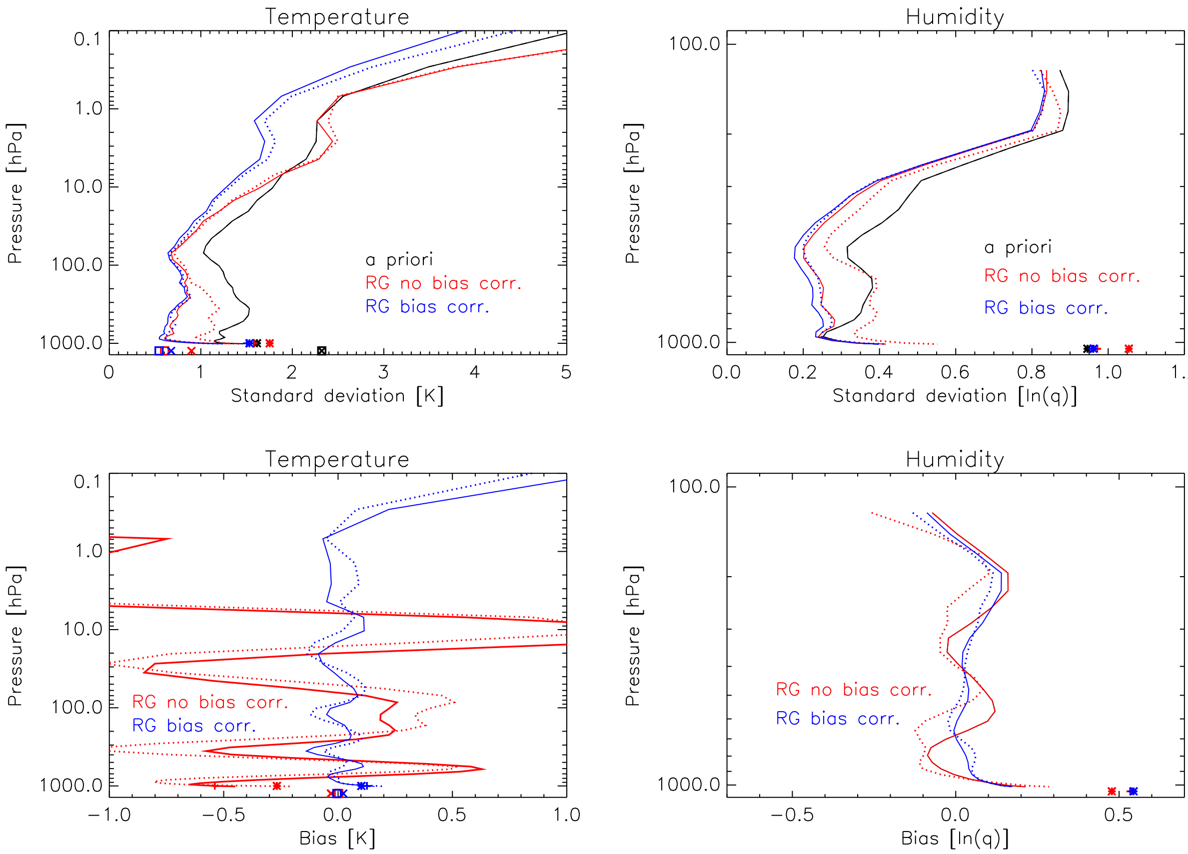

Figure 15: Error characteristics of cross retrievals with and without bias correction for retrievals using RTTOV from spectra simulated with Gastropod (AS69 atmospheres, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

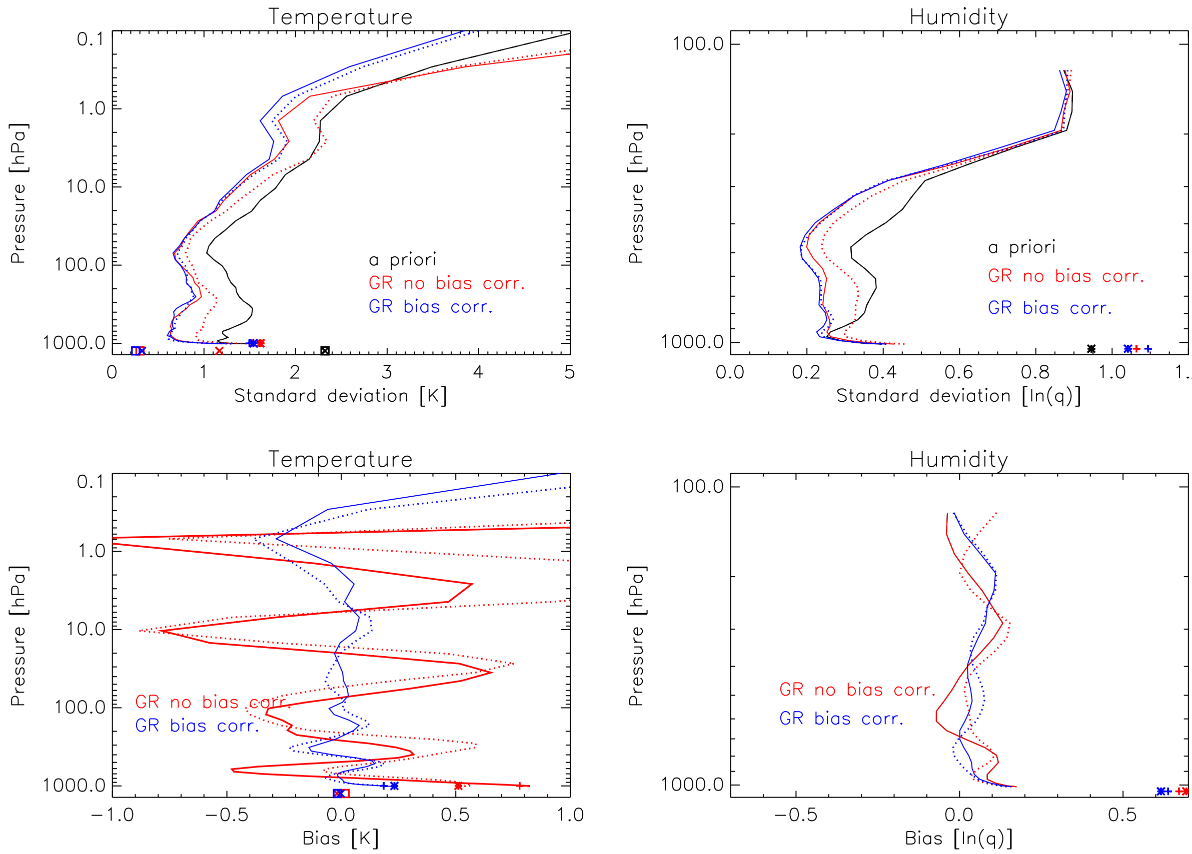

Figure 16: Error characteristics of cross retrievals with and without bias correction for retrievals using Gastropod from spectra simulated with RTTOV (AS69 atmospheres, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

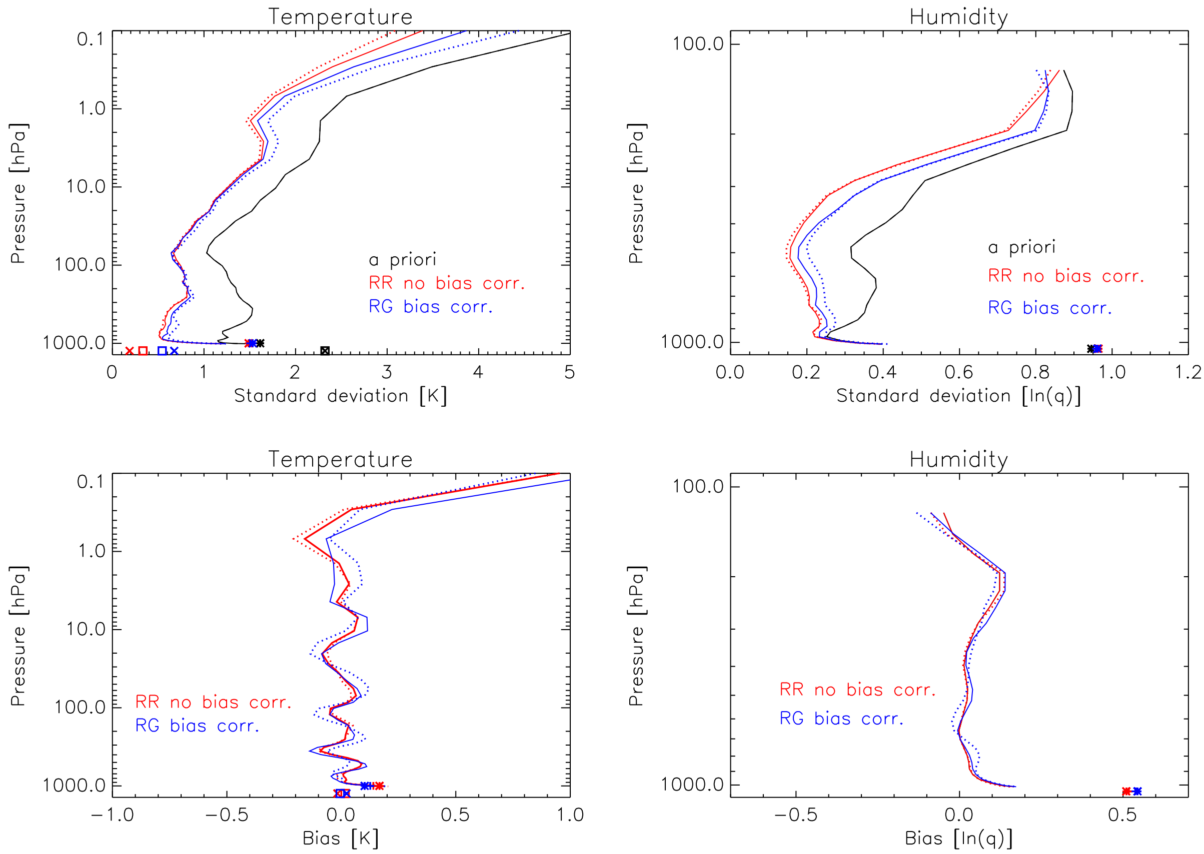

Figure 17: Comparison of the error characteristics of RTTOV bias corrected cross retrievals (from spectra simulated with Gastropod) and RTTOV reference retrievals (AS69 atmospheres, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

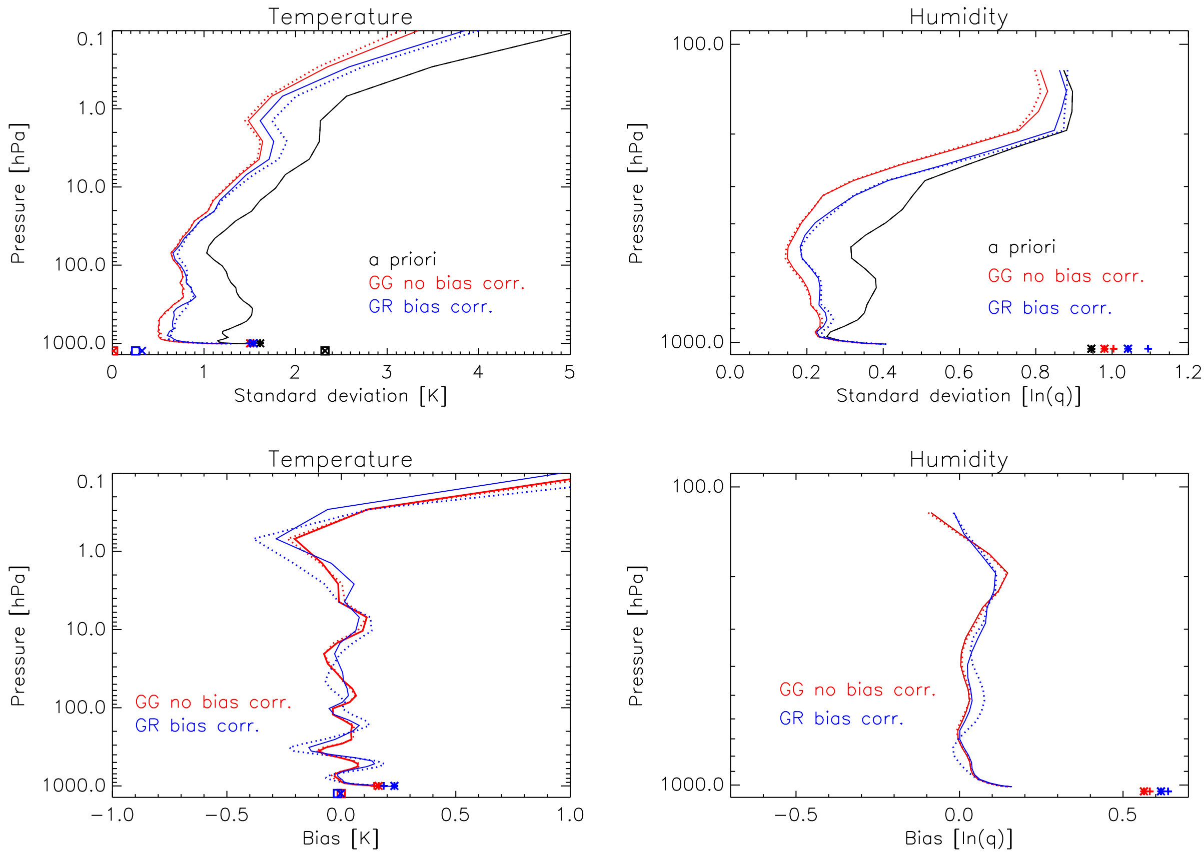

Figure 18: Comparison of the error characteristics of Gastropod bias corrected cross retrievals (from spectra simulated with RTTOV) and Gastropod reference retrievals (AS69 atmospheres, NESDIS channel selection). All line styles and symbols are as defined in Figure 9.

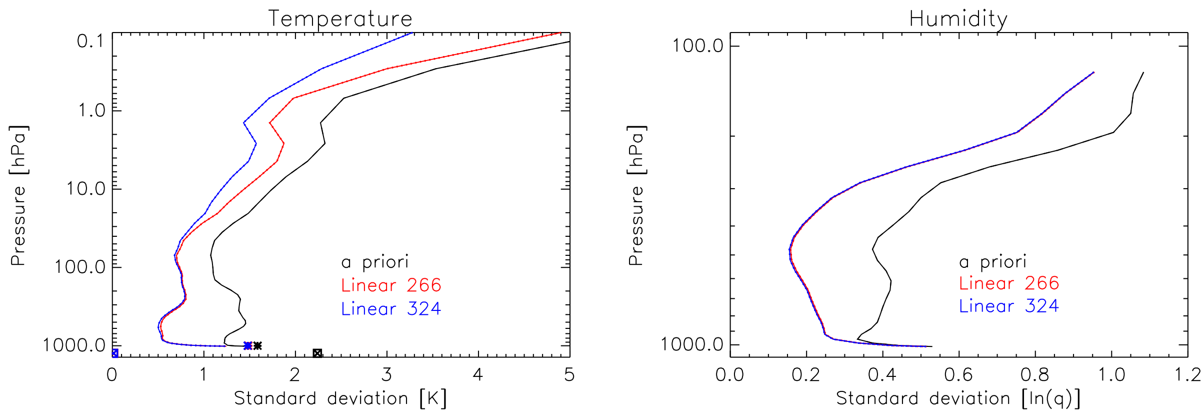

Figure 19: Differences in retrieval errors (predicted by optimal linear theory) for AS69 retrievals using the NESDIS channel selection (324) and the 266 channel subset thereof. The linear retrieval errors for surface humidity is 1.40 for both channel selections (c.f. a background error of 1.45). These errors do not appear on the humidity standard deviation plot. All line and symbol styles are as defined previously in Figure 1.

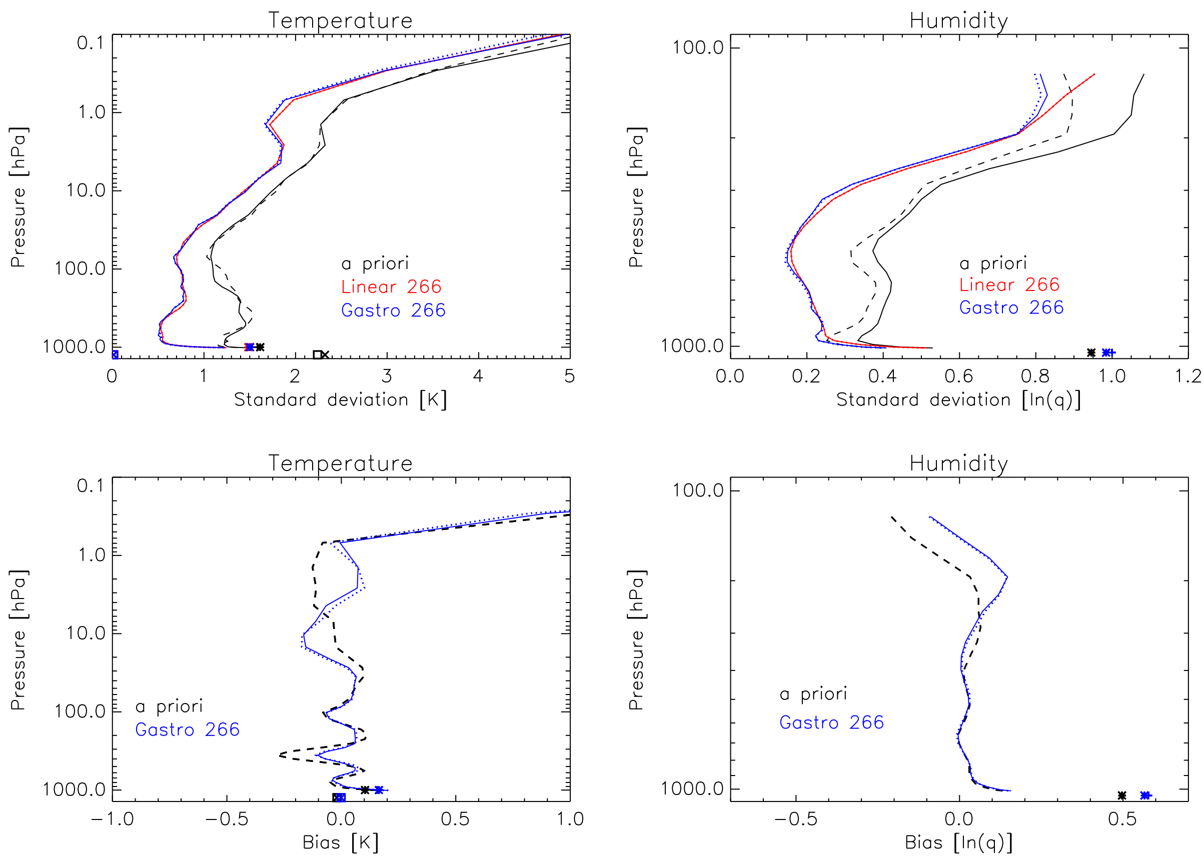

Figure 20: Error characteristics of reference retrievals using the 266 channel subset of the NESDIS channel selection for the ensemble of atmospheric states AS69, compared with optimal linear theory. Background and optimal linear retrieval errors for surface humidity are 1.45 and 1.40 respectively and do not appear on the humidity standard deviation plot. All line and symbol styles are as defined previously in Figure 1.

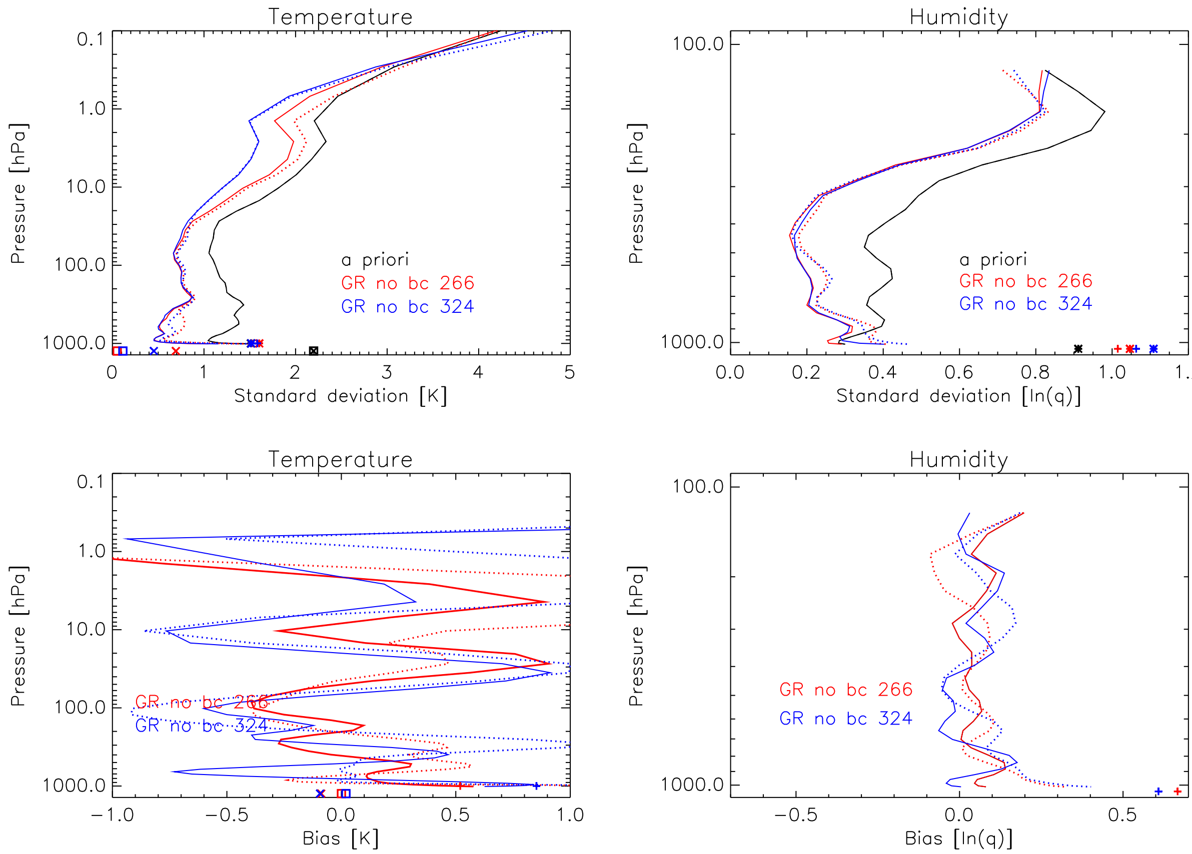

Figure 21: Comparison of the error characteristics of cross retrievals without bias correction for Gastropod retrievals using the 324 NESDIS channel selection, and a 266 channel subset thereof (atmosphere P012, reference spectra simulated with RTTOV). The bias in surface humidity retrievals with a diagonal approximation to **R** is 1.16 for the 324 channel set and 1.00 for the 266 channel set. These data do not appear in the humidity bias plot. All line styles and symbols are as defined in Figure 9.

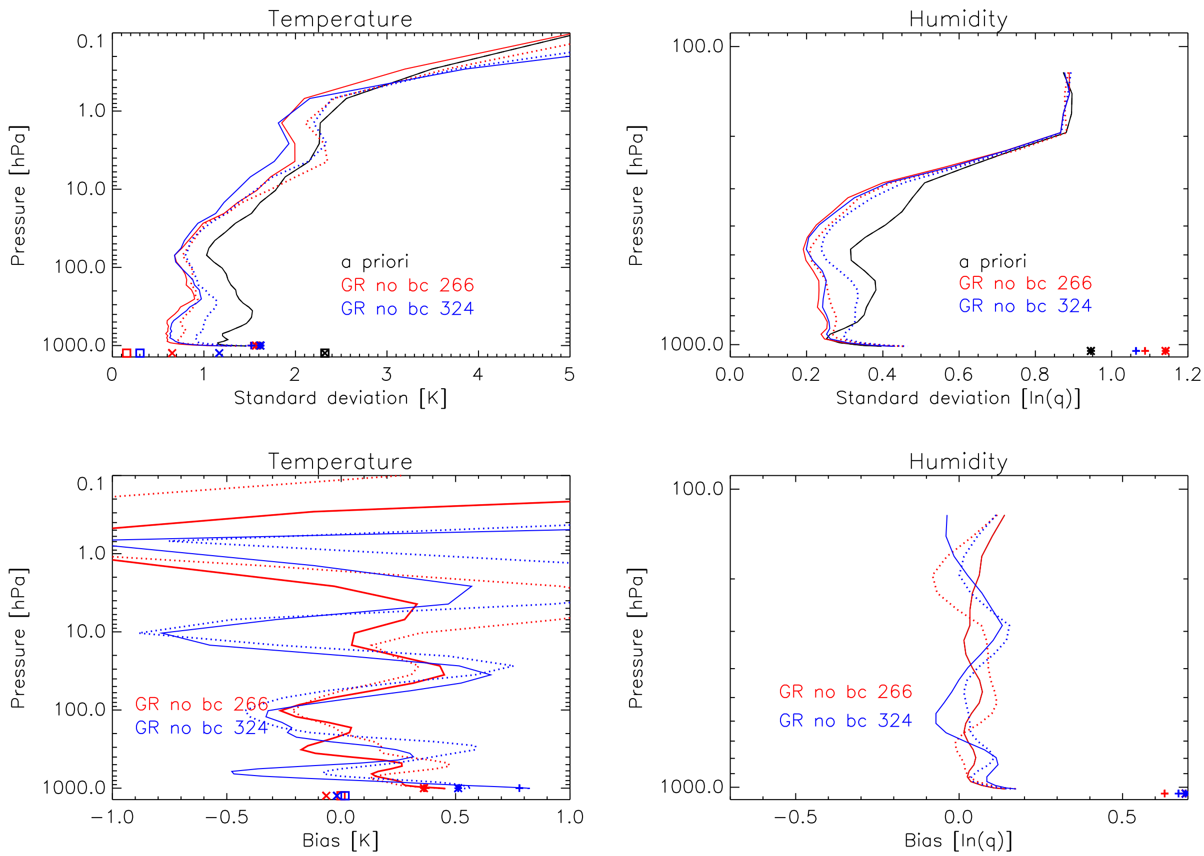

Figure 22: Comparison of the error characteristics of cross retrievals without bias correction for Gastropod retrievals using the 324 NESDIS channel selection, and a 266 channel subset thereof (atmospheres AS69, reference spectra simulated with RTTOV). All line styles and symbols are as defined in Figure 9.

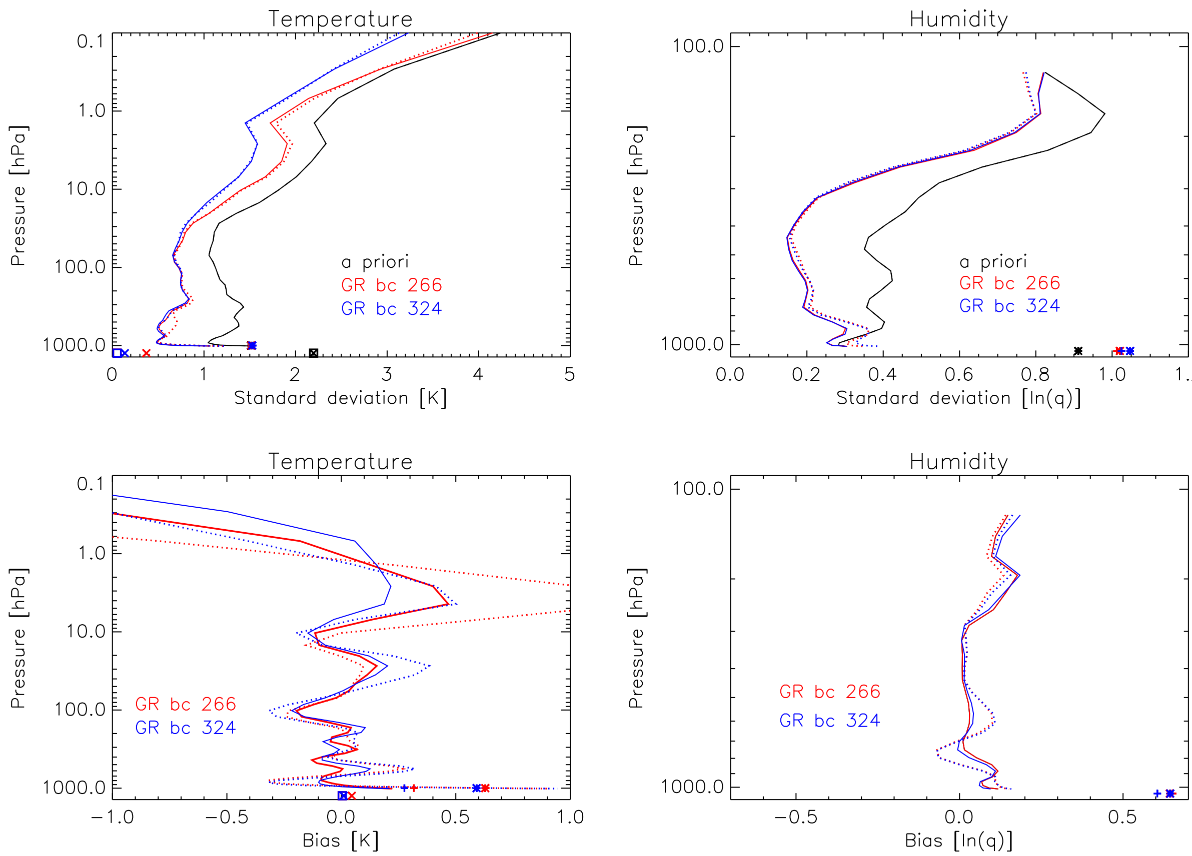

Figure 23: Comparison of the error characteristics of cross retrievals with bias correction for Gastropod retrievals using the 324 NESDIS channel selection, and a 266 channel subset thereof (atmosphere P012, reference spectra simulated with RTTOV). All line styles and symbols are as defined in Figure 9.

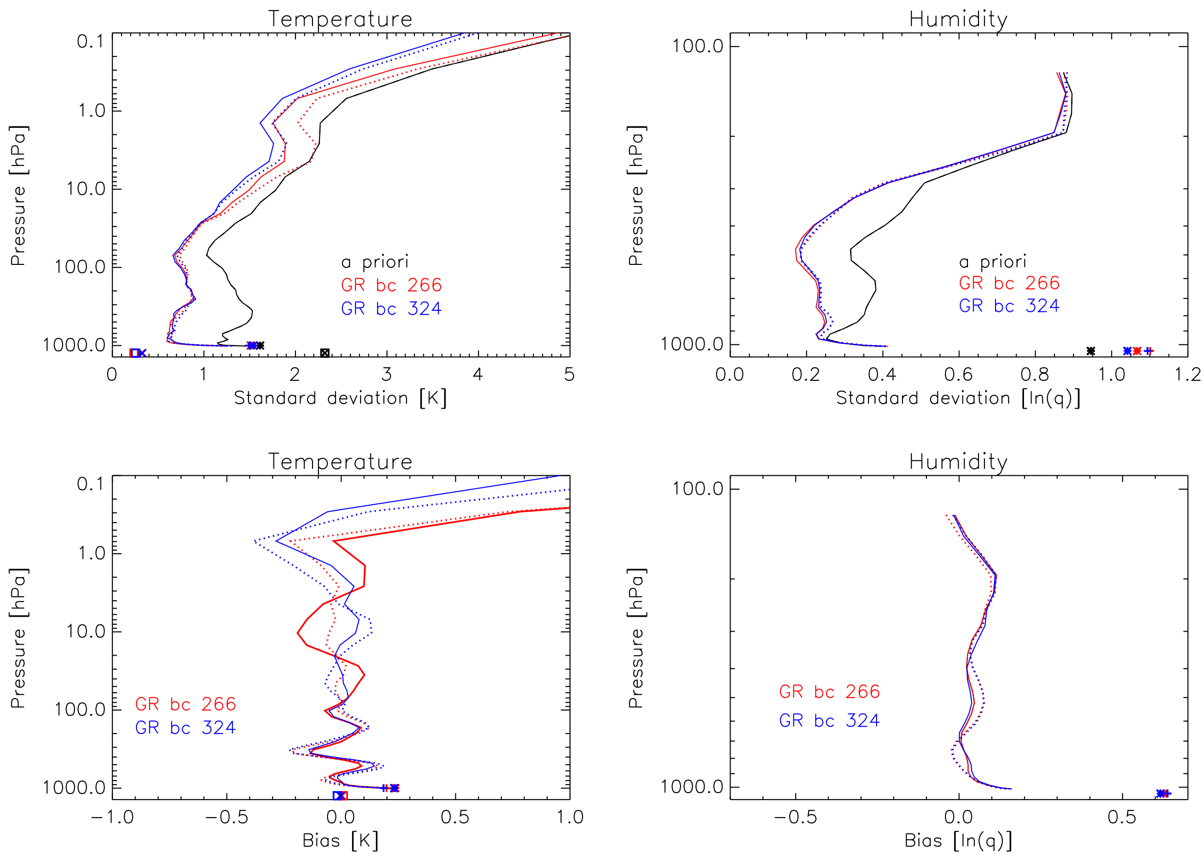

Figure 24: Comparison of the error characteristics of cross retrievals with bias correction for Gastropod retrievals using the 324 NESDIS channel selection, and a 266 channel subset thereof (atmospheres AS69, reference spectra simulated with RTTOV). All line styles and symbols are as defined in Figure 9.

Series	ret	ref	bias	chan	N_{real}	N_{ret} full **R**	N_{ret} diag **R**	pDFS Monte-C full **R**	pDFS Monte-C diag **R**
P012	R	R	-	324	100	99	100	17.8	17.8
P012	G	G	-	324	100	100	100	17.8	17.8
P012	R	G	F	324	100	97	96	12.9	8.7
P012	G	R	F	324	100	99	95	13.6	11.6
P012	R	G	T	324	100	99	99	15.6	14.7
P012	G	R	T	324	100	99	97	15.6	14.7
AS69	R	R	-	324	138	135	137	16.1	16.3
AS69	G	G	-	324	138	138	138	16.0	16.2
AS69	R	G	F	324	138	131	123	7.3	0
AS69	G	R	F	324	138	130	106	8.9	2.2
AS69	R	G	T	324	138	133	133	13.5	11.6
AS69	G	R	T	324	138	130	131	12.4	10.8
P012	G	G	-	266	100	100	100	16.2	16.4
P012	G	R	F	266	100	99	91	13.7	10.1
P012	G	R	T	266	100	99	96	14.1	13.1
AS69	G	G	-	266	138	138	138	14.6	14.8
AS69	G	R	F	266	138	133	121	10.4	6.3
AS69	G	R	T	266	138	131	131	11.5	9.4

Table 2: Summary of retrieval characteristics for experiments using fast model differences as a proxy for fast model errors. All entries are as defined in Table 1.

Series	ret	ref	bias	chan	Linear DFS full **R**	Linear DFS diag **R**
P012	G	-	-	324	17.8	15.5
AS69	G	-	-	324	17.3	15.1
P012	G	-	-	266	16.1	13.7
AS69	G	-	-	266	15.6	13.4

Table 3: Summary of optimal (full specification of **R**) and suboptimal (diagonal approximation to **R**) retrieval characteristics predicted by linear theory for the set of experiments tabulated in Table 2. All entries are as defined in Table 1.

4 Assesment of the impact of errors in the assumed ozone profile on retrieval accuracy

A study has been undertaken to assess the sensitivity of temperature and humidity retrieval accuracy to errors in the assumed ozone profile.

Retrievals were performed for the AS69 ensemble with the ozone profile set to the ensemble mean ozone profile (as opposed to the ozone profile assumed in the synthetic radiance simulation, as previously). The retrievals assuming perfect knowledge of ozone will be referred to as standard retrievals and the retrievals with the ensemble mean ozone profile will be referred to as climatological ozone retrievals hereinafter.

The forward model error covariance matrix and flat bias correction for the climatological ozone retrievals include ozone representation errors. Specifically, considering the situation where retrievals are performed with model M2 from synthetic spectra simulated by model M1, the forward model error covariance and bias is estimated from the differences

$$f_{\mathrm{M1}}(\mathrm{x\_qT_{true}}\ |\mathrm{x\_O_{3true}}) - f_{\mathrm{M2}}(\mathrm{x\_qT_{true}}\ |\mathrm{x\_O_{3clim}}),$$

where f is the forward model and x_qT and x_O_3 the temperature and humidity and ozone sub-vectors of the state vector x.

Inclusion of the ozone representation error increases the diagonal elements of $\mathbf{F}$ by an order of magnitude in the 10 micron ozone band, but by less than a factor of two in the 720 wavenumber region of the CO_2 ν_2 band.

Retrievals were performed with the full 324 NESDIS channel selection and a 298 channel subset which excludes the 26 NESDIS channels in the 10 micron ozone band. All synthetic radiance spectra were bias corrected prior to performing the 1D_Var retrieval.

Linear theory (see Figure 25 and Table 5) predicts that there is essentially no difference between standard and climatological retrieval accuracy for the AS69 ensemble and full specification of $\mathbf{F}$. There is a small improvement in accuracy in the climatological retrieval with a diagonal approximation to $\mathbf{F}$, presumably due to reduced weight or no contribution from channels in the 10 micron ozone band, where forward model error correlations are important.

1D_Var retrievals generally bear out the predictions from linear theory. Changes are more complicated, because the number of retrievals which converge is slightly different (1–3 fewer cross-retrievals converge in the climatological AS69 run than the standard run) and the RG and GR cross-retrievals runs differ in the detail of the observed changes. Nonetheless, stratospheric T retrieval errors (particularly 5-0.5 hPa) are slightly higher for climatological retrievals with full specification of $\mathbf{F}$, and slightly lower for climatological retrievals with a diagonal specification of $\mathbf{F}$ in both sets of cross retrievals.

An example of a comparison of retrieval errors from standard and climatological bias-corrected cross retrievals is illustrated in Figure 26. Degrees of freedom for signal are tabulated for the standard and two cliamtological cross-retrieval runs in Table 4.

From these simulations we conclude that the conclusions drawn from the standard retrieval runs are not likely to be substantially affected by uncertainty in the ozone profile assumed in retrievals (of temperature and humidity) provided ozone representativity errors are specified accurately in bias correction and the forward model error covariance matrix.

Retrieval accuracy is not significantly reduced if the channels in the 10 micron ozone band are excluded completely, which would clearly reduce the effect of suboptimal specification of ozone representativity errors in practice.

Obviously this study does not address the impact of model error in the case where the ozone profile is included in the set of parameters to be retrieved.

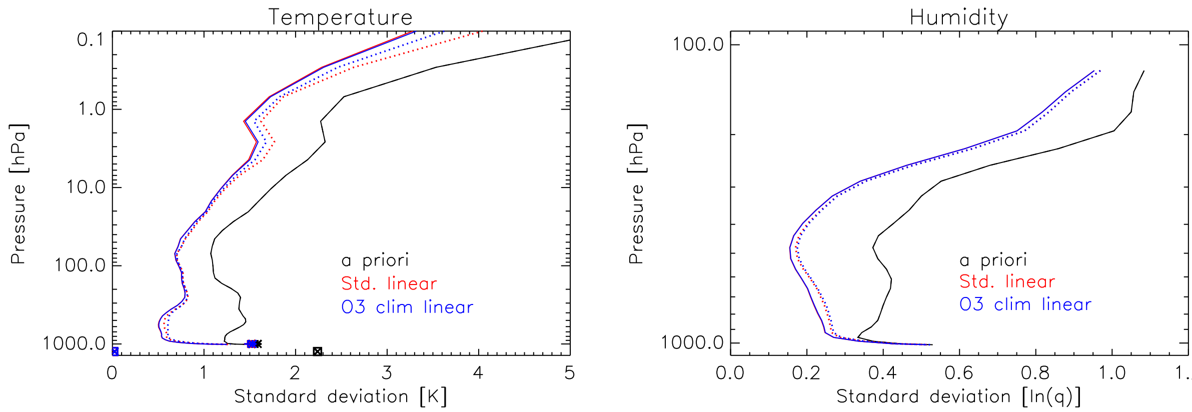

Figure 25: Differences in retrieval errors (predicted by optimal linear theory) for standard AS69 retrievals using the NESDIS channel selection (324) and retrievals using the 298 channel subset thereof, and including ozone representativity errors in the specification of the forward model error covariance matrix. All line and symbol styles are as defined previously in Figure 1.

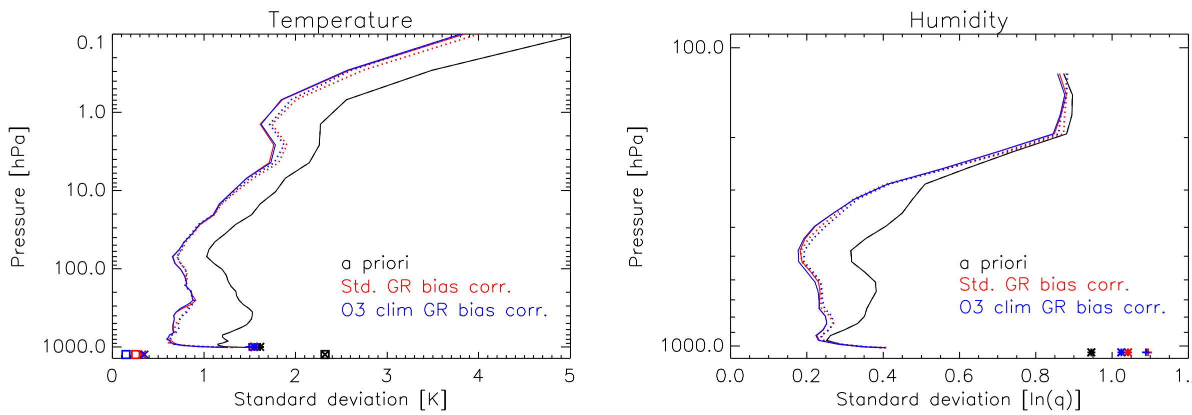

Figure 26: Error characteristics of bias-corrected cross retrievals using the 298 channel subset of the NESDIS channel selection for the ensemble of atmospheric states AS69 (including ozone representativity errors in the specification of **F**), compared with standard AS69 bias-corrected cross-retrievals. All line and symbol styles are as defined previously in Figure 1.

Series	ret	ref	bias	chan	N_{real}	pDFS Monte-C full $\mathbf{R}$	diag $\mathbf{R}$
AS69	R	R	-	324	138	16.1	16.3
AS69	G	G	-	324	138	16.0	16.2
AS69 O3 clim	R	R	T	324	138	15.9	15.7
AS69 O3 clim	G	G	T	324	138	15.8	15.7
AS69 O3 clim	R	R	T	298	138	15.9	15.8
AS69 O3 clim	G	G	T	298	138	15.9	15.8
AS69	R	G	T	324	138	13.5	11.6
AS69	G	R	T	324	138	12.4	10.8
AS69 O3 clim	R	G	T	324	138	13.2	11.5
AS69 O3 clim	G	R	T	324	138	12.3	10.7
AS69 O3 clim	R	G	T	298	138	13.4	11.7
AS69 O3 clim	G	R	T	298	138	12.5	10.7

Table 4: Comparison of retrieval characteristics for standard experiments and bias-corrected retrievals with climatological variation of ozone included. All entries are as defined in Table 1.

Series	ret	ref	bias	chan	Linear DFS full $\mathbf{R}$	diag $\mathbf{R}$
AS69	G	-	-	324	17.3	15.1
AS69 O3 clim	G	-	-	324	17.2	15.3
AS69 O3 clim	G	-	-	298	17.2	15.3

Table 5: Summary of optimal (full specification of $\mathbf{R}$) and suboptimal (diagonal approximation to $\mathbf{R}$) retrieval characteristics predicted by linear theory for the set of experiments tabulated in Table 4. All entries are as defined in Table 1.

5 Summary and conclusions

The IASI_1DVar code has been used to perform retrievals for ensembles of atmospheric states to assess both the accuracy of fast model retrievals and the impact of model error correlations on retrieval accuracy. Retrievals were performed for an ensemble of perturbations to a tropical atmosphere (P012) and for ensembles of perturbations to an ensemble of 69 atmospheric states (AS69).

Some practical difficulties were encountered in making direct comparisons with linear theory, due to noisy estimates of ensemble background and retrieval error covariances, and profile screening steps required for consistency with profile checks in IASI_1DVar . In addition to standard graphical comparisons, analysis methods (using projection of estimated covariance matrices onto the eigenvectors of **B**) were developed to diagnose and account for these problems when characterising retrieval accuracy.

The first component of the extended study focussed on verification of previous predictions of suboptimal retrieval accuracy due to fast model transmittance prediction errors, and their spectral correlation. Results from the IASI_1DVar retrievals essentially confirm the predictions of linear theory: Gastropod transmittance prediction errors do not have a significant impact on retrieval accuracy for retrievals using the NESDIS channel selection, but these errors do compromise retrieval accuracy with the full AIRS channel set. Retrieval accuracy is largely insensitive to the specification of **R** for retrievals using the NESDIS channel selection, but full specification of **R** is crucial for retrievals using the full AIRS channel set. In this case the information content of observations is almost completely compromised when a diagonal approximation is made to **R**, while retrieval accuracy approaches that of optimal linear theory with full specification of **R**.

These results also support the conclusion of previous studies [Sherlock et al., 2003] that Jacobian errors can have a significant impact on retrieval accuracy (particularly for retrievals using the full AIRS channel set). Accounting for Jacobian errors using linear theory carries a significant computational (reference line-by-line calculations are needed to estimate Jacobian errors), and thus monte carlo approaches (which can also be readily extended to simulate other aspects of an operational data assimilation system (e.g. bias correction)), are probably the preferred method to assess the impact of fast model errors and suboptimal data assimilation choices on retrieval accuracy.

The second component of the extended study characterised retrieval accuracy in an operational context, using fast model differences (resulting principally from spectroscopic differences and transmittance prediction errors) as a proxy for real fast model errors. In this situation the interpretation of results is more complicated, because retrieval accuracy (for a given channel selection) depends critically on the accuracy of bias correction and the specification of the observation error covariance matrix, and the impact of these different aspects can depend on atmospheric state.

Results from the IASI_1DVar retrieval experiments suggest that if fast model differences are indeed a good proxy for fast model errors, and if flat bias corrections can be estimated accurately, then assimilation of the full NESDIS channel selection with a diagonal approximation to **R** is generally useful. There is essentially no loss in accuracy due to fast model differences for temperature retrievals, but there is a loss in the accuracy of humidity retrievals. In particular, the benefit of data assimilation for retrieval of upper tropospheric humidity may be completely lost, and a diagonal approximation to **R** may compromise (retrieval errors exceeding background errors) lower tropospheric humidity retrievals in some atmospheric situations. If bias correction is imperfect, the results of the IASI_1DVar retrievals indicate retrieval bias will increase (as expected), and retrieval accuracy will generally be very sensitive to the specification of **R**. Sensitivity studies we have performed suggest these conclusions also hold when background ozone profiles are subject to error.

Given that AIRS fast model differences are comparable with current O–B statistics, these results suggest operational channel selections and associated specification of the observation error covariance matrix should take estimates of inter-channel error correlations and the accuracy and stability of bias correction coefficients into account. Ideally, monte-carlo type 1D-Var retrievals, like those undertaken in this study, could be used the characterize and minimize the impact of suboptimal retrieval choices in operational data assimilation.

Acknowledgements

This study was co-funded by NIWA, under the Foundation for Research Science and Technology contract C01X0218. Thanks to Andrew Collard for code revisions and discussions during the course of this work.

References

F. Chevallier. Sampled databases of atmospheric profiles from the ECMWF 50-level forecast model. Technical Report SAF-RR-4, European Centre for Medium-range Weather Forecasts, Reading, United Kingdom, 1999. [Available from the Librarian, ECMWF, Shinfield Park, Reading RG2 9AX, United Kingdom.].

A. Collard and S. Healy. The combined impact of future space-based atmospheric sounding instruments on numerical weather prediction analysis fields: a simulation study. *Quart. J. Roy. Meteor. Soc.*, 129:2741–2760, 2003.

M. Matricardi, F. Chevallier, and S. Tjemkes. An improved general fast radiative transfer model for the assimilation of radiance observations. Technical Report 345, European Centre for Medium Range Weather Forecasts, Reading, United Kingdom, 2001. [Available from the Librarian, ECMWF, Shinfield Park, Reading RG2 9AX, United Kingdom.].

C. D. Rodgers. Characterisation and error analysis of profiles retrieved from remote sounding measurements. *J. Geophys. Res.*, 95(D5):5587–5595, 1990.

V. Sherlock. Impact of RTIASI fast radiative transfer model error on IASI retrieval accuracy. Technical Report FR-319, Met Office, Exeter, United Kingdom, 2000. [Available from the National Meteorological Library, Fitzroy Road, Exeter, United Kingdom.].

V. Sherlock, A. Collard, S. Hannon, and R. Saunders. The Gastropod fast radiative transfer model for advanced infrared sounders and characterization of its errors for radiance assimilation. *J. Appl. Meteor.*, 42(12):1731–1747, 2003.
Code, coefficients and documentation online at gastro.sourceforge.net.

L. L. Strow, S. Hannon, S. De Souza-Machado, and H. Motteler. An overview of the AIRS radiative transfer model. *IEEE Trans. Geosci. Remote Sens.*, 41(2):303–313, 2003.

R. A. Toth. Air- and N_2-broadening parameters of water vapour: 604 to 2271 cm^{-1}. *J. Mol. Spectrosc.*, 201(2):218–243, 2000.

P. D. Watts and A. P. McNally. The sensitivity of a minimum variance retrieval scheme to the value of its principal parameters. In *Proc. of the Fourth Int. TOVS Study Conf.*, pages 399–412, [Available from the CIMSS, Univ. Wisconsin-Madison, 1225 W. Dayton St., Madison WI 53706, U.S.A.], 16-22 March 1988. Cooperative Institute for Meteorological Satellite Studies. Igls, Austria.