Stratospheric and Mesospheric Data Assimilation: The role of middle atmospheric dynamics

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Volume 3 of "*Data Assimilation for Atmospheric, Oceanic and Hydrologic Applications*." The first volume was published in 2009, and the second in 2013. Both volumes were published by the Springer, with 27 chapters each, which were based on papers presented at the Sasaki Symposium on data assimilation (DA) in the AOGS meetings along with some invited papers. Prof. Yoshi Sasaki passed away on Mar. 12, 2015. He was a pioneer in atmospheric data assimilation who introduced and applied the variational methods. We plan to dedicate this book to the late Yoshi Sasaki as a memorial volume.

ABSTRACT

The middle atmosphere refers to the stratosphere and mesosphere and features dynamics and circulations that are fundamentally different from those of the troposphere. The large-scale meridional circulations in the middle atmosphere operate on seasonal and longer time scales and are largely forced by the breaking of upward propagating waves. The winter stratosphere is dominated by large-scale waves and a polar vortex which confines constituents and which is sometimes punctuated by stratospheric sudden warmings. In contrast, the summer stratosphere is quiescent. Meanwhile, the meridional circulation in the mesosphere is mainly driven by the breaking of a broad spectrum of gravity waves that have propagated upward from the troposphere. These facets of middle atmosphere dynamics have implications for, and pose unique challenges to, data assimilation systems whose models encompass this region of the atmosphere. In this work, we provide an overview of middle atmosphere data assimilation in the context of the dynamics of this region. The purpose is to demonstrate how the dynamics can be used to explain the behavior of data assimilation systems in the middle atmosphere, and also to identify challenges in assimilating measurements from this region of the atmosphere. There are two overarching themes. Firstly, we consider the vertical propagation of information through waves, resolved and parameterized, and background error covariances. Secondly, we delve into the dynamical sources of model errors and techniques for their estimation.

1. Introduction

The past decade has seen operational weather forecasting centers raise their model lids to the middle or upper mesosphere. The NASA's Global Modeling and Assimilation Office (GMAO) raised its model lid height to 80 km in January 2004. The European Centre for Medium-Range Weather Forecasts (ECMWF) did the same in February 2006, as did the Met Office in November 2009. The Canadian Meteorological Centre (CMC)'s model lid moved to 0.1 hPa (roughly 65 km) in June 2009 (Charron et al. 2012). Given that the primary focus of an operational weather forecasting centre is on producing real time forecasts for the troposphere, the extra computational expense invested in raising the model lid to such heights merits an explanation. There are two main motivating factors for making this change. On the one hand, a precise model representation of the stratosphere is expected to increase predictive skill of extended range (10 days to subseasonal) forecasts (Tripathi et al. 2014, Gerber et al. 2012, Charlton et al. 2004, 2005b) but more importantly there is a significant number of nadir satellite observations that are sensitive to the middle atmosphere, Figure 1 shows the normalized weighting functions from the Advanced Microwave Sounding Unit (AMSU)-A instrument. Several channels (12-14) exhibit peak sensitivity to upper stratospheric temperature and many others (6-11) have peak or significant sensitivity to lower or mid stratosphere temperature. In order to assimilate these channels, a model would need a good background forecast up to 0.1 hPa, so its sponge layer should begin above this level. This then implies a model lid in the middle mesosphere. Thus the stratosphere and most of the mesosphere are now part of the weather forecasting domain.

Since weather forecast models form the basis of major reanalysis efforts such as ERA-Interim (Dee et al. 2011), JRA-55 (Kobayashi et al. 2015) or MERRA (Rienecker et al. 2011), there are now long time series of analyses of the middle atmosphere which serve the climate community. These reference datasets are widely used for assessing and validating climate models, for understanding measurements and driving chemistry transport models (CTMs). Thus a whole community is inspecting assimilation products in the middle atmosphere, providing feedback on successes and deficiencies. In particular, middle atmosphere dynamicists, climatologists and chemists have noted differences in the various reanalysis products and established an international effort (Stratospheric Processes and their Role in Climate (SPARC) Ranalysis Intercomparison Project or S-RIP) to systematically compare the products and provide guidance to climate scientists as to where and when they are reliable as well as to data assimilators (http://www.sparc-climate.org/activities/reanalysis/). The very existence of S-RIP points to the value placed on middle atmosphere analyses by climate scientists.

There are yet other reasons for assimilating observations of the middle atmosphere, such as driving models with chemistry to quantify stratospheric ozone loss (Shepherd et al. 2014), assessing changes in the transport of constituents (and the Brewer-Dobson circulation) (Hegglin et al. 2014), and better understanding large-scale dynamic events such as sudden stratospheric warmings and their potential impacts or responses under climate change scenarios. Finally, the stratosphere has a memory that can be exploited for improving the skill of seasonal forecasts (Stockdale et al. 2015, Sigmond et al. 2013, Marshall and Scaife 2009, Boer and Hamilton 2008) providing yet another motivation for the assimilation of observations into models capable of depicting the middle atmosphere.

Middle atmosphere data assimilation has therefore become increasingly relevant to operational and research atmospheric data assimilation efforts. While the same general techniques of data assimilation are applied to all regions of the atmosphere simultaneously, there are reasons to afford middle atmosphere data assimilation separate consideration. Firstly, the dynamics of the middle atmosphere differ from those of the troposphere and, as will be shown below, this has important implications for understanding the behavior of data assimilation systems. Secondly, the degree to which a forecast model captures these dynamics provides insight into the nature of model errors in this region of the atmosphere. Finally, the observing system targeting this region of the atmosphere poses unique challenges. While radiosondes have formed the backbone of tropospheric assimilation systems (whether directly or through the anchoring of bias correction schemes applied to satellite measurements), they only reach as high as the middle stratosphere, leaving much of the middle atmosphere devoid of in situ measurements. Operational satellites sensing the middle atmosphere are primarily nadir sounders such as AMSU (Advanced Microwave Sounding Unit). Since these instruments are sensitive to broad layers of the atmosphere, the vertical structure of the stratosphere and mesosphere cannot be well resolved. Fortunately, with the routine assimilation of Global Positioning System (GPS) Radio Occultation (RO) measurements, the vertical structure of the lower to mid stratosphere can be better resolved (Cardinali and Healy, 2014; Healy and Thépaut, 2006). However, above 35 km, the data become noisier and only weakly constrain the full state despite effectively constraining the bias of satellite measurements. Thus, the vertical structure of the atmosphere above the mid stratosphere remains difficult to estimate.

The goal of this article is to present a subjective overview of middle atmosphere data assimilation, from the perspective of middle atmosphere dynamics but targeted to a data assimilation audience. The intent is not to be exhaustive, but rather, illustrative, while maintaining a focus on identifying particular issues and challenges in the middle atmosphere of coupled troposphere-middle atmosphere data assimilation systems. Constituent assimilation is an enormous topic that is relevant for the middle atmosphere, but one that is not considered here. The distribution of constituents is determined by atmospheric transport and mixing as well as chemical reactions. An overview of transport in the middle atmosphere is provided by Andrews et al. (1987) and Shepherd (2007) while Monge-Sanz et al. (2013) discuss the role of assimilation techniques on constituent transport in the context of chemistry transport models. Recent reviews of chemical data assimilation are provided by Bocquet et al. (2015) and Sandu and Chai (2011).

The article is organized as follows. In section 2 a brief overview of middle atmosphere dynamics is provided while in section 3 we look at middle atmosphere data assimilation through the lens of middle atmosphere dynamics. Some additional challenges and issues of middle atmosphere data assimilation not previously mentioned are identified in section 4 and a summary of the chapter is presented in section 5.

2. Brief overview of middle atmosphere dynamics

In order to understand how forecasting and assimilation systems respond to perturbations such as analysis increments, it is necessary to introduce a few concepts about middle atmosphere dynamics. A very brief introduction of the dynamic features that have some impact on data assimilation is given here, but more detailed accounts are available in textbooks (e.g. Andrews et al. 1987, Vallis 2006) and articles (e.g. Shepherd 2000, 2002, 2007; McLandress 1998; Smith 2004).

The middle atmosphere refers to the stratosphere and mesosphere and extends from roughly 10 to 80 km above the Earth's surface. Temperature increases with height in the stratosphere due to the absorption of ultraviolet radiation by ozone and decreases with height in the mesosphere as the ozone concentration drops off. The stratosphere is statically stable and the climatological winds are to a first approximation zonal. If we consider the two-dimensional, steady, geostrophic and hydrostatic equations, in the absence of a momentum source, the atmosphere would be in radiative equilibrium balance with outgoing terrestrial radiation balancing incoming solar radiation. This means a cold dark winter pole and a warm sunlit summer pole. Through thermal wind balance, zonal winds increase with height. However, as shown in **Figure 2a**, radiative-equilibrium temperature calculations yield temperatures near the winter pole (dashed lines) that are far too cold compared to observed values (solid lines), and zonal wind speeds that are much too strong (compare dashed and solid lines in **Figure 2b**). McLandress (1998) added a simple Rayleigh friction term as a forcing term in the zonal momentum equation which is linearly proportional to zonal wind with the proportionality constant increasing with height. The resulting temperatures and zonal wind speeds are closer to observations (compare dotted and solid lines in **Figure 2**) than the radiative equilibrium solution (dashed lines). The conclusion is that some kind of momentum source/sink is needed to explain the observed zonal mean temperatures and winds, as was first hypothesized by Leovy (1964).

The origin of this momentum source/sink is breaking waves, which exert a drag or forcing on the zonal mean flow and drive a mean meridional circulation. In the winter stratosphere, large-scale quasi-stationary Rossby waves forced by topography and land-sea contrasts are able to propagate upward through the stratospheric westerlies where they increase in amplitude as density decreases. Eventually they break, impart their (negative) momentum to the zonal mean flow, exerting a drag on the wintertime westerlies. This creates poleward motion through a Coriolis torque and by continuity, descent (and warming through adiabatic compression) over the winter pole. Thus, large-scale waves drive this thermally-indirect circulation, called the Brewer-Dobson circulation. The Brewer-Dobson circulation is important not only for explaining stratospheric temperature distributions, but also for transporting constituents, as is apparent in the accumulation of ozone over the winter pole in **Figure 3**. The conditions for vertical propagation of quasi-stationary Rossby waves (see Andrews et al. 1987, chapter 4.5 or Vallis 2006, chapter 13.3) in the case of a constant wind (U) are that U>0 (eastward) and U remains below a critical value (U_c). Thus, these waves cannot propagate into the stratosphere in summer when zonal winds are easterly. Furthermore, in the winter when they can propagate vertically, large-scale waves (wavenumbers 1 to 3) are favoured because the critical wind speed (U_c) decreases rapidly with increasing wavenumber. Thus the winter stratosphere is dominated by waves having large horizontal scales. Due to the fact that quasi-stationary Rossby waves are unable to propagate in easterly zonal wind, the summer stratosphere is characterized by an absence of these waves and so by temperatures closer to radiative equilibrium.

The stratospheric jets also act to filter much smaller-scale waves (i.e., gravity waves) which would otherwise propagate up to the mesosphere. In winter when stratospheric winds are westerly and increasing with height, gravity waves with eastward phase speeds may reach their critical level (where the zonal phase velocity equals the zonal wind) in the stratosphere. This removal or "filtering" of eastward propagating waves at their critical levels leads to predominantly westward propagating gravity waves reaching the mesosphere (assuming a westward-eastward isotropic launch gravity wave spectrum). When those waves break in the mesosphere they deposit westward momentum (Lindzen 1981). Similarly, in the summer hemisphere, easterly winds filter westward propagating gravity waves at their critical levels, so that gravity waves which break in the mesosphere deposit eastward momentum. In the mesosphere, this deceleration of the westerlies in the winter hemisphere and deceleration of the easterlies in the summer hemisphere caused by gravity wave momentum deposition create a poleward motion in the winter hemisphere, but equatorward motion in the summer hemisphere. By continuity, there is descent over the winter pole and ascent over the summer pole. Thus small scale gravity waves are responsible for driving the pole-to-pole Murgatroyd-Singleton circulation in the mesosphere seen in the upper part of **Figure 3**.

Since the spectrum of Rossby waves propagating upward in the winter stratosphere is dominated by the largest modes, as synoptic scale waves are filtered in the lower stratosphere, these large-scale waves are expected to be well represented in global numerical models. On the other hand, gravity waves are small-scale waves which propagate almost vertically. Therefore, global numerical models are typically not able to directly represent these waves. In order to incorporate the momentum forcing produced by small-scale gravity waves in global numerical models, the drag exerted by the upward propagation and breaking of small-scale gravity waves on the zonal mean flow is accounted for through "gravity wave drag" parameterizations. These parameterizations are divided in two groups: parameterizations of waves of orographic origin and non-orographic gravity wave drag schemes. The generation characteristics of orographically generated waves are well known and have been shown to have a large impact in the lower stratosphere and in particular on the Brewer-Dobson circulation (Li et al 2008, McLandress and Shepherd 2009). Gravity waves from other sources such as fronts, convection, and geostrophic adjustment are modelled through non-orographic gravity wave parameterizations (e.g. Hines 1997, Scinocca 2003) and are expected to have a large impact on the upper stratosphere and the mesosphere.

3. Impact of middle atmosphere dynamics on data assimilation

The fact that the middle atmosphere is largely driven by waves propagating up from the troposphere has implications for data assimilation. The fundamental difference in stratospheric dynamics between winter and summer also impacts interpretation of data assimilation results and inputs (such as background error covariances). Finally, the importance of gravity waves (that are generated in the troposphere and propagate upward) to the mesospheric circulation means that these signals (which are frequently treated as noise in the troposphere) might need to be better simulated or estimated in the troposphere and lower stratosphere. In this section, we explore how middle atmosphere dynamics impact the inputs and results of data assimilation systems.

3.1. Upward propagation of information

3.1.1. Propagation of information and errors through resolved waves

Figure 4 shows averaged analyzed temperature vertical profiles (over the global domain) from a set of data assimilation experiments using a 3D-variational (3D-Var) system for which only the strength of an externally applied filter is varied. As a result of changing the strength of the filter, a large impact on mesospheric temperatures is found. Specifically, the stronger the filter, the colder the global mean mesopause temperature. A difference of 20 K at 90 km is seen between experiments. These results were surprising because the Canadian Middle Atmosphere Model (CMAM) (Scinocca et al. 2008) which was employed in the data assimilation system extends to about 95 km but the observations were inserted only below about 45 km. Thus the filter was targeting imbalance arising from increments below 45 km. Yet below 45 km, the temperature profile averaged over all coincident measurement locations was virtually identical regardless of which filter was employed. This is because the averaging over all profiles smooths whatever degree of noise is present in the profiles obtained with different filters. However, the waves defined by the increments in the troposphere (whether real or spurious) propagate up to the mesosphere where they break and create a drag (momentum forcing) which impacts the zonal mean flow. If they do not break by 80 km they encounter the model sponge layer which is designed to absorb such waves thus preventing their reflection from the model lid at 95 km. The sponge layer is a numerical device acting on departures from the zonal mean flow (Shepherd et al. 1996) that is intended to mimic the fact that in the absence of the model lid these waves would reach higher altitudes where they would break, deposit momentum and create turbulent dissipation generating heating. Eventually the radiation to space balances the wave-generated heating resulting in the temperature profiles seen in **Figure 4**. Thus although the heating is artificially created here through the enforced dissipation of these upward propagating waves, the same process would occur in the real atmosphere though at higher altitudes because of molecular viscosity. Indeed Lűbken et al. (2002) show that gravity waves are an important source of heating in the mesopause region. Thus, in **Figure 4**, a stronger, more dissipative filter results in smaller wave momentum flux reaching the mesosphere and less enforced wave breaking and resultant heating in the sponge layer. This hypothesis was confirmed by comparing the temperature variance of time series of analyses from the various experiments (Sankey et al. 2007). The stronger the filter, the smaller the variance. Thus resolved waves in the troposphere and stratosphere can propagate up to the mesosphere and impact the zonal mean or even the global mean flow. The implication is that tropospheric tuning of data assimilation systems can have large impacts on mesospheric analyses. On the other hand, the sensitivity of the mesosphere can also be used to tune assimilation parameters (such as filter strength, as was done in Sankey et al. 2007).

Nezlin et al. (2009) demonstrated that even without observations above 45 km, the large scale dynamics (up to wavenumber 10) in the mesosphere could be improved. They also showed that the quality of mesospheric analyses was sensitive to the accuracy of observations taken below 45 km. Both of these facts attest to the vertical propagation of information. (Here we use the term "information" to describe that part of the true atmospheric signal that a given model can resolve.) The observations constrain the atmospheric signal at a given height, and then the dynamics of the model propagates this observational information upward producing an impact at heights where no observations had been assimilated. Since the middle atmosphere is largely forced by upward propagating waves, both information and errors propagate vertically through waves in data assimilation systems. While Nezlin et al. (2009) demonstrated that the vertical propagation of information in a 3D-Var system (the CMAM-Data Assimilation System (DAS)) is theoretically possible through the use of simulated observations, Xu et al. (2011a,b) demonstrated that CMAM-DAS mesospheric winds do indeed compare well to independent measurements on long time scales. This confirms that vertical propagation of information from the troposphere to the mesosphere actually occurs in assimilation systems since no observations in the mesosphere had been assimilated. The same effect is seen in the intraseasonal variability of mesospheric zonal-mean temperature and constituents (carbon monoxide) in a set-up where the CMAM is nudged towards the ERA-Interim reanalysis in the troposphere and stratosphere, and the model is seen to agree well with MLS (Microwave Limb Sounder) observations in the mesosphere (McLandress et al. 2013).

Even without mesospheric observations, the migrating diurnal and semi-diurnal tidal signals in the mesosphere can be captured (Sankey et al. 2007, Wang et al. 2011, Xu et al. 2011a,b, Hoppel et al. 2013). Since these signals are generated by the absorption of solar radiation by water vapour in the troposphere and by ozone in the stratosphere, observations from the troposphere and stratosphere constrain these signals well. Thus agreement of a model’s mesospheric tidal amplitudes with observations indicates that the vertical propagation of the signal into the mesosphere is at least partially captured by the model. Of course, assimilation of mesospheric observations, greatly improves agreement with observations (Hoppel et al. 2013).

3.1.2. Propagation of information through background error covariances

The two orders of magnitude increase with height in forecast error variance seen in the bottom left panel of **Figure 5** largely reflects the increasing amplitude of gravity waves from the stratosphere to the mesosphere. As a result, spurious increments in the mesosphere can be produced (top left panel) when the large forecast error variances are combined with small but nonzero correlations in the wings of the weighting function. For example, the analysis increment at 0.01 hPa in the top left panel of **Figure 5** appears at a height where the weighting function for an observation at 10 hPa is virtually zero (i.e. the wings of the weighting function) (top right panel) because the correlation function (bottom right panel, black curve) is not exactly zero at 0.01 hPa. Setting such tiny correlations (which are due to statistical noise) to exactly zero removes much of the spurious mesospheric analysis increments (dashed lines in top left panel). In fact, removing such spurious increments in the mesosphere is imperative when an assimilation system assimilates no mesospheric observations and is therefore unable to damp such errors. In the mesosphere, such spurious increments may be persistent (because of the presence of model and/or observation biases) and can actually lead to physically nonsensical results after only a few weeks of assimilation. Thus information propagated to the mesosphere through background error covariances is not necessarily desirable. Similarly, erroneous small scale vertical structures in background error covariances cannot be damped by measurements if the observing system is lacking in detailed vertical information. This is the case in the upper stratosphere where nadir temperature sounders are the dominant source of information.

Since observations of the middle atmosphere are predominantly from satellite-based radiance measurements, the problem of vertical localization of covariances needed for some ensemble-based data assimilation techniques in radiance space is worth noting. The issue is that these types of measurements are related to model quantities integrated in space so that the concept of localization is unclear. Yet the localization of error covariances is important for practical application of ensemble Kalman filters to comprehensive and complex meteorological models. Such localization is frequently done in observation space for computational expediency. The problem identified by Campbell et al. (2010) is that location and distance are ill defined quantities in radiance space so that observation-space localization applied to the usual case of channels with overlapping sensitivities cannot achieve the correct Kalman gain even when observations are known to be perfect. Ideally, the vertical localization must therefore be at least as broad as the weighting functions but not so broad that the suppression of spurious correlations due to sampling errors become ineffective. On the other hand, localization in model space does not suffer from this problem.

3.1.3. Propagation of information through gravity wave drag schemes

Gravity wave drag (GWD) schemes can also propagate information from the troposphere and stratosphere to the mesosphere. GWD schemes parameterize (represent simplifications of) the processes of gravity wave generation in the troposphere, vertical propagation and nonlinear saturation. The output of such a scheme is a drag or forcing term for the momentum equations. GWD schemes are needed in climate models because their coarse horizontal resolutions lead to insufficient forcing of the meridional circulation and insufficient downwelling (and warming) over the winter pole (as well as insufficient upwelling and cooling over the summer pole). Thus, without a GWD scheme, climate models can suffer from the "cold pole" problem, which is particularly evident in the southern hemisphere where there are fewer forced planetary waves (Austin et al., 2003).

GWD schemes can also vertically propagate information in data assimilation systems (Ren et al. 2008). Observations are used to define winds in the troposphere and stratosphere which filter resolved gravity waves which might otherwise reach the mesosphere. Similarly, the parameterized impact of subgrid scale gravity waves in GWD schemes produce a force on the mesospheric flow (McLandress et al. 2013). The benefit of a GWD scheme on mesospheric analyses was demonstrated by Ren et al.

(2011). Background or 6-h forecasts were closer to independent observations of mesospheric temperature (from SABER retrievals) when a GWD scheme was used (**Figure 6**). The benefit was quite large if no mesospheric observations were assimilated, but still apparent even if they were assimilated. Since mesospheric analyses obtained with a model using a GWD scheme but with no mesospheric observations were close to independent measurements, it is evident that GWD is able to propagate useful information to the mesosphere. At ECMWF, the same GWD scheme used in Ren et al. (2011) was implemented operationally, and shown to improve the bias in temperature at the stratopause at the winter pole in 5-day forecasts (Orr et al., 2010).

3.2. Understanding forecast improvements

The winter polar stratosphere is dominated by westerly winds that increase with height and define a polar vortex (polar night jet). In the Northern Hemisphere, this vortex is occasionally disrupted by stratospheric sudden warming (SSW) events during which temperatures can rise dramatically (by 50 K in one week). Simultaneously, the climatological westerly winds weaken and may even become easterly. Mesospheric coolings can also occur in conjunction with stratospheric warmings. Since SSW events are primarily driven by planetary waves propagating up from the troposphere, such events involve vertical coupling from the troposphere to the mesosphere. Baldwin and Dunkerton (2001) showed that the dominant mode of slowly varying wintertime variability called the Northern Annular Mode (or NAM) has a spatial structure which is similar from the surface to over 50 km altitude, thus indicating a coupling of the troposphere and stratosphere. (At the surface the pattern is sometimes called the Arctic Oscillation.) The NAM pattern at 10 hPa is a disk of similarly signed values around the pole with oppositely signed values in a ring or annulus around this. A projection of the geopotential height onto this pattern indicates the relative strength of the polar vortex. A strongly positive projection indicates a stronger than normal polar vortex, while a strongly negative projection indicates a weaker than normal vortex. Moreover, when time series of strongly positive or negative NAM events are composited, the vertical coupling becomes apparent. Specifically, a large stratospheric event, such as an SSW, will appear in the mid-stratosphere (10 hPa is often used as a reference level) about ten days prior to its appearance at the surface. Once the NAM signal appears in the troposphere (300 hPa), the same sign of the NAM index persists in the troposphere for around 60 days. During this time, the troposphere is characterized by a particular climatology. For instance, during a strong vortex event, cool winds would flow over eastern Canada, North Atlantic storms would bring rain and mild temperatures to northern Europe and drought conditions would prevail in the Mediterranean (Thompson and Wallace 2001). Thus, the stratospheric modulation of tropospheric climate suggests a predictive skill which can be exploited on the week to seasonal timescales (e.g. Douville 2009). Charlton et al. (2004, 2005b) also showed that stratospheric initial conditions can impact tropospheric forecast skill on the 10-15 day timescale. Various mechanisms have been proposed to explain the stratospheric modulation of tropospheric climate on the week to seasonal timescale but there is no consensus yet as to which is the most important one (Charlton et al. 2005a, Tripathi et al. 2014).

On shorter (medium range weather forecasting) time scales, middle atmosphere dynamics are still useful for understanding forecast improvements. When the Canadian Meteorological Centre raised the lid of its operational forecast model from 10 to 0.1 hPa, most (over 80%) of the improvement in forecast skill (of both stratosphere and troposphere) was achieved without new measurements in the upper stratosphere (AMSU-A ch. 11-14 and GPS RO between 30-40 km) (Charron et al. 2012). This means that an improved modeling of the stratosphere is sufficient to obtain improved upper stratospheric analysis (where no new data were assimilated). Moreover, the improvement was greatest in the winter for both hemispheres. Thus improvement depended more on season (when the stratosphere was dynamically active) than on hemisphere (or observation distribution). Furthermore, when additional observations in the upper stratosphere were assimilated, they were beneficial in winter but not in summer. These results are understandable in the context of middle atmosphere dynamics. Just as tropospheric observations are most useful when dynamic activity (such as baroclinic wave development) is occurring, stratospheric observations are most beneficial when the stratosphere is dynamically active (in winter).

Because of the prevalence of gravity waves and divergent motions in the mesosphere (Koshyk et al. 1999), and the unlikelihood of sparse observations being able to resolve these waves, it is not obvious how beneficial the assimilation of mesospheric observations will be. By comparing forecasts started from analyses in the middle atmosphere (100-0.1 hPa) with those started from climatology in the middle atmosphere, Hoppel et al. (2008) found that the assimilation of middle atmospheric observations were beneficial for winter high latitudes up to the 10-day forecast lead time. In the summer, when the stratosphere is quiescent and dominated by zonal mean flow, persistence or climatology works reasonably well so the benefit of assimilation is not as apparent. On the other hand, mesospheric observations also help to improve the depiction and forecasts of certain planetary waves in the mesosphere as well as reducing biases in zonal mean fields stemming from model errors (Hoppel et al. 2013).

3.3. Model error

3.3.1. Bias estimation

Since not all the resolved waves will be correctly analysed because the observing system can detect only certain spatial scales, and some of the resolved waves are forced in the models by parameterization schemes which are imperfect (e.g. deep convection), we should expect errors in the meridional circulation. Errors in the forcing of a meridional circulation should then lead to latitudinally varying biases. Thus, we should expect bias in zonal mean fields in stratospheric forecasts. Observations (such as those from nadir sounders) also have biases and require a pre-assimilation bias-correction procedure, so the challenge is to separate these two sources of biases. Moreover, observation bias correction schemes often rely on an assumption of unbiased forecasts—which is clearly invalid in the stratosphere. Dee and Uppala (2009) noted that improvement in the stratospheric bias of ERA-interim over ERA-40 was achieved through the introduction of variational bias correction (Derber and Wu 1998).

In this procedure, bias correction parameters are added to the control vector so that all observations—including those which are not corrected, such as radiosondes--are used to determine their values. This then forces a consistency among observations which are being bias corrected (e.g. the same instrument on different platforms). Of course, even with variational bias correction, the bias so-determined could be due to either a bias in observations or observation operators or to a bias in the model forecast. Since the bias correction is applied to the observation, only the former type of bias is desired. Thus care must be taken to ensure that the recovered bias is truly due to the observations. To some extent, the anchoring of the assimilation system by uncorrected observations (such as radiosondes) reduces the likelihood that model bias will be detected. However, in the upper stratosphere and mesosphere where few uncorrected observations exist, the danger of correcting for model bias is considerable. Thus Dee and Uppala (2009) chose to leave the top peaking channel (SSU channel 3 or AMSU-A channel 14) uncorrected in the ERA-interim, in order to anchor the system. This resulted in a reduced warm bias near the model top. Since a warm bias had independently been attributed to the model forecast (McNally 2004) the results were positive. So although variational bias correction has proven to be a valuable tool for reanalyses as well as operational assimilation systems, the problem of separating model and measurement bias in the upper stratosphere or mesosphere remains (Hoppel et al. 2013). Leaving a certain instrument uncorrected still creates difficulty when it is present on multiple platforms, or when the observing system changes (e.g. when the top peaking channel changed from SSU ch. 3 to AMSU-A ch. 14). Furthermore, whatever bias exists in the uncorrected measurement will appear in the analyses. Several distinct temporal inhomogeneities in global-mean ERA-Interim temperatures were identified by McLandress et al. (2014).

3.3.2. Unresolved gravity wave drag estimation

The breaking of small-scale gravity waves in the upper stratosphere and mesosphere plays an important role in driving the meridional circulation and thus the impact of these small-scale waves can be detected in large-scale observations such as nadir or AMSU-A satellite measurements. Therefore, the systematic biases found in the model compared to observations may be associated to a large extent with those small-scale gravity wave breaking processes that are not resolved in the model but have a large global impact. Data assimilation techniques which are used to produce analyses can also be used to help diagnose systematic model error. For example, McLandress et al (2012) used the time averaged zonal mean zonal wind analysis increments to identify missing gravity wave drag in the southern hemisphere while Pulido (2014) employed systematic differences of potential vorticity between analyses and forecasts to determine momentum forcing via potential vorticity inversion. In addition, data assimilation techniques can also be used to estimate the missing momentum forcing in the model as a product of the assimilation. Since this missing forcing may be associated to a large extent with gravity wave drag due to unresolved waves, this information can then be used to constrain gravity wave drag parameterization schemes. For example, Pulido and Thuburn (2005) applied a 4D variational assimilation (4D-Var) technique to estimate the missing momentum forcing in the model instead of estimating an initial state. The optimal momentum forcing is the one whose model state evolution is associated with the minimum of the cost function.

One helpful aspect of middle atmosphere data assimilation is that the only two processes that are parameterized in models at that height range are radiation and the dissipation of small-scale gravity waves. Since the physics of radiation is well known and only has a large impact on long (seasonal) time scales, the missing zonal momentum forcing at these heights on shorter time scales may be mainly attributed to small-scale gravity waves (Pulido and Thuburn 2006). The optimal momentum forcing estimated with 4D-Var resembles that expected from the filtering of an isotropic gravity wave spectrum (Lindzen, 1981), with large deceleration centres at high latitudes during the winter and summer (Pulido and Thuburn, 2008). On the other hand, it is less evident that the estimated forcing at high latitudes during equinox is associated with an isotropic gravity wave spectrum.

3.3.3. Parameter estimation

Models have a large number of parameters that are not directly observable. Currently, climate modelers infer the values of such unknown parameters manually by comparing the climatology of model integrations with the observed climatology. These inferred parameters may then change if resolution, parameterizations or other parameter values are changed in the model. Data assimilation provides an objective approach to the estimation of unknown model parameters (Ruiz et al 2013). Online parameter estimation techniques based on the ensemble Kalman filter or 4DVar usually define an augmented state which is composed of the model state and also the parameters to be estimated. However, the parameters are not directly constrained by observations as is the model state. Instead, the parameters are constrained through background error correlations between the parameters and model state variables.

Gravity wave drag parameters related to the launch wave spectrum and to the saturation and breaking properties of the waves (which determine the gravity wave drag vertical profile) are poorly known from observations. Various techniques have been employed to estimate reasonable values for such parameters. Watanabe (2008) used the results of a high resolution global simulation to determine the characteristics of wave momentum fluxes and to estimate the launch wave spectrum parameters in the Hines parameterization scheme. Some efforts have also been devoted to using high resolution satellite observations (e.g. Atmospheric InfraRed Sounder or AIRS, High Resolution Dynamics Limb Sounder or HIRDLS) to constrain the launch gravity wave spectrum (Alexander et al. 2010). In addition, inverse techniques based on data assimilation have been used to estimate gravity wave parameters. Pulido et al. (2012) proposed an offline data assimilation technique based on a genetic algorithm that uses the estimated missing momentum forcing to constrain launch momentum flux and saturation parameters. Tandeo et al (2015) proposed an ensemble Kalman filter (EnKF) coupled to an expectation maximization algorithm to estimate parameters from an orographic gravity wave drag scheme and also to estimate initial background error covariances which are essential for convergence of the filter in a perfect model experiment. They show that in the presence of model error the filter may converge to different optimal parameters depending on the choice of the first guess value. In general, the estimation of parameters using data assimilation techniques faces a number of unique challenges which require further development or refinement. These challenges are associated with the highly nonlinear nature of the model state response to parameters changes in the context of current assimilation techniques (EnKF and 4DVar) which are based on the linear-Gaussian assumption. To deal with this limitation, some potential solutions have been proposed such as the combination of an offline genetic algorithm with a 4DVar technique (Pulido et al 2012), the use of a hybrid EnKF-particle filter, with EnKF for the state variables and a particle filter applied to the parameters (Santitissadeekorn and Jones 2015) and the afore-mentioned EnKF combined with an Expectation-Maximization algorithm (Tandeo et al 2015). A second major challenge is parameter estimation in the presence of model error. In this regard, a recent study found a positive impact particularly when parameter estimation was combined with model error treatment approaches (Ruiz and Pulido, 2015). A third challenge is the interaction between different parameterizations. While this issue is particularly important for tropospheric data assimilation (e.g. interactions between a planetary boundary layer scheme and a convective scheme), it is not as relevant for middle atmosphere data assimilation, as noted earlier.

4. Challenges in middle atmosphere data assimilation

While in section 3, we have already noted some challenges in middle atmosphere data assimilation in the context of the topics discussed earlier, in this section we focus on issues that have not yet been raised or fully considered.

A characteristic of the observing system for the middle atmosphere is the difficulty of obtaining in situ measurements apart from radiosondes and aircraft observations. Thus, as noted earlier, the vertical structure above the lower stratosphere is not well observed from operational satellites since nadir sounders are sensitive to temperatures over thick layers. On the other hand, GPS radio occultation measurements have been very beneficial not only for their information content and vertical resolution (e.g. Cardinali and Healy, 2014; Healy and Thépaut, 2006) but also for their very low bias which allows them to serve as anchors in bias correction schemes for satellite observations (Cucurull et al, 2014). The constraint of GPS RO data on analyses, however, diminishes as the data become noisier in the upper stratosphere, even as their effectiveness for anchoring the bias correction of satellite data extends throughout the stratosphere (e.g. Cucurull et al. 2014, Charron et al. 2012). Limb sounders such as MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) on Envisat (Environmental satellite), Atmospheric Chemistry Experiment (ACE) aboard SciSat, Microwave Limb Sounder (MLS) on EOS AURA and Sounding of the Atmosphere Using Broadband Emission Radiometry (SABER) aboard TIMED also provide (or did provide) useful information on vertical structure, but these instruments have been on research not operational satellites. As a result, these observations are useful for reanalyses and non-operational assimilation systems but not in operational systems unless they are available in real time (as in the case of MIPAS). Moreover, concern has been expressed over the lack of plans for new limb sounders in the future (Errerra et al., 2015). In the tropics where simple dynamical balances between mass and wind fields are lacking, wind observations are vital but sparse. The Atmospheric Dynamics Mission (ADM-Aeolus) will measure winds globally up to 30 km using an active sensor which will help to better constrain the tropical lower stratosphere but in the mesosphere where unbalanced motions are important, the absence of wind measurements remains an issue. Furthermore, ADM-Aeolus will only measure line-of-sight winds, not vector winds, so a reasonable first guess is required in order to use the information. The only real time observations of the mesosphere are from the SSMIS instrument, however Hoppel et al. (2013) note that apart from the F19 and F20 deployments of the Defense Meteorological Satellite Program (DMSP), there are no other plans for upper atmospheric sounding channels on other satellite sensors raising the possibility of an unconstrained mesosphere analysis in the future. Given that the mesosphere provides the upper boundary for the stratosphere, negative impact on the quality of meteorological forecasts from a paucity of mesospheric measurements is plausible.

The usual filtering of or the imposition of balance constraints on the initial state in the data assimilation cycle (Daley 1991) to eliminate gravity waves should be avoided to keep relevant information for the middle atmosphere. On the other hand, most data assimilation techniques which are intermittent (e.g. EnKF, 3DVar) produce temporal discontinuities in the state variables when observations are assimilated, therefore the generation of spurious gravity waves is inevitable with these techniques (e.g. Sankey et al., 2007). A promising way to avoid this issue is the use of an incremental analysis update (IAU) approach (Bloom et al., 1996) or nudging techniques (Lei et al., 2012). The idea behind these approaches is to distribute the forcing toward observations along the whole assimilation window, in the first case through a uniform forcing term (i.e. the analysis increment), or in the second case through a linear damping forcing term (nudging term) that pushes the model toward the analyses. These approaches give a smooth evolution of the model state so that they avoid the spurious generation of gravity waves due to spin-up processes and in turn avoid the need to apply external filters. The smooth model state evolution then permits cleaner momentum budget studies. The use of IAU was also found helpful for capturing mesospheric tides (Sankey et al. 2007, Wang et al. 2011). Since the migrating diurnal tide is already captured by general circulation models, its signal in the mesosphere can also be captured even without mesospheric observations, if care is taken when filtering analysis increments. The incremental analysis update approach was employed in combination with 3D variational assimilation to produce Modern-Era Retrospective Analysis for Research and Applications (MERRA) reanalyses by the NASA-GEOS data assimilation system (Rienecker et al 2011). A 4D extension of the IAU procedure was developed by Lorenc et al. (2015) and is used in the hybrid ensemble variational assimilation scheme which is used for deterministic medium range weather forecasts at Environment Canada (Buehner et al. 2015).

Section 3.1 highlighted the fact that information propagates vertically with resolved and unresolved waves, but it is worth remarking that by the same mechanisms, errors can also propagate vertically. For example, Nezlin et al. (2009) show that increasing the observation error applied to simulated tropospheric observations deteriorates the quality of stratospheric and mesospheric analyses. Thus the tuning of assimilation schemes for tropospheric forecast quality may have unintended impacts on the analyses of the middle atmosphere (e.g. Sankey et al. 2007). On the other hand, the upscale propagation of errors and concomitant loss of predictability characteristic of the troposphere is not as severe in the middle atmosphere (Ngan and Eperon, 2012). Moreover, increased resolution and better resolved gravity waves may actually help to improve predictability on longer time scales. This may sound counter intuitive given the flat kinetic energy spectrum in the mesosphere due to large amplitude gravity waves (Koshyk et al. 1999), but the hypothesis of Ngan and Eperon (2012) is that predictability can be increased if the gravity waves are better resolved because the upscale error cascade is slower for these waves than for balanced modes. Whether the results of this theoretical study are borne out in operational data assimilation systems is yet to be determined.

The impact of the stratosphere on tropospheric forecasts has primarily been associated with certain "extreme" dynamical events in the stratosphere such as sudden warmings. However, there remain many questions associated with the stratospheric influence on tropospheric forecasts, such as whether the influence extends beyond such extreme events and how far in advance extreme events can be predicted. These are some of the questions that are being addressed by a new international collaboration within SPARC called the Stratospheric Network on Assessment of Predictability (SNAP, http://www.sparc-climate.org/activities/assessing-predictability/). Operational weather centers have seen improvements in tropospheric forecasts when raising their model lids (e.g. Charron et al. 2012), however such changes are made simultaneously with other assimilation system changes. Thus another goal of SNAP is to try to isolate the extent to which accurate stratospheric forecasts contribute to tropospheric predictability.

5. Summary

Information can be propagated vertically in data assimilation systems through covariances, vertically propagating waves, and gravity wave drag schemes. As a result, very large scales in the mesosphere can be improved even without assimilating any mesospheric measurements. The fact that the middle atmosphere is driven by vertically propagating waves has important implications for data assimilation systems. (1) Tropospheric waves (whether correctly simulated or not) impact zonal mean fields in the stratosphere and mesosphere. This means that apparently random signals (e.g. waves) can produce nonlocal systematic errors (e.g. a zonal mean bias). (2) Since not all waves are correctly simulated, and the large wavenumber part of the spectrum is not resolved, we should expect bias (errors in zonal mean) in the mesosphere and stratosphere. This has implications for observation bias correction schemes that assume the background forecast is unbiased. (3) Mesospheric analyses are sensitive to errors in tropospheric analyses. On the other hand, perhaps we can use this sensitivity to help choose assimilation parameters in the troposphere. (4) Information propagates up (through resolved waves during the forecast step). Some of the large scales in the mesosphere can be improved even with no mesospheric observations if tropospheric wave forcing is captured and the middle atmosphere is well modelled. The assimilation of observations will additionally improve mesospheric analyses on large scales thus providing a better upper boundary condition with which to constrain forecasts of the troposphere and lower stratosphere, particularly on longer time scales.

Given the fact that the middle atmosphere is largely driven by vertically propagating waves including gravity waves, and the fact that global climate models often have coarse resolution, it is necessary to parameterize the impact of the dissipation of subgrid scale waves on the zonal mean flow thus introducing a potential source of model error. Data assimilation is useful for estimating the missing drag attributed to such waves as well as for estimating parameters involved in gravity wave drag schemes.

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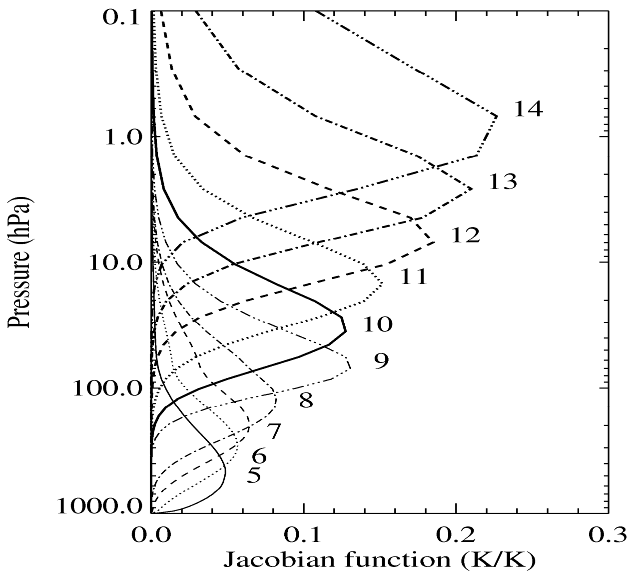

Figure 1: AMSU-A weighting functions on the 43 RTTOV levels computed using the US standard atmosphere. Each function is identified by a channel number on the right. Only weighting functions for channels 5 to 14 are shown. Figure courtesy of D. Shawn Turner.

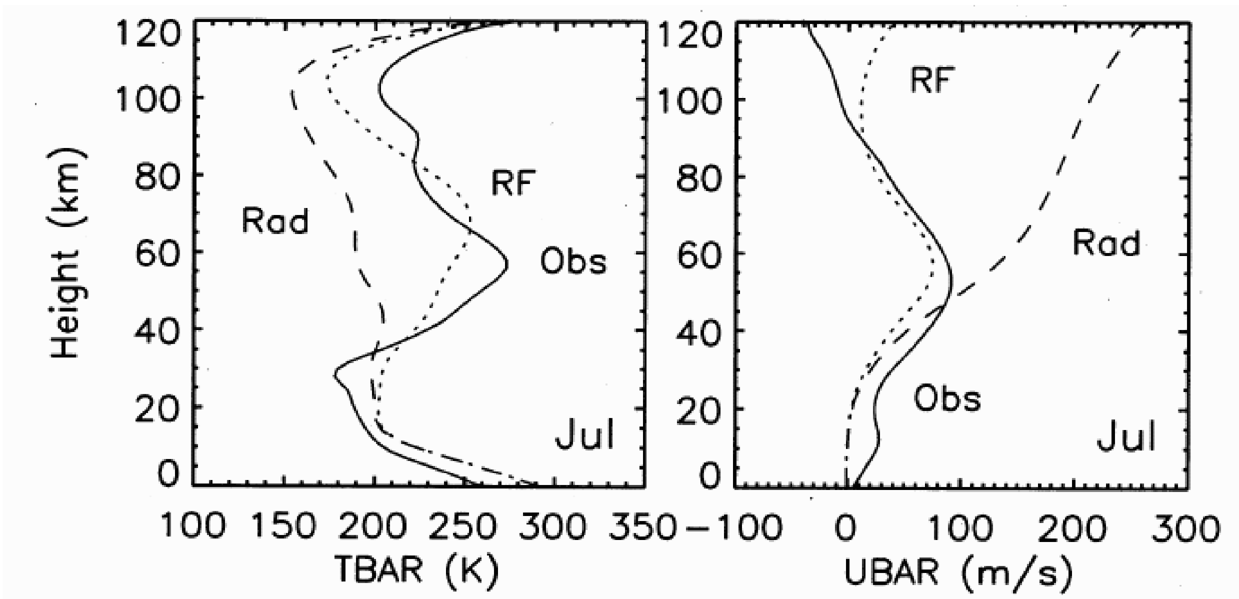

Figure 2: Zonal mean temperature at 90 S (left) and zonal wind field at 40 S (right) during austral winter. Observations from the COSPAR International Reference Atmosphere (CIRA) are shown as solid lines. (COSPAR=COmmittee on SPAce Research). The profiles obtained from radiative equilibrium are shown in dashed curves. Assuming a momentum force that is negative in the winter hemisphere and positive in the summer hemisphere yields a better fit to observations (dotted curves). From McLandress (1998).

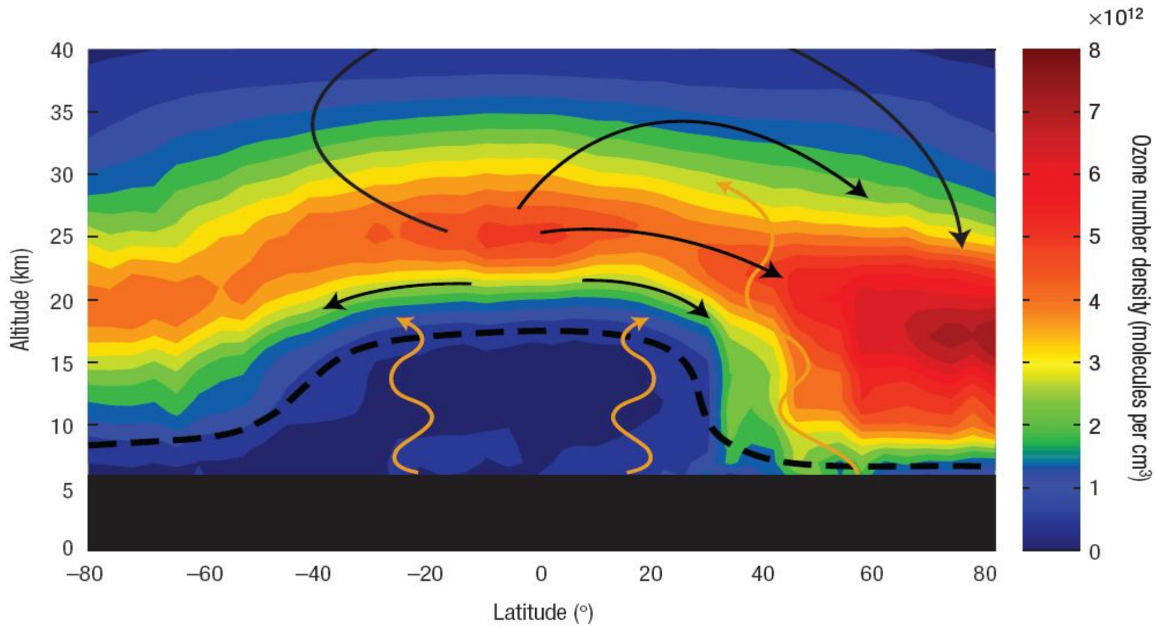

Figure 3: Cartoon of the Brewer-Dobson circulation. Meridonal circulation is indicated by black arrows. The tropopause is indicated by a heavy dashed line. The ozone distribution for March 2004 from OSIRIS is shown in colours with values indicated by a colour bar on the right. From Shaw and Shepherd (2008).

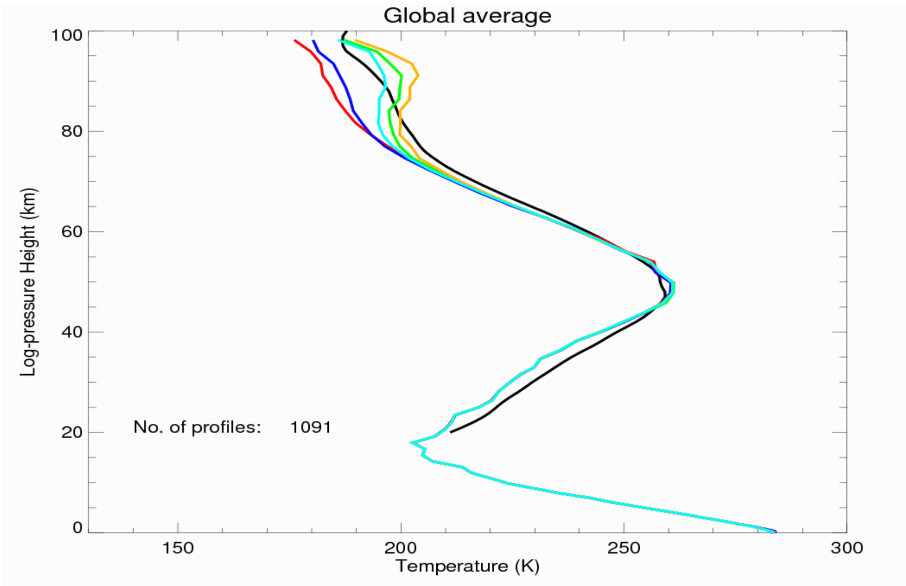

Figure 4: Average of CMAM-DAS temperature profiles sampled at SABER locations over the globe during 25 January 2002. The temperatures are from analyses obtained from assimilation experiments which were identical except for the externally applied filter. In all cases, observations were assimilated below 45 km only. The colours are black (SABER data), cyan (DF with 12-h cutoff), yellow (DF with 6-h cutoff), green (IAU with 6-h cutoff), blue (IAU with 4-h cutoff), and red (IAU with constant coefficients). Filter strength increases as follows: yellow-green-cyan-blue-red. From Sankey et al. (2007).

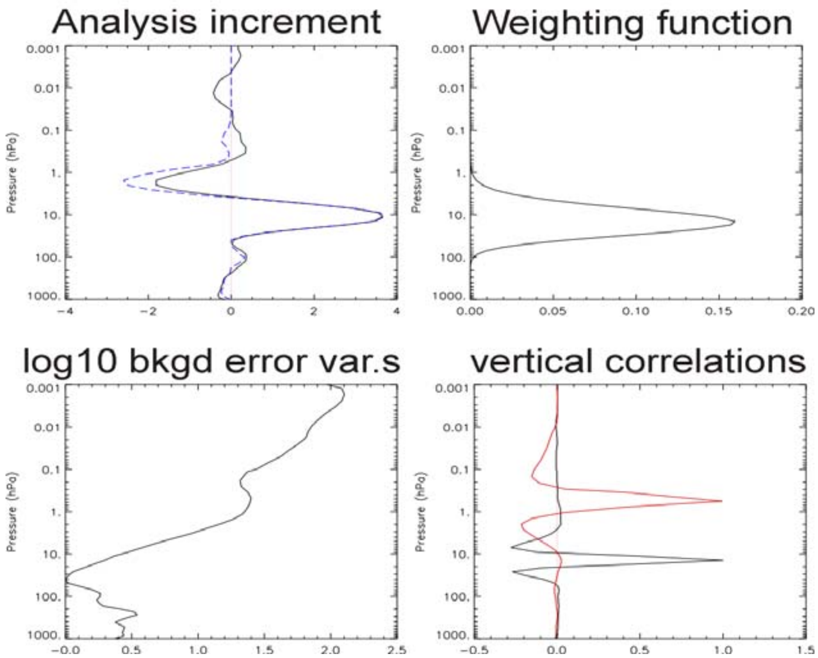

Figure 5: A 1-D assimilation of AMSU channel 11. Top left: Temperature analysis increments obtained when vertical correlations are unmodified (solid) or modified so that near zero values are exactly zero (dashed). Top right: weighting function for AMSU-A channel 11. Bottom left: log10 of temperature background error variance used with the CMAM-DAS. Bottom right: Two sample vertical correlation functions. From Polavarapu et al. (2005).

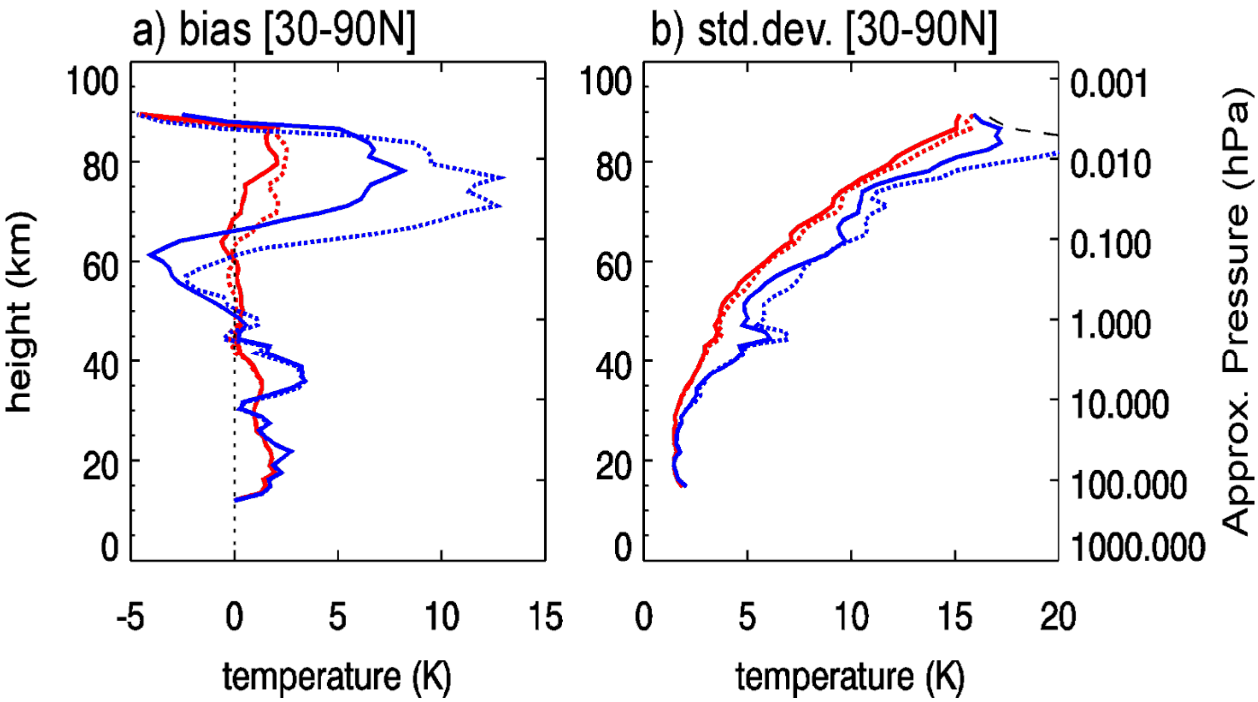

Figure 6: Fit of 6h temperature forecasts to SABER observations during 1-14 February 2006 using the CMAM data assimilation system. Assimilation cycles were run with parameterized gravity wave drag scheme (solid lines) or without it (dashed lines). Results from experiments in which SABER temperatures were assimilated are shown in red while those from experiments that did not assimilate those measurements are shown in blue. Panel (a) shows the bias from these 4 experiments while panel (b) shows the standard deviation for the northern hemisphere high latitudes. From Ren et al. (2011).