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Combining Data from the Distributed GRUAN Site Lauder-Invercargill, New Zealand, to Provide a Site Atmospheric State Best Estimate of Temperature

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Abstract. A Site Atmospheric State Best Estimate (SASBE) of the temperature profile above the GCOS (Global Climate Observing System) Reference Upper-Air Network (GRUAN) site at Lauder, New Zealand, has been developed. Data from multiple sources are combined within the SASBE to generate a high temporal resolution data set that includes an estimate of the uncertainty on every value.

The SASBE has been developed to enhance the value of measurements made at the distributed GRUAN site at Lauder and Invercargill (about 180 km apart), and to demonstrate a methodology which can be adapted to other distributed sites. Within GRUAN, a distributed site consists of a cluster of instruments at different locations.

The temperature SASBE combines measurements from radiosondes and automatic weather stations at Lauder and Invercargill, and ERA5 reanalysis, which is used to calculate a diurnal temperature cycle to which the SASBE converges in the absence of any measurements.

The SASBE provides hourly temperature profiles at 16 pressure levels between the surface and 10 hPa for the years 1997 to 2012. Every temperature value has an associated uncertainty which is calculated by propagating the measurement uncertainties, the ERA5 ensemble SDs, and the ERA5 representativeness uncertainty through the retrieval chain. The SASBE has been long-term archived and is identified using the following digital object identifier (doi): doi:10.5281/zenodo.1195779

The study demonstrates a method to combine data collected at distributed sites. The resulting best-estimate temperature data product for Lauder is expected to be valuable for satellite and model validation as measurements of atmospheric essential climate variables are sparse in the Southern Hemisphere. The SASBE could, for example, be used to constrain a radiative transfer model to provide top-of-the-atmosphere radiances with traceable uncertainty estimates.

1 Introduction

Measurements of the upper-air are essential for atmospheric research and weather forecasts. While high vertical resolution temperature profiles can be retrieved from space-based instruments, these retrievals require validation, which is typically done

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by comparison with ground-based or *in situ* measurements. Ground-based techniques to observe upper-air temperatures include lidar and microwave radiometer, while *in situ* measurements are typically made using balloon-borne radiosondes. While radiosondes provide vertically highly-resolved profiles of temperature, pressure and humidity, they are only used at about 800 upper-air sites worldwide (Ingleby, 2017), which typically launch two sondes per day. Given the limited spatio-temporal sampling of the radiosonde measurements, their use for satellite validation can be challenging as the number of collocations within a given time interval and distance is small (see e.g. Calbet, 2016). However, if measurements from different instruments, or from collocated sites, can be combined in a best-estimate data product, the value of those measurements can be enhanced.

Site Atmospheric State Best Estimates (SASBEs; Tobin et al., 2006) combine measurements from multiple instruments to create a vertically-resolved, high temporal resolution time series of an atmospheric essential climate variable (ECV; GCOS-200, 2016; Bojinski et al., 2014) above a site. SASBEs aim to encompass all suitable knowledge of the state of the target variable at the specific site and include an estimate of the uncertainty on each value therewith satisfying the requirements of GCOS-170 (2013). Tobin et al. (2006) developed a SASBE for the Atmospheric Radiation Measurement (ARM) site Southern Great Plains[1], which was used to validate retrievals of temperature and water vapour from the Atmospheric Infrared Sounder (AIRS; Aumann et al., 2003). Maillard Barras et al. (2015) present a methodology to combine *in situ* ozonesonde and space-based microwave radiometer measurements from SOMORA into an ozone SASBE. The authors found improved agreement between the ozone SASBE and the Microwave Limb Sounder (AURA/MLS) in comparison to the agreement with the operational SOMORA retrieval which does not include ozonesonde profiles.

The combination of measurements from different sensors with ancillary information in a SASBE, enhances the information content of available observations. Furthermore, it can simplify the use of observations if the SASBE is provided in a well-documented open-access database.

As upper-air measurements in the Southern Hemisphere are especially sparse, it is essential to exploit all available observations. A well-equipped atmospheric measurements site, operated by the New Zealand National Institute of Water and Atmospheric Research (NIWA), is based at Lauder on the South Island of New Zealand. This site is part of the GCOS[2] Reference Upper-Air Network (GRUAN; GCOS-112, 2007), which was established to fill the need for reference-quality measurements of upper-air ECVs. Bodeker et al. (2016) document the development of GRUAN over the first ten years after its establishment; a governance structure is in place, 24 sites have joined the network as of 2016, and a first reference-quality data product, accounting for all known biases, and including a traceable uncertainty estimate, is publicly available (see Dirksen et al., 2014).

Within GRUAN, a cluster of instruments at different locations can be operated as a distributed site. If the measurements made at one location are used to estimate measurements made elsewhere, the uncertainty estimates on the estimated measurements must include the original measurement uncertainty plus the additional uncertainty induced by the transfer algorithm (GCOS-170, 2013). A method to enhance the value of a distributed GRUAN site by combining measurements from distributed instruments is presented here. Measurements made at Invercargill (46.413° S, 168.3173° E, 1 m) are used as predictors of the temperatures above Lauder (45.0383° S, 169.6843° E, 370 m) and, as required, the uncertainty added by the transfer algorithm

[1]the site has since joined GRUAN
[2]Global Climate Observing System

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is calculated and included in the best-estimate of the temperature. GRUAN is also setting new standards regarding the careful documentation of data sets, i.e. every GRUAN data product has an accompanying peer-reviewed publication describing the bias correction, retrieval steps and uncertainty components. Following GRUAN's tenets, this paper documents a method to create a temperature SASBE for Lauder, New Zealand. This SASBE will be published in the PANGAEA archive with the digital object identifier.

The temperature SASBE presented here combines measurements performed at the distributed GRUAN site Lauder and Invercargill both based in the lower South Island of New Zealand. The SASBE comprises hourly temperature profiles above Lauder and associated uncertainty estimates at 16 vertical levels, i.e. surface, 925 hPa, 850 hPa, 700 hPa, 500 hPa, 400 hPa, 300 hPa, 250 hPa, 200 hPa, 150 hPa, 100 hPa, 70 hPa, 50 hPa, 30 hPa, 20 hPa, and 10 hPa. The value of the upper-air observations is enhanced by (i) considerable improvement of the temporal resolution, (ii) the availability of an uncertainty estimate with every temperature value, and (iii) better documentation of the data set.

This paper presents the observational data sets used herein, followed by a detailed description of the SASBE methodology used. The SASBE is presented in Section 4 and the paper concludes with a discussion outlining possible applications for the temperature SASBE at Lauder.

2 Observational Data and Reanalysis

The temperature SASBE combines radiosonde and automatic weather station data collected at Lauder and Invercargill. These measurements are supplemented with ERA5 reanalysis (Hersbach and Dee, 2016) which are used to provide an estimate of the diurnal temperature cycle above the sites. The atmospheric research facility at Lauder is operated by NIWA and the operational measurement site at Invercargill is run by the New Zealand MetService. Lauder is a certified GRUAN site which also includes radiosonde profiles from Invercargill in its data stream, based on the concept of a distributed site. The radiosonde data used in the SASBE described here were not GRUAN processed as the time frame used here was prior to the availability of GRUAN profiles for Lauder. Nonetheless, the purpose if this paper is to demonstrate the construction of a SASBE for a GRUAN site for implementation across GRUAN. Lack of GRUAN data for this demonstration in no way compromises the validity of the method. Within this study, basic estimates of the 1-σ uncertainty for radiosonde temperatures are used. If available, traceable uncertainty estimates should be used instead, such as those provided with the GRUAN radiosonde data product.

The ERA5 reanalysis is the fifth generation of atmospheric reanalysis produced by the European Centre for Medium-Range Weather Forecasts (ECMWF). The ERA5 data are used in this study to provide diurnal temperature cycles above Lauder and Invercargill from which anomalies can be calculated. ERA5 reanalysis data for the years 2010 to 2017 are used here as this was the period of data available at the beginning of 2018. Eventually, ERA5 will be available from 1950 onwards and monthly updates with a maximum latency of three months are planned. ERA5 has an hourly temporal resolution, a 31 km horizontal grid worldwide with 137 vertical levels up to 0.01 hPa. It is the first reanalysis which includes uncertainties calculated by running a 10-member ensemble of data assimilations at 62 km resolution with 3-hourly output. The temperature and its uncertainty are interpolated to the location of the Lauder and Invercargill upper-air sites. Additional temporal interpolation is required to obtain uncertainty estimates on the hourly ERA5 temperatures.

To clarify the sources of the data and the various identification numbers for the stations, Table 1 summarises the data sources, while Table 2 provides the station details.

Dataset	Source	Available at
Lauder radiosonde	Network for the Detection of Atmospheric Composition Change	ftp://ftp.cpc.ncep.noaa.gov/ndacc/station/lauder/
Lauder AWS	New Zealand's National Climate Database	https://cliflo.niwa.co.nz/
Invercargill radiosonde	MetService; New Zealand's National Climate Database	https://cliflo.niwa.co.nz/
Invercargill AWS	New Zealand's National Climate Database	https://cliflo.niwa.co.nz/
ERA5 reanalysis	ECMWF Copernicus Climate Change Service	https://climate.copernicus.eu/products/climate-reanalysis

Table 1. The data sets used. For those data sets available in New Zealand's National Climate Database, Table 2 gives the Agent number and Network number which are required to identify the site. The Invercargill radiosonde measurements are obtained from two sources, (i) the New Zealand's Climate Database (low resolution), and (ii) as high resolution profiles in the original Vaisala output format (MetService). The high resolution Vaisala files, which also include a range of metadata, have been processed into netCDF files (Bruno Kinoshita, personal communication) and are used for the years they are available. AWS abbreviates automatic weather station.

Station	WMO ID	Cliflo Identifiers	OSCAR Entry
Lauder	93817		https://oscar.wmo.int/surface/index.html#/search/station/stationReportDetails/12986
Lauder AWS		Agent 5535, Network I59065	https://oscar.wmo.int/surface/index.html#/search/station/stationReportDetails/12986
Invercargill	93844	Agent: 5814, Network: I68433	https://oscar.wmo.int/surface/index.html#/search/station/stationReportDetails/12991
Invercargill AWS	93845	Agent: 12444, Network: I68437	https://oscar.wmo.int/surface/index.html#/search/station/stationReportDetails/12992

Table 2. Station details for Lauder and Invercargill, including the World Meteorological Organization (WMO) station identifier (ID). The Agent and Network number are required to identify the station in New Zealand's National Climate Database. The Observing Systems Capability Analysis and Review (OSCAR) Tool is WMO's official repository of metadata on surface-based observations.

3 Methodology

The availability of upper-air measurements is limited, especially in the Southern Hemisphere. Therefore, combining those observations available with ancillary information in a SASBE will enhance the value of the upper-air record. The temperature SASBE presented here is aiming to combine all available knowledge about the temperature profile at the lower South Island of New Zealand in a temperature SASBE for Lauder, located centrally within the lower South Island. One source of knowledge about the temperatures above Lauder is the ERA5 reanalysis which is used to calculate a diurnal temperature cycle. This diurnal cycle builds the foundation for the SASBE presented here, i.e. the SASBE converges towards the ERA5 diurnal cycle in the absence of any other sources of data. However, the upper-air site at Lauder, New Zealand, performs weekly radiosondes launches. The temperature anomaly of the radiosonde measurement with respect to the ERA5 diurnal cycle is calculated

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and, around the launch time of the radiosonde, the temperature SASBE diverts from the diurnal cycle towards the observed temperature. At the exact time of the measurement, the SASBE adapts the measured value, and with further time difference to the measurement relax back to the diurnal cycle. The persistence (autocorrelation) of temperature anomalies can be used to determine how fast the SASBE converges towards the diurnal cycle. At the exact time of the radiosonde measurement, the autocorrelation function is 1, i.e. the measurement is perfectly correlated with itself. With further time difference the autocorrelation decreases and the SASBE converges towards the diurnal cycle.

While the upper-air research site in Lauder has a wide range of instruments, the temperature profile is only measured once weekly with radiosondes. Fortunately, about 180 km southwest of Lauder, the operational upper-air site at Invercargill measures the temperature profile twice daily. While the absolute temperatures above Lauder and Invercargill might differ, the temperature anomalies are well-correlated (see Section 3.1.2). Therefore, the Invercargill temperature anomalies with respect to the ERA5 diurnal cycle may be used to infer temperature anomalies above Lauder. Because these inferred anomalies provide knowledge about the temperature above Lauder they can be integrated into the SASBE to induce excursions from the diurnal cycle. As for the Lauder radiosonde anomalies, their influence should decrease with further time distance from the measurement time.

Within the SASBE, the inferred temperature anomalies should have less weight than the measurements made at Lauder, i.e. they should be punished for originating from Invercargill, and should furthermore not be granted any weight at the time of a Lauder measurement. This is achieved by including the weight ϕ which is again based on the autocorrelation of temperature anomalies at Lauder. At any given time t, ϕ is the value of the autocorrelation function for the time difference to the closest Lauder launch time (see Fig. 1).

The concept of the SASBE is schematically shown in Fig. 1. The details of the preparation of the individual components and the combination of them in the temperature SASBE is described in the following sections. In the following all calculations are presented for one pressure level only.

3.1 Preparing the individual components of the SASBE

3.1.1 Calculating the upper-air diurnal temperature cycle above Lauder and Invercargill

The diurnal temperature cycle above Lauder and Invercargill is calculated from the hourly ERA5 reanalysis by fitting four Fourier pairs for the hour of the day (h), and four Fourier pairs for the day of the year (d). Bilinear interpolation in space is used to retrieve ERA5 reanalysis temperature at the exact location of the Lauder and Invercargill upper-air sites, respectively.

$$T_{Diur} = \zeta_0 + \sum_{i=1}^{4} \zeta_{i\cdot 2-1} \cdot \sin\left(\frac{i \cdot 2\pi h}{24}\right) + \zeta_{i\cdot 2} \cdot \cos\left(\frac{i \cdot 2\pi h}{24}\right) \tag{1}$$

where all ζs are expanded in a Fourier series with 4 pairs to account for the annual cycle, i.e.:

$$\zeta_i = \zeta_{i_0} + \sum_{j=1}^{4} \zeta_{i_{j\cdot 2-1}} \cdot \sin\left(\frac{j \cdot 2\pi d}{365.25}\right) + \zeta_{i_{j\cdot 2}} \cdot \cos\left(\frac{j \cdot 2\pi d}{365.25}\right) \tag{2}$$

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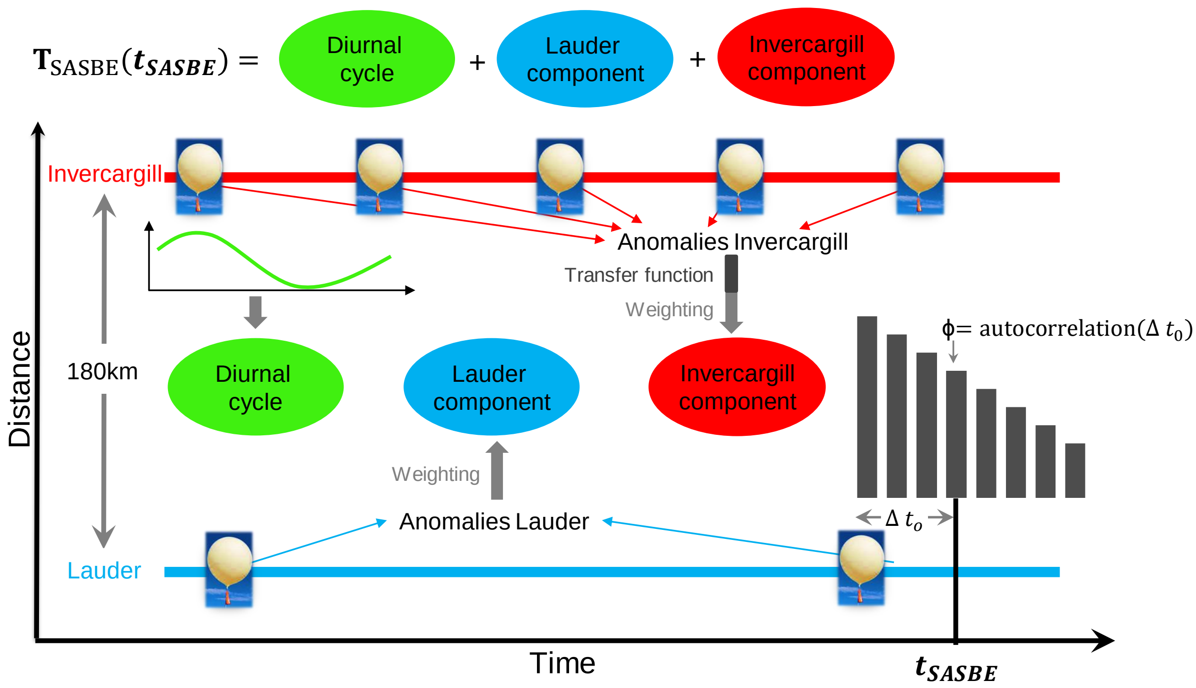

Figure 1. Schematic explanation of the temperature SASBE and its components. The diurnal cycle is determined from ERA5 as described in Section 3.1.1. To calculate the Invercargill component, a transfer function (see Sect. 3.1.2) and some weighting is applied to the temperature anomalies at Invercargill. To calculate the Lauder component, the temperature anomalies are weighted (see Sect. 3.2). Also shown is the weight ϕ, which is determined by the value of the autocorrelation function for the time difference between t and the closest Lauder radiosonde launch.

This leads to $9 \cdot 9 = 81$ fit coefficient which are estimated for Lauder and for Invercargill and can be used to calculate a climatological mean diurnal temperature cycle for every day of the year, with a smooth transition from day to day.

The 1-σ uncertainty on the regression coefficients is calculated based on the method described in Bodeker and Kremser (2015), using the 3-hourly 10-member ensemble SDs provided within ERA5, interpolated to an hourly resolution. The fitting uncertainty on the diurnal cycle is calculated as:

$$\sigma_{fit} = \sqrt{\sum_{i=1}^{81} \sigma^2_{\zeta_i} \left(\frac{\partial T_{Diur}}{\partial \zeta_i} \right)^2} \tag{3}$$

This uncertainty indicates how good the regression model fits the 8 years of hourly reanalysis data. However, this uncertainty does not indicate how representative the ERA5 diurnal cycle is for the temperatures measured above Lauder or Invercargill. Therefore, another uncertainty component, the representativeness uncertainty ($\sigma_{representativeness}$), is included and the uncertainty on the diurnal cycle is estimated as:

$$\sigma_{T_{Diur}} = \sqrt{\sigma^2_{fit} + \sigma^2_{representativeness}} \tag{4}$$

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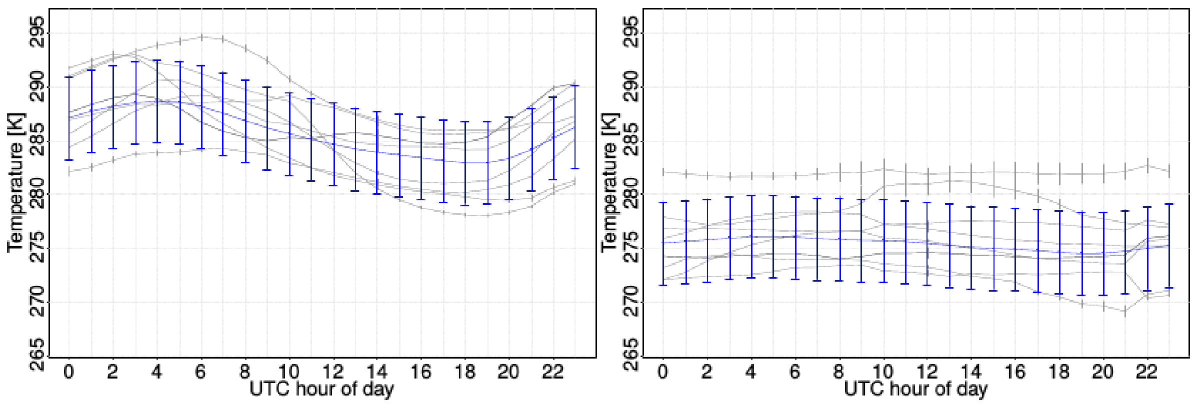
The representativeness uncertainty is estimated as the standard deviation of the differences between the radiosonde temperature and T_{Diur} for every available radiosonde launch at Lauder/Invercargill, respectively.

The fitted diurnal cycle with its associated uncertainty and the ERA5 temperatures at the respective day of the year are shown in Fig. 2 at 925 hPa for two selected days of the year. Depending on the site and the pressure level, the representativeness uncertainty reaches values from approximately 2.8 K to 5.6 K and dominates the uncertainty on the diurnal cycle.



(a) 1st day of year (b) 183rd day of year

Figure 2. Fitted diurnal cycle (blue) and ERA5 temperatures for two example days of the year from 2010 to 2016 (grey), at 925 hPa above Lauder. The ERA5 ensemble standard deviation is shown as vertical bars around the grey lines and the uncertainty on the fitted diurnal cycle is shown in the blue error bars.

3.1.2 Inferring temperature anomalies above Lauder from temperature measurements above Invercargill

While radiosondes are launched weekly at the research facility in Lauder, twice daily radiosonde observations are performed at the operational upper-air site in Invercargill. Hence, using radiosonde profiles from Invercargill to estimate the temperature above Lauder greatly increases the availability of data to be included in the SASBE. Using the Invercargill measurements as a proxy for the atmospheric state above Lauder demonstrates how data collected at distributed GRUAN sites can be combined.

Although the absolute temperature values at Lauder (inland) and Invercargill (coastal) are likely quite different, the temperature anomalies with respect to their respective diurnal cycles are correlated. For a maximum time difference between the Lauder and Invercargill radiosonde launch of 1.5 hours, the correlation of the anomalies is between $R = 0.69$ and $R = 0.92$, with a mean correlation of $R = 0.85$. This correlation of anomalies is exploited to estimate temperature anomalies above Lauder based on temperature profiles from radiosondes launched at Invercargill.

The temperature anomaly (T') with respect to the diurnal cycle is calculated from the radiosonde measurement and the diurnal cycle calculated at the respective site as $T'(t) = T_{RS}(t) - T_{Diur}(t)$. The 1-$\sigma$ uncertainty on the temperature anomalies is calculated as $\sigma_{T'(t)} = \sqrt{\sigma^2_{T_{RS}(t)} + \sigma^2_{T_{Diur}(t)}}$. When the separation in launch time between Lauder and Invercargill is less

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than 1.5 hours, the data are used to train a regression model (see Eq. (5)) that is applied to estimate temperature anomalies above Lauder from the temperature anomaly of a radiosonde launched from Invercargill.

Four basis functions are used in the regression, i.e. the offset term that accounts for the constant bias between Lauder and Invercargill (Term 1), the temperature anomaly above Invercargill (Term 2), the difference (always Invercargill minus Lauder) in the surface pressure (ΔSP, Term 3), and the difference in the surface temperature anomaly ($\Delta ST'$, Term 4).

$$\widehat{T}'_{Lau} = \underbrace{\gamma}_{\text{Term 1}} + \underbrace{\beta \cdot T'_{Inv}}_{\text{Term 2}} + \underbrace{\eta \cdot \Delta SP}_{\text{Term 3}} + \underbrace{\kappa \cdot \Delta ST'}_{\text{Term 4}} + \underbrace{\epsilon}_{\text{Term 5}} \tag{5}$$

γ, β, η, and κ are the regression coefficients and ϵ (Term 5) is the residual which cannot be explained with the regression model. Term 2 is expanded with a Fourier series, where θ is the wind direction at the respective pressure level above Invercargill.

$$\beta = \beta_0 + \beta_1 sin(2\pi\theta) + \beta_2 cos(2\pi\theta) + \beta_3 sin(4\pi\theta) + \beta_4 cos(4\pi\theta) \tag{6}$$

Including the Fourier pairs and normalising all basis functions (except γ) by subtracting their mean value leads to:

$$\widehat{T}'_{Lau} = \gamma + \beta_0 \cdot (T'_{Inv} - \overline{T'_{Inv}}) + \beta_1 \cdot \left(T'_{Inv}\sin(2\pi\theta) - \overline{T'_{Inv}\sin(2\pi\theta)}\right) + \beta_2 \cdot \left(T'_{Inv}\cos(2\pi\theta) - \overline{T'_{Inv}\cos(2\pi\theta)}\right) + \beta_3 \cdot \left(T'_{Inv}\sin(4\pi\theta) - \overline{T'_{Inv}\sin(4\pi\theta)}\right) + \beta_4 \cdot \left(T'_{Inv}\cos(4\pi\theta) - \overline{T'_{Inv}\cos(4\pi\theta)}\right) + \eta \cdot (\Delta SP - \overline{\Delta SP}) + \kappa \cdot (\Delta ST' - \overline{\Delta ST'}) + \epsilon \tag{7}$$

The overbar denotes the mean of the basis function. At 925 hPa the wind direction is not recorded in the input dataset and therefore a simplified regression model (see Eq. (8)), excluding the Fourier expansion is applied.

$$\widehat{T}'_{Lau} = \gamma + \beta \cdot (T'_{Inv} - \overline{T'_{Inv}}) + \eta \cdot (\Delta SP - \overline{\Delta SP}) + \kappa \cdot (\Delta ST' - \overline{\Delta ST'}) + \epsilon \tag{8}$$

The residuals (ϵ) are plotted in Fig. 3 for varying maximum time differences $\Delta t_{regression}$ between the Lauder and Invercargill launch times. Decreasing the time difference, in general, decreases the residuals at most levels slightly. However, at 30 hPa the regression model trained on collocations from within 6 hours leads to the smallest residuals. Further analysis shows that the correlation between Lauder and Invercargill temperature anomalies is larger for a maximum time difference of 3 hours ($R = 0.78$) and 6 hours ($R = 0.76$) than for 1.5 hours ($R = 0.69$). The sample size for collocations within 1.5 hours is small and contains some large differences between the Lauder and Invercargill anomalies. The increased persistence in the stratosphere, combined with the small sample size, leads to a larger correlation when expanding the time difference. Since the maximum time difference of 1.5 hours minimizes the residuals at most pressure levels, it is used as $\Delta t_{regression}$. This choice is ultimately an expert decision and further options could be tested to ensure an optimal choice is made by, e.g. different maximum time differences could be applied at each pressure level. For the purpose of demonstrating this methodology, a constant value has been selected with the expectation that the results would not change significantly for reasonable variation of $\Delta t_{regression}$. At the surface, plotted at 965 hPa in Fig. 3 for convenience, the residuals are zero based on the availability of hourly surface data. The calculation of the residuals at the surface level provides a test of the regression model. Within the SASBE, the measurements of the automatic weather station are used at the surface level.

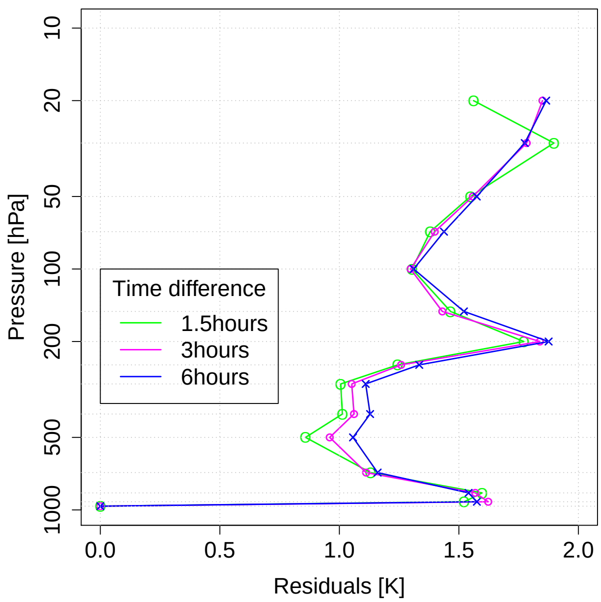

Figure 3. Temperature residuals for the regression model described in Eq. 5. The regression model is trained with three different datasets containing Lauder and Invercargill radiosonde measurements with launch times having a maximum time difference of 1.5 hours (green, 324 collocations), 3 hours (pink, 646 collocations), and 6 hours (blue, 879 collocations).

The uncertainties on the Invercargill and Lauder measurements and anomalies, and on the regression coefficients, are propagated through Eq. (7) and Eq. (8), following standard error propagation rules (e.g. Bevington and Robinson, 2003). Uncertainties of different variables are assumed to be uncorrelated since the error covariance matrices are unknown. The uncertainty on the estimated Lauder temperature anomaly is then calculated including the partial derivatives with respect to all variables. The uncertainty for the full regression model is shown in Eq. (9) and a simplified version is applied at the 925 hPa level.

$$\sigma_{\widehat{T}'_{Lau}} = \sqrt{\begin{aligned}&\sigma_\gamma^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\gamma}\right)^2+\sigma_{\beta_0}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\beta_0}\right)^2+\sigma_{\beta_1}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\beta_1}\right)^2+\sigma_{\beta_2}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\beta_2}\right)^2+\sigma_{\beta_3}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\beta_3}\right)^2\\&+\sigma_{\beta_4}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\beta_4}\right)^2+\sigma_{T'_{Inv}}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial T'_{Inv}}\right)^2+\sigma_\theta^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\theta}\right)^2+\sigma_\eta^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\eta}\right)^2\\&+\sigma_{\Delta SP}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\Delta SP}\right)^2+\sigma_\kappa^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\kappa}\right)^2+\sigma_{\Delta ST'}^2\left(\frac{\partial\widehat{T}'_{Lau}}{\partial\Delta ST'}\right)^2\end{aligned}} \tag{9}$$

Instrument and variable	Uncertainty
Automatic weather station temperature	0.2 K
Automatic weather station pressure sensor	0.5 hPa
Vaisala RS92 temperature	0.25 K
Vaisala RS80 temperature	0.5 K
Vaisala RS80/RS92 wind direction	3°

Table 3. Estimates of uncertainties associated with the measurements used in the SASBE.

As a result, every estimated Lauder temperature anomaly has an individual uncertainty estimate which includes the uncertainty on the measurements and Invercargill anomaly, as well as the uncertainty introduced by the regression model.

Unfortunately, there appears to be considerable uncertainty about uncertainties associated with radiosonde measurements. With the exception of the GRUAN radiosonde data product, which is corrected for all known biases, and provides an uncertainty best-estimate on every value, the different terminology used by different authors of publications using radiosonde measurements leads to confusion. Furthermore, the uncertainty estimates are not traceable and are commonly provided as a general estimate, rather than as an individual value for each measurement.

For the purpose of this temperature SASBE, rather than unravelling the different estimates of uncertainties for the same instruments, we set the 1-σ uncertainty to the values given in Table 3. The exact values of the uncertainties might differ from these estimates, but this is irrelevant to the mechanics of the methodology and to the temperature estimate itself, but could inflate or deflate the uncertainty bars. The 1-σ temperature uncertainty for the Vaisala RS92 is set to 0.25 K based on Vaisala (2013), which is in agreement with Steinbrecht et al. (2008). This uncertainty is doubled for the Vaisala RS80, which is the older radiosonde model manufactured by Vaisala. The uncertainty on the wind direction measured with the RS92 and RS80 instruments is estimated as 3° at the 1-σ level. The 1-σ uncertainties for the automatic weather stations at Lauder and Invercargill are set to 0.2 K and 0.5 hPa for temperature and pressure respectively.

3.2 Combining the individual components of the SASBE

The temperature SASBE for Lauder is calculated from the different components presented in the Sections 3.1.1 and 3.1.2. The diurnal temperature T_{Diur} builds the foundation for the SASBE. Estimates of the temperature anomaly above Lauder ($\widehat{T'}_{Lau}$) inferred from radiosonde launches at Invercargill are available 12-hourly (the $\widehat{\ }$ symbol is used for inferred quantities). The Lauder temperature anomalies (T'_{Lau}) are available once weekly.

At any time t the SASBE temperature $T_{SASBE}(t)$ may be influenced by several radiosonde measurements made at Lauder and Invercargill (the maximum time difference of measurements influencing the temperature SASBE is set to 30 days). Weighting determines how much weight is given to a certain temperature anomaly. The weight ϕ determines how much influence the Lauder and Invercargill measurements have. At the time of a radiosonde measurement at Lauder $\phi = 1$ which implies that the entire weight is given to the Lauder temperature anomalies. With further time difference from the closest launch at Lauder (Δt_0), ϕ decreases based on the autocorrelation function (acf). Autocorrelation is the correlation of a time series with a lagged

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(delayed) version of itself (Wilks, 2011). Here ϕ is calculated from ERA5 temperature anomalies with respect to the ERA5 diurnal cycle as:

$$\phi = acf(\Delta t_0), \quad \text{if} \quad \phi < 0.5 \quad => \quad \phi = 0.5 \tag{10}$$

The lowest value of ϕ is restricted to 0.5 to minimize the maximum weight given to the Invercargill component. The choice of this threshold is ultimately an expert decision. A quantitative comparison of different values for ϕ could be made by analysing the effects of different lower thresholds for ϕ during the period of an extensive measurement campaign.

Furthermore, another weight is required to determine how much influence any individual temperature anomaly from Lauder or Invercargill has. These weights are taking into account the time difference (Δt_i,Δt_j) of an individual launch to the time for which the SASBE is calculated. For Lauder temperature anomalies these weights, w_i, are calculated as:

$$w_i = \frac{1}{\Delta t_i^2} \cdot \frac{1}{\sum_{i=1}^{N} \Delta t_i^2} \tag{11}$$

from the N Lauder launch times t_i. For the estimated anomalies inferred from Invercargill measurement these weights, w_j are calculated from the M Invercargill launch times t_j as:

$$w_j = \frac{1}{\Delta t_j^2} \cdot \frac{1}{\sum_{i=1}^{N} \frac{1}{\Delta t_i^2} + \sum_{i=1}^{M} \frac{1}{\Delta t_j^2}} \tag{12}$$

The weights for Lauder anomalies are normalized with the sum over all Lauder weights and the anomalies implied from measurements in Invercargill are normalized with the sum of their own weight plus the sum of the Lauder weights. This insures that the inferred temperatures have limited influence.

If a positive temperature anomaly was determined from a radiosonde measurement at a given time, there is some confidence that the anomaly would still be positive in the hours before and afterwards. However, as a best-estimate, the temperature anomaly a few hours after the measurement may conservatively be assumed lower than at the time of the measurement. This effect is included into the SASBE by attenuating the temperature anomaly with the autocorrelation function. This attenuated anomaly T^* is calculated as:

$$T^*_{i_{Lau}}(t) = T'_{Lau}(t_i) \cdot acf(\Delta t_i) \tag{13}$$

with $\Delta t_i = |t - t_i|$ for Lauder. The attenuated estimate of anomalies above Lauder inferred from Invercargill radiosonde measurements is calculated as:

$$\widehat{T}^*_{j_{Lau}}(t) = \widehat{T}'_{Lau}(t_j) \cdot acf(\Delta t_j) \tag{14}$$

where $\Delta t_j = |t - t_j|$.

Taking the different weights and the decaying temperature anomalies into account, the SASBE temperature is calculated as:

$$T_{SASBE}(t) = \underbrace{T_{Diur}(t)}_{\text{Diurnal cycle}} + \underbrace{\sum_{i=1}^{N} \phi \cdot w_i \cdot T^*_{i_{Lau}}(t)}_{\text{Lauder component}} + \underbrace{\sum_{j=1}^{M} (1-\phi) \cdot w_j \cdot \widehat{T}^*_{j_{Lau}}(t)}_{\text{Invercargill component}} \tag{15}$$

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As the SASBE requires an uncertainty estimate on every temperature value, the uncertainties are propagated through Eq. (15). In a first step, Eq. (15) is rewritten, by expanding the terms for the weighted temperature anomaly, as:

$$T_{SASBE}(t) = T_{Diur}(t) + \sum_{i=1}^{N} \phi \cdot w_i \cdot acf(\Delta t_i) \cdot [T_{RS_{Lau}}(t_i) - T_{Diur}(t_i)]$$
$$+ \sum_{j=1}^{M} (1-\phi) \cdot w_j \cdot acf(\Delta t_j) \cdot \left[\widehat{T}_{RS_{Lau}}(t_j) - T_{Diur}(t_j)\right] \tag{16}$$

where $T_{RS_{Lau}}$ is the temperature measured with a radiosonde above Lauder and $\widehat{T}_{RS_{Lau}}$ is a regression model estimated (see Sect.3.1.2) temperature above Lauder based on the Invercargill radiosonde flight and the diurnal temperature cycle above Lauder. The uncertainty on the temperature SASBE is calculated from the following components:

$$\sigma_{T_{SASBE}(t)} = \sqrt{\sigma^2_{T_{Diur}} \left(\frac{\partial T_{SASBE}}{\partial T_{Diur}}\right)^2 + \sigma^2_{T_{RS_{Lau}}} \left(\frac{\partial T_{SASBE}}{\partial T_{RS_{Lau}}}\right)^2 + \sigma^2_{\widehat{T}_{RS_{Lau}}} \left(\frac{\partial T_{SASBE}}{\partial \widehat{T}_{RS_{Lau}}}\right)^2} \tag{17}$$

with the partial derivatives:

$$\frac{\partial T_{SASBE}}{\partial T_{Diur}} = 1 - \sum_{i=1}^{N} \phi \cdot w_i \cdot acf(\Delta t_i) - \sum_{j=1}^{M} (1-\phi) \cdot w_j \cdot acf(\Delta t_j) \tag{18}$$

$$\frac{\partial T_{SASBE}}{\partial T_{RS_{Lau}}} = \sum_{i=1}^{N} \phi \cdot w_i \cdot acf(\Delta t_i) \tag{19}$$

and

$$\frac{\partial T_{SASBE}}{\widehat{T}_{\partial RS_{Lau}}} = \sum_{j=1}^{M} (1-\phi) \cdot w_j \cdot acf(\Delta t_j) \tag{20}$$

respectively, and therefore:

$$\sigma_{T_{SASBE}(t)} = \sqrt{\sigma^2_{T_{Diur}} \left(1 - \sum_{i=1}^{N} \phi \cdot w_i \cdot acf(\Delta t_i) - \sum_{j=1}^{M} (1-\phi) \cdot w_j \cdot acf(\Delta t_j)\right)^2}$$
$$\overline{+ \sigma^2_{T_{RS_{Lau}}} \left(\sum_{i=1}^{N} \phi \cdot w_{i_{Lau}} \cdot acf(\Delta t_i)\right)^2 + \sigma^2_{\widehat{T}_{RS_{Lau}}} \left(\sum_{j=1}^{M} (1-\phi) \cdot w_j \cdot acf(\Delta t_j)\right)^2} \tag{21}$$

The uncertainty on the estimated RS temperature ($\widehat{T}_{RS_{Lau}}$) is estimated as:

$$\sigma_{\widehat{T}_{RS_{Lau}}} = \sqrt{\sigma^2_{T_{RS_{Inv}}} \left(\frac{\partial \widehat{T}_{RS_{Lau}}}{\partial T_{RS_{Inv}}}\right)^2 + \sigma^2_{T_{Diur_{Lau}}} \left(\frac{\partial \widehat{T}_{RS_{Lau}}}{\partial T_{Diur_{Lau}}}\right)^2 + \sigma^2_{T_{Diur_{Inv}}} \left(\frac{\partial \widehat{T}_{RS_{Lau}}}{\partial T_{Diur_{Inv}}}\right)^2} \tag{22}$$

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Here, $\sigma_{T_{Diur_{Lau}}}$ and $\sigma_{T_{Diur_{Inv}}}$ include the uncertainty based on the fit only (see Eq. (3)), to avoid including the representativeness uncertainty multiple times in the SASBE.

The uncertainty on the best-estimate temperature ($\sigma_{T_{SASBE}(t)}$), at the 1-σ level, is calculated for every temperature value in the SASBE and is shown as black uncertainty bars in the top panels of Figs. 4-7.

4 Results

The temperature SASBE for Lauder is available in hourly resolution for 1997 to 2012 at 16 vertical levels. An estimate of the uncertainty is available with every temperature value. At the surface, the temperature SASBE consists of the measurements from the automatic weather station in Lauder. If no temperature or pressure measurement is available at a given time, the values are linearly interpolated if measurements are available within ±1 hour (temperature) or ±12 hours (pressure). In this study, the uncertainty added by the interpolation is not taken into account.

As an example, Figs. 4-7 show the hourly temperature SASBE at 925 hPa, and its individual components, for 6th to 9th December 2010, respectively. The panel (a) in each figure shows the SASBE temperature (black line) and its associated 1-σ uncertainty bars. Also shown is the diurnal cycle and its uncertainty (green), as well as the results of a denial study (red), which calculates a best-estimate of the temperature assuming that no radiosonde measurements are available at Lauder. At times when no radiosonde measurement above Lauder influences the temperature SASBE, the temperature of the denial study equals the temperature SASBE. Blue stars show the temperature measured with a radiosonde above Lauder, if available, and red stars show the temperature that is inferred from the Invercargill radiosondes by transferring the anomalies to Lauder using a regression model as described in Section 3.1.2. At times when a measurement is available above Lauder, the SASBE temperature is identical to the radiosonde measurement, as it receives the full weight, i.e. $\phi = 1$ (see panel (d)).

The panel (b) shows the uncertainty added by the individual components and the total uncertainty on the SASBE, i.e. the terms of Eq. (17). At the exact time of a Lauder radiosonde measurement, the uncertainty on the SASBE equals the radiosonde uncertainty, and increases with time away from a measurement at Lauder, as the other terms influence the SASBE and therefore increase the uncertainty.

Panel (c) shows the weighted contribution from the Lauder radiosonde anomalies $\left(\sum_{i=1}^{N} \phi \cdot w \cdot T^*_{i_{Lau}}(t)\right)$ in blue and the weighted contribution from the estimated Lauder anomalies $\left(\sum_{j=1}^{M} \phi \cdot w_j \cdot \widehat{T}^*_{j_{Lau}}(t)\right)$ in red.

The bottom panel shows the weights ϕ and $(1-\phi)$ which are given to the Lauder anomalies and estimated Lauder anomalies, respectively. Typically two radiosondes are launched daily from Invercargill at about 10 UTC and 22 UTC (as shown in Figs. 4 to 7), while typically one radiosonde is launched from Lauder each week, here visible in Fig. 5. Close to the time of the Lauder radiosonde launch, the uncertainty on the SASBE decreases as it is increasingly dominated by the radiosonde uncertainty.

It can further be seen in Fig. 5 that using the Invercargill measurements as a proxy for the temperature above Lauder is an improvement compared to using only *a priori*. This becomes obvious when comparing the differences between the SASBE and (i) denial study, and (ii) the diurnal cycle at the time of a Lauder radiosonde measurement. As the temperature of the denial study is closer to the SASBE than the diurnal cycle, including information from Invercargill would be beneficial at this

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instance. However, it can be questioned whether using estimates of temperature anomalies above Lauder which are based on measurements from Invercargill is generally superior to using the ERA5 diurnal cycle alone. Analysis of the normalizes squared residuals between the Lauder radiosonde measurements and (i) the diurnal cycle and (ii) the diurnal cycle plus temperature anomalies estimated using the regression model and the Invercargill radiosondes indicate that integrating measurements from Invercargill into the temperature SASBE for Lauder improves the SASBE (figures not shown here).

The results of this study indicate that radiosonde measurements from Invercargill, together with a transfer algorithm, add value to the temperature SASBE for Lauder. This is also reflected in the uncertainties on the SASBE temperature which decrease in the vicinity of a radiosonde measurement from Invercargill, which has been transferred to Lauder and is included into the SASBE. To transfer the information of radiosonde temperatures, the correlation of temperature anomalies between Lauder and Invercargill is exploited. While the SASBE presented here will not at all times give an accurate estimate of the true temperature, it is a best estimate of this unknown true value, which includes an estimate of the uncertainty to indicate the confidence that users of the SASBE should have in the temperature estimate at a given time.

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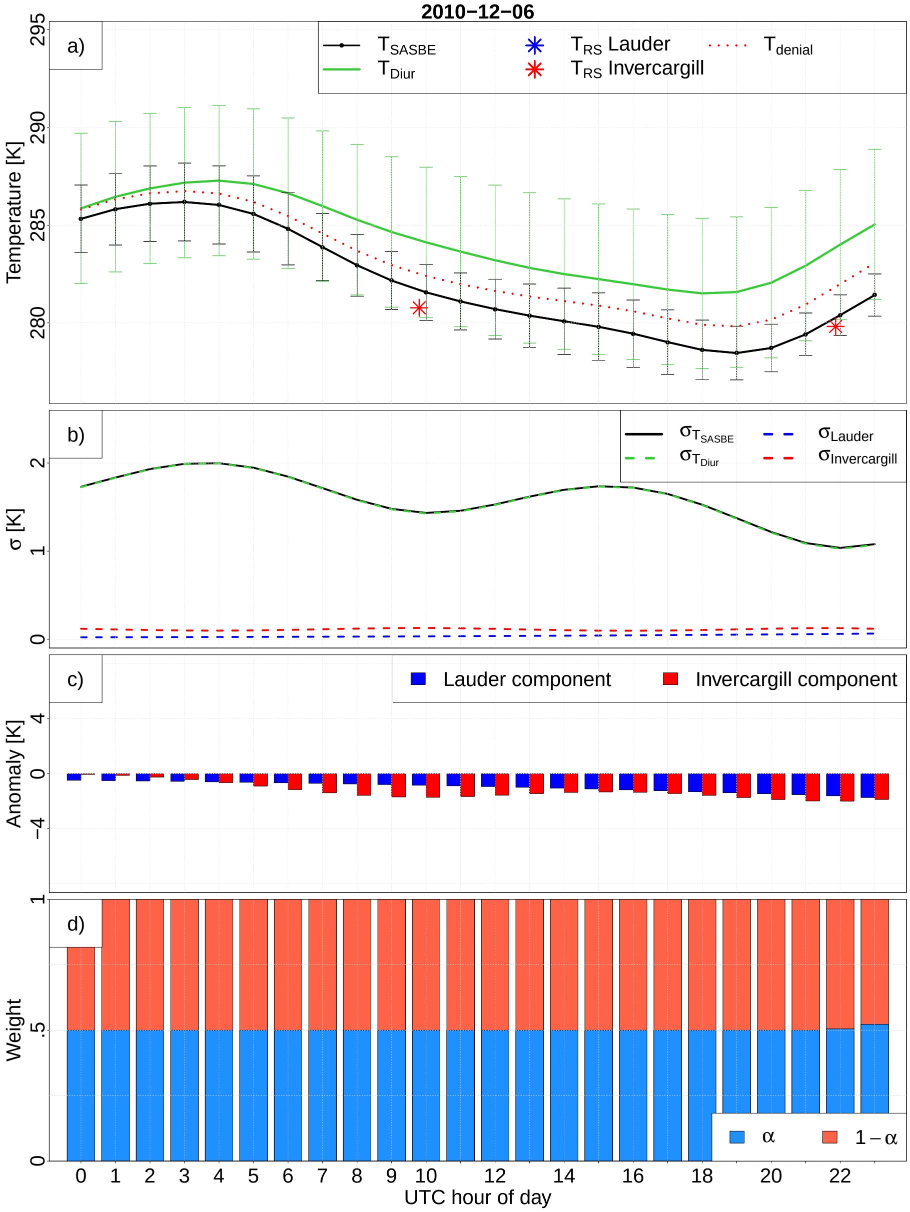

Figure 4. Temperature SASBE at 925 hPa and its individual components for the 6th December 2010. Top panel: Temperature SASBE (black line), diurnal cycle (green line), denial study (i.e. pretending no measurements exist at Lauder, dotted red line), and radiosonde temperature measurement if available (Invercargill: red star, Lauder: blue star; only shown on days when an observation is available). Second panel: uncertainty components from Eq. (17), i.e. uncertainty added by: the diurnal cycle (red), the Lauder radiosonde anomaly (blue), and the estimated Lauder anomaly (red). The combined uncertainty ($\sigma_{T_{SASBE}(t)}$) is shown as black line. Third panel: Weighted Lauder radiosonde temperature anomaly ($\sum_{i=1}^{N} \phi \cdot w \cdot T^{*}_{i_{Lau}}(t)$, blue bars) and weighted estimated Lauder temperature anomaly ($\sum_{j=1}^{M} \phi \cdot w_j \cdot \widehat{T}^{*}_{j_{Lau}}(t)$, red bars). Bottom panel: weights ϕ and $(1-\phi)$ which determine how much weight is given to the Lauder radiosonde temperature anomalies and estimated Lauder anomalies based on radiosonde measurements taken above Invercargill.

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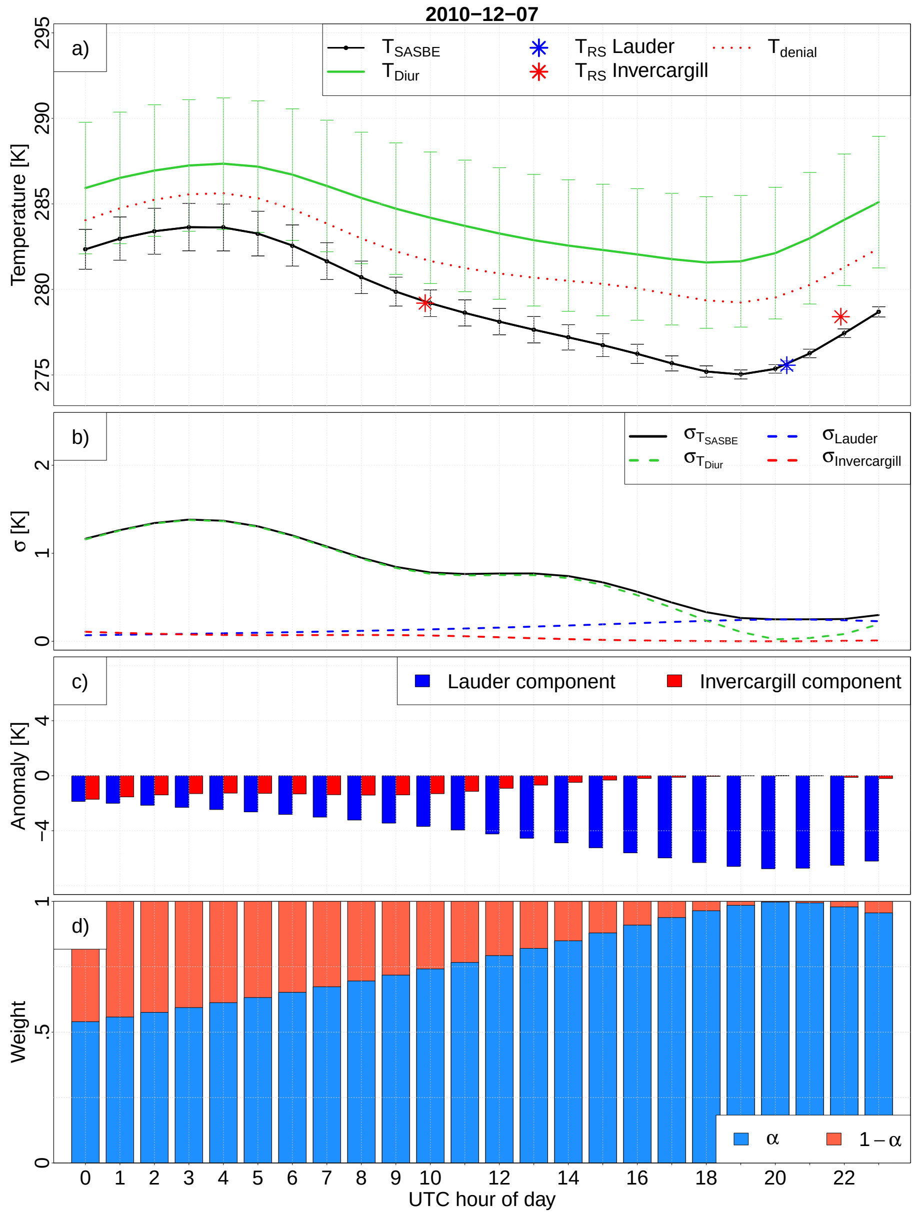

Figure 5. As Fig 4, but for the 7th December 2010.

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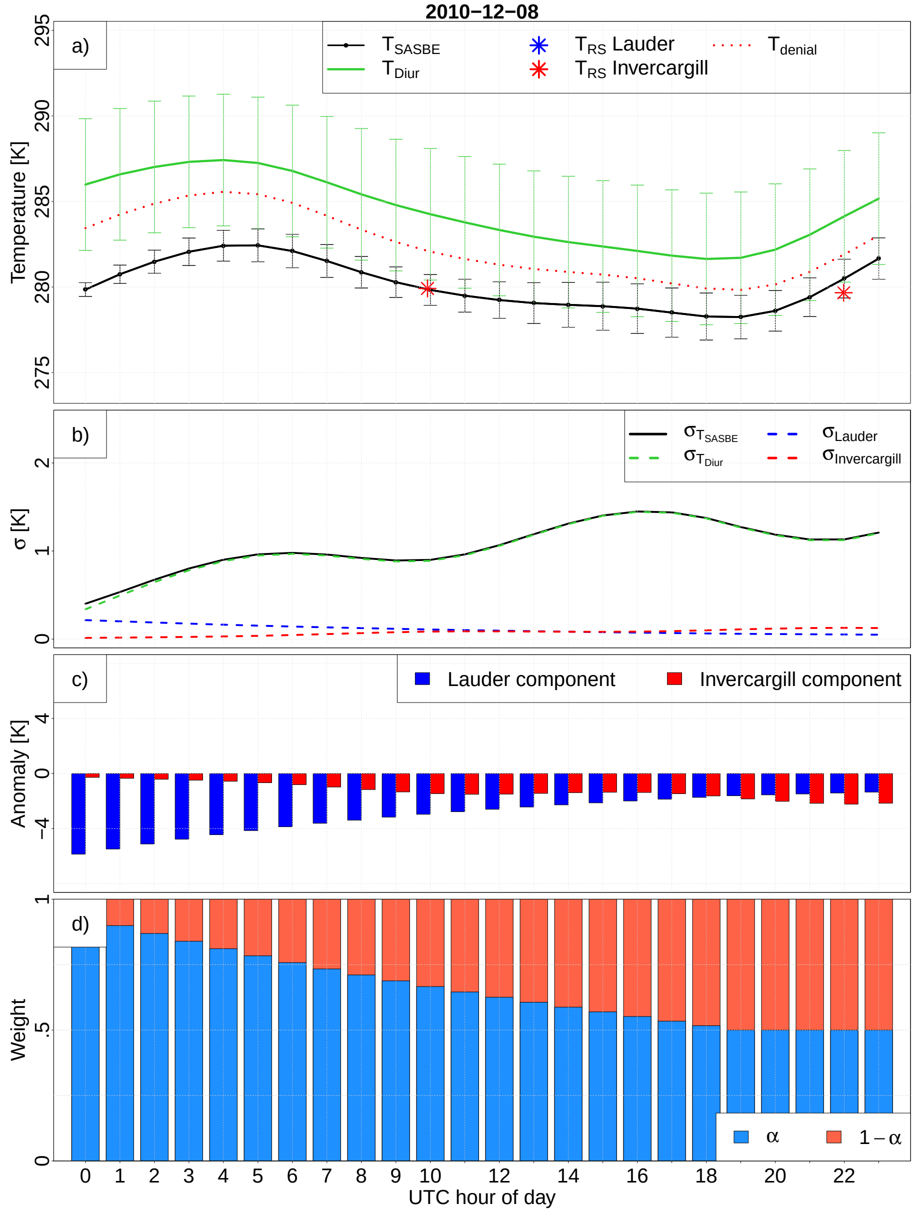

Figure 6. As Fig 4, but for the 8th December 2010.

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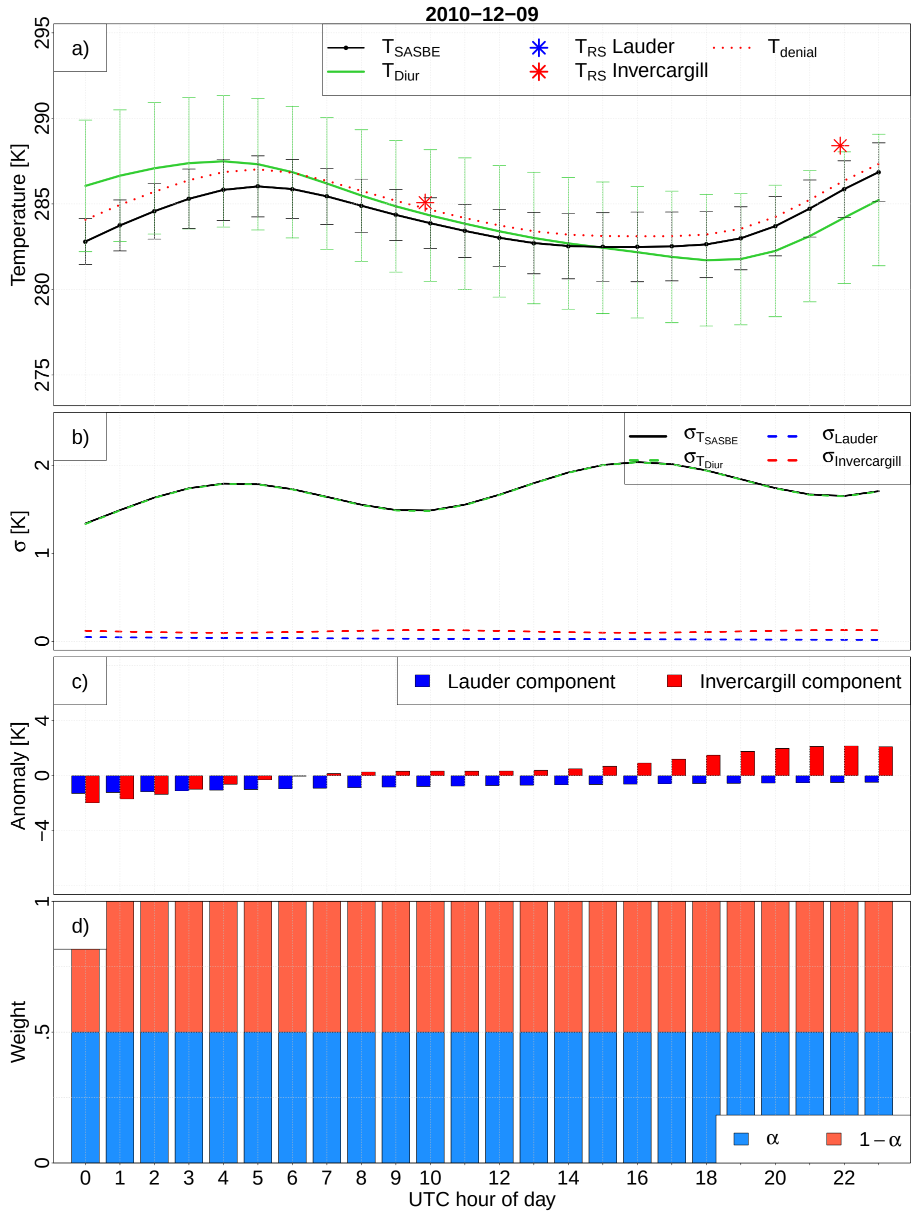

Figure 7. As Fig 4, but for the 9th December 2010.

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5 Conclusions

This study demonstrates a method to combine the temperature measurements made at a distributed upper-air site into a Site Atmospheric State Best Estimate (SASBE). Distributed sites within the context of GRUAN are clusters of instruments at different locations which collectively submit data to the GRUAN archive. Examples of such GRUAN sites are Cabauw/De Bilt, The Netherlands, Beltsville/Sterling, US, and Lauder/Invercargill, New Zealand. While the instrumentation might differ at other upper-air sites, the methodology described here can be adapted for other distributed sites.

Within the development of this data product, some pragmatic choices have been made. While other researchers might choose some parameters differently, the methodology itself remains unaffected. Parameters to be selected include the maximum separation in time used to choose data to train the regression model, and the maximum weight given to the estimated anomalies. Furthermore, different options for the calculation of the weights might be possible.

The new data product presented here, provides an hourly resolved best-estimate of the temperature above Lauder, New Zealand, at 16 vertical levels from the surface to 10 hPa. This SASBE combines radiosonde and automatic weather station measurements from Lauder and Invercargill with a diurnal cycle calculated from the new ERA5 reanalysis by ECMWF. The information from radiosonde measurements made at Invercargill is transferred to Lauder using a regression model. While it would be preferable to have high temporal resolution (e.g daily) measurements available at Lauder, using the radiosonde measurements from Invercargill improves the estimate of the temperature compared to merely using the ERA5 diurnal cycle. Using the temperature anomalies of radiosondes launched from Invercargill with respect to the diurnal cycle, introduces uncertainty, which is calculated by error propagation through the regression model. This meets the requirements outlined by GCOS-170 (2013) regarding the handling of uncertainties when transferring information from the location of a measurement to another location. Thus, this study presents a methodology for how to estimate temperatures at a given site based on measurements made elsewhere.

As ERA5 has an hourly resolution and provides uncertainties calculated by a 10-member ensemble, it is well-suited to provide a default diurnal cycle which defines the SASBE in the absence of any measurements. The representativeness uncertainty of the ERA5 diurnal cycle is additionally taken into account. As measurements become available, the temperature SASBE diverges from the diurnal cycle towards the measurements. At the time a radiosonde measurement is made above Lauder, the temperature SASBE is defined entirely by the measurement. The uncertainty is lowest at this time and equals the measurement uncertainty. With further time difference from a Lauder radiosonde measurement, the uncertainty on the SASBE increases. The availability of an estimated temperature anomaly based on the measurements made at Invercargill decreases the uncertainty on the SASBE temperature in comparison to using entirely the diurnal cycle. While the SASBE will not always represent the true temperature, it is a best-estimate of the true temperature constructed by combining different sources of information about the temperature above Lauder. The uncertainty on the data product indicates the confidence that a user should have in the temperature estimate at a given time. The uncertainty is an essential part of the SASBE, and users of the data product are urged to be cognizant of the uncertainties when using the temperature SASBE.

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Due to its high temporal resolution, and the included estimate of the uncertainty, the SASBE is well-qualified for the validation of space-based sensors. Most overpasses of a satellite during the years 1997-2012 will lead to a close collocation in time, given the hourly resolution of the SASBE. Using individual radiosonde measurements rather than a SASBE can minimise the number of collocations significantly, as was the case in Calbet et al. (2017), who analysed differences between the Infrared Atmospheric Sounding Interferometer (IASI, Siméoni et al., 1997) and GRUAN radiosonde profiles, but was limited to using data from one GRUAN site only. If the satellite data product, i.e. the retrieved temperature profile, is provided with an uncertainty estimate, a quantitative comparison between the SASBE and the temperature retrieval is possible. The comparisons can either be made using direct collocations or by applying a numerical weather prediction model as a transfer standard (Tradowsky et al., 2017) to eliminate effects caused by imperfect spatial and, to a smaller degree, temporal collocation. However, most space-based sensors do not measure ECVs directly. For example, radiometers such as AIRS and IASI measure the top-of-the-atmosphere radiance and a radiative transfer model is required to retrieve atmospheric ECVs. As the retrieval of atmospheric temperatures from radiance is an ill-posed problem, it can be preferable to validate space-based radiometers in their native measurement space (see e.g. Calbet et al., 2017). With a radiative transfer model and additional water vapour profiles, the temperature SASBE can be used to provide such a radiance space validation as it has been described in Tradowsky et al. (2016). The uncertainties provided in the SASBEs can be propagated into uncertainties in the top-of-the-atmosphere radiances, by using a Monte Carlo approach. For this purpose, the top-of-the-atmosphere radiances are calculated many times (e.g. 100s of model runs) with slightly changed input variables (i.e. temperature, ozone and water vapour). Every input variable is varied between its upper and lower uncertainty bound and different combinations of the variables are used to calculate the top-of-the-atmosphere radiances. The uncertainty on the modelled radiances is then obtained from the spread of the calculated top-of-the-atmosphere radiances for different variations of the input variables. The modelled radiances can then be compared with radiances obtained from satellite-based radiometers above the specific location. This method has the advantage that it validates the space-based radiometers in radiance space without requiring a retrieval and the *a priori* information required within the retrieval.

The temperature SASBE may also be used as *a priori* for the retrieval of other ECVs at Lauder, i.e. a temperature profile is required as *a priori* for the retrieval of an ozone profile from the stratospheric ozone lidar based at Lauder (Brinksma et al., 1997). As the radiosonde measurements made at Lauder have not been assimilated into numerical weather prediction models prior to 2016, the SASBE can be used as an approximately independent validation data set for model calculations (not entirely independent as the Invercargill measurements have been assimilated). Its hourly resolution and the availability of uncertainties make the SASBE especially valuable. The ERA5 reanalysis is used to calculate the diurnal cycle and the anomalies with regards to this diurnal cycle above Lauder and Invercargill. However at times close to a Lauder radiosonde measurements, the SASBE is primarily determined by the Lauder radiosonde temperature. Thus, the SASBE may be valuable to assess the accuracy of the ERA5 reanalysis when applying close collocation criteria for the time (i.e. around the radiosonde measurement time). While this is not different to using the Lauder radiosondes directly, the SASBE is available in an easier accessible and consistent format.

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This publication describes the development of a temperature SASBE for the GRUAN site at Lauder, New Zealand. A method to combine measurements from distributed sites is presented which accounts for the additional uncertainty that is induced by using the measurement of an ECV made at one location as a proxy for the ECV at another location nearby. This is an essential first step to enhance the value of distributed GRUAN sites.

6 Data availability

The temperature SASBE for Lauder, New Zealand, has been long-term archived and is indexed as doi:10.5281/zenodo.1195779. Users are encouraged to contact the first author of the paper to inform her about the use of the data product.

Author contributions. J.S. Tradowsky developed the methodology for the SASBE, wrote the software, and drafted the paper. G.E. Bodeker supervised and supported the development of the methodology and provided detailed comments on the draft paper. R.R. Querel, P.J.H. Builtjes, and J. Fischer supervised the work and provided comments to the draft paper.

Competing interests. The authors declare no competing interest.

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