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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 standard deviations, and the ERA5 representativeness uncertainty through the retrieval chain. The SASBE has been long-term archived and is identified using the digital object identifier https://doi.org/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 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.

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 10 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 (colocated) locations can be operated as a distributed site. If, at such a distributed site, the measurements made at one location are used to estimate measurements made elsewhere, the uncertainty on the estimated measurements must include the original measurement uncertainty plus the additional uncertainty introduced 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 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 paper first presents the observational data sets used herein, followed by a detailed description of the SASBE methodology used. The SASBE is presented in Sect. 4, followed by a discussion of method, results, and possible applications. A short conclusion completes the paper.

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 for which the SASBE is calculated is 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 1σ uncertainty for radiosonde temperatures are used. If available, traceable uncertainty estimates such as those pro-

[1] The site has since joined GRUAN.

[2] Global Climate Observing System.

vided with the GRUAN radiosonde data product (Dirksen et al., 2014) should be used instead.

The ERA5 reanalysis is the fifth generation of atmospheric reanalysis produced by the European Centre for Medium-Range Weather Forecasts (ECMWF). ERA5 data for the years 2010 to 2017 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. Eventually, ERA5 will be available from 1950 onwards and monthly updates with a maximum latency of 3 months are planned, however at the beginning of 2018 only 8 years of data were available. 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.

3 Methodology

A method 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 on the lower South Island, is presented here. The SASBE is calculated at 16 vertical levels, i.e. surface, 925, 850, 700, 500, 400, 300, 250, 200, 150, 100, 70, 50, 30, 20, and 10 hPa, which are the so-called standard pressure level of radiosondes transmitted in the alphanumeric TEMP format. Currently, the global operational upper-air network is migrating towards high-resolution radiosonde reports in the BUFR format (Ingleby and Edwards, 2015). In the interest of clarity, the method is described as applied to one selected pressure level below.

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 and, around the launch time of the radiosonde, the temperature SASBE diverts from the diurnal cycle towards the observed temperature. 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, which implies that the SASBE adapts the measured value. 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 Sect. 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 attenuated as they originate from a different location, 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 their combination is described in the following sections.

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. Bilinear interpolation in space is used to retrieve ERA5 reanalysis temperature at the exact location of the Lauder and Invercargill upper-air sites, respectively. Then, four Fourier pairs for the hour of the day (h), and four Fourier pairs for the day of the year (d) are fitted to the data (see Eqs. 1 and 2). Inclusion of the higher harmonics of the diurnal cycle, which represent the temporal variability due to atmospheric tides (Haurwitz, 1964), is possible due to the hourly resolution of ERA5. The ability to resolve atmospheric tides is typically limited by the temporal resolution of, e.g. satellite-based instruments (Huang et al., 2010).

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) 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, 2017) and are used for the years they are available. AWS abbreviates automatic weather station.

Data set	Source	Available at (last access: 5 December 2018)
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 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.

Station	WMO ID	Cliflo Identifiers	OSCAR entry (last access: 5 December 2018)
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

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

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

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

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

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

This uncertainty indicates how well 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 ($\sigma_{\mathrm{representativeness}}$), is included and the uncertainty on the diurnal cycle is estimated as follows:

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

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 and 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 2 selected days of the year. Depending on the site and the pressure level, the representativeness uncertainty reaches values from approximately 2.8 to 5.6 K and dominates the uncertainty on the diurnal cycle.

3.1.2 Inferring temperature anomalies above Lauder from temperature measurements above Invercargill

Although the absolute temperature values at Lauder (inland) and Invercargill (coastal) differ, the temperature anomalies with respect to their respective diurnal cycles are correlated. For a maximum time difference of 1.5 h between the Lauder and Invercargill radiosonde launch, the correlation of the anomalies is between $R = 0.69$ and $R = 0.92$ depending on the pressure level, with a mean correlation of $R = 0.85$. This correlation of anomalies is exploited to estimate temperature

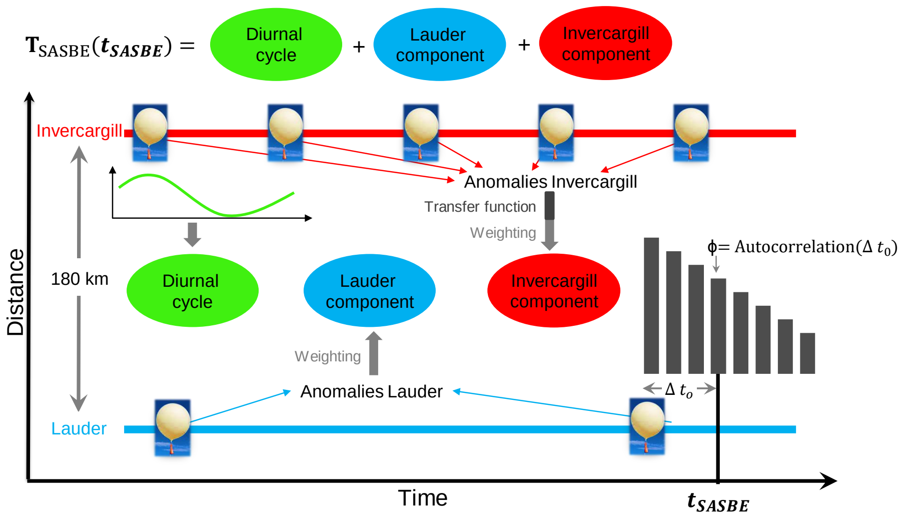
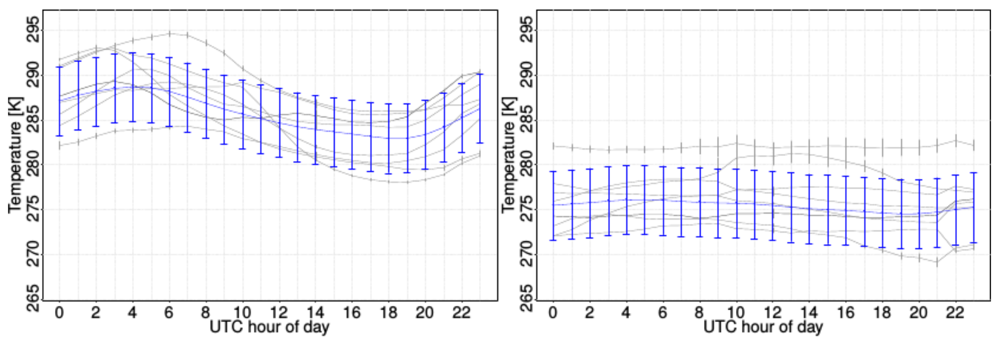


Figure 1. Schematic explanation of the temperature SASBE and its components. The diurnal cycle is determined from ERA5 as described in Sect. 3.1.1. To calculate the Invercargill component, a transfer function (see Sect. 3.1.2) and some weighting is applied to the temperature anomalies at Invercargill. 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.



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

Figure 2. Fitted diurnal cycle (blue) and ERA5 temperatures for 2 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.

anomalies above Lauder based on temperature anomalies of radiosondes launched at Invercargill with respect to the diurnal cycle.

The temperature anomaly (T') at a given pressure level with respect to the diurnal cycle is calculated from the radiosonde measurement and the diurnal cycle calculated at the respective site as $T'(t) = T_{\mathrm{RS}}(t) - T_{\mathrm{Diur}}(t)$. The 1$\sigma$ uncertainty on the temperature anomalies is calculated as $\sigma_{T'(t)} = \sqrt{\sigma^2_{T_{\mathrm{RS}}(t)} + \sigma^2_{T_{\mathrm{Diur}}(t)}}$. When the separation in launch time between Lauder and Invercargill is less than 1.5 h, the data are used to train a regression model (Eq. 5) that is applied to "translate" temperature anomalies from Invercargill to Lauder.

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 (ΔST$'$, Term 4).

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

where 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 for the wind direction θ to account for the dependence of the correlation between the Lauder and Invercargill temperature anomaly on the meteorological conditions, such as a lag/lead in the temperature anomaly based on the wind direction.

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

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

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

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

$$\begin{aligned}\widehat{T}'_{\text{Lau}} = \gamma + \beta \cdot \left(T'_{\text{Inv}} - \overline{T'_{\text{Inv}}}\right) + \eta \cdot (\Delta\text{SP} - \overline{\Delta\text{SP}}) \\ + \kappa \cdot \left(\Delta\text{ST}' - \overline{\Delta\text{ST}'}\right) + \epsilon \quad (8)\end{aligned}$$

The residuals (ϵ) are plotted in Fig. 3 for varying maximum time differences $\Delta t_{\text{regression}}$ between the Lauder and Invercargill launch times. Decreasing the time difference, in general, decreases the residuals slightly at most levels. However, at 30 hPa the regression model trained on collocations from within 6 h 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 h ($R = 0.78$) and 6 h ($R = 0.76$) than for 1.5 h ($R = 0.69$) at the 30 hPa level. The sample size for collocations within 1.5 h 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. However, since the maximum time difference of 1.5 h minimises the residuals at most pressure levels, it is used as $\Delta t_{\text{regression}}$. This choice is ultimately an expert decision and further options could be tested to ensure an optimal choice is made, e.g. by testing different maximum time differences for 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 $\Delta t_{\text{regression}}$. 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,

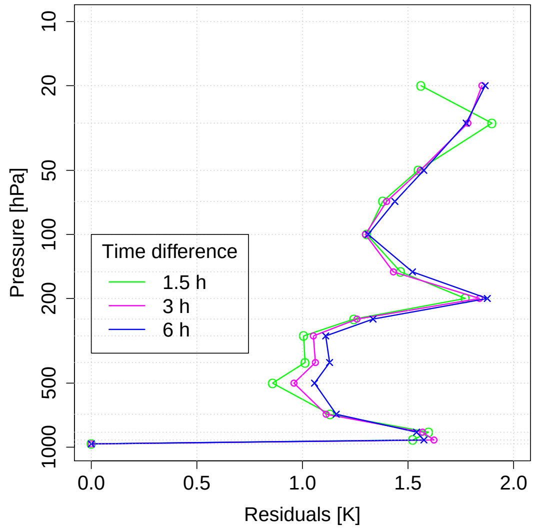


Figure 3. Temperature residuals for the regression model described in Eq. (5). The regression model is trained with three different data sets containing Lauder and Invercargill radiosonde measurements with launch times having a maximum time difference of 1.5 h (green, 324 collocations), 3 h (pink, 646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

the measurements of the automatic weather station are used at the surface level.

The uncertainties on the Invercargill and Lauder measurements and anomalies, and on the regression coefficients, are propagated through Eqs. (7) and (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.

$$\begin{aligned}\sigma_{\widehat{T}'_{\text{Lau}}} = \Bigg[&\sigma_\gamma^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \gamma}\right)^2 + \sigma_{\beta_0}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \beta_0}\right)^2 + \sigma_{\beta_1}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \beta_1}\right)^2 \\ &+ \sigma_{\beta_2}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \beta_2}\right)^2 + \sigma_{\beta_3}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \beta_3}\right)^2 + \sigma_{\beta_4}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \beta_4}\right)^2 \\ &+ \sigma_{T'_{\text{Inv}}}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial T'_{\text{Inv}}}\right)^2 + \sigma_\theta^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \theta}\right)^2 + \sigma_\eta^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \eta}\right)^2 \\ &+ \sigma_{\Delta\text{SP}}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \Delta\text{SP}}\right)^2 + \sigma_\kappa^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \kappa}\right)^2 + \sigma_{\Delta\text{ST}'}^2 \left(\frac{\partial \widehat{T}'_{\text{Lau}}}{\partial \Delta\text{ST}'}\right)^2 \Bigg]^{1/2} \quad (9)\end{aligned}$$

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 1σ 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 1σ 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.

3.2 Combining the individual components of the SASBE

The temperature SASBE for Lauder is calculated from the different components presented in the Sect. 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 ($\widehat{T}'_{\mathrm{Lau}}$) 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 approximately weekly.

At any time t the SASBE temperature $T_{\mathrm{SASBE}}(t)$ 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) and Invercargill measurements gain weight. Autocorrelation is the correlation of a time series with a lagged (delayed) version of itself (Wilks, 2011). Here ϕ is calculated from ERA5 temperature anomalies with respect to the ERA5 diurnal cycle as follows:

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

The lowest value of ϕ is restricted to 0.5 to limit 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.

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

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°

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 follows:

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

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

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

The weights for Lauder anomalies are normalised with the sum over all Lauder weights and the anomalies implied from measurements in Invercargill are normalised 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 to be 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 follows:

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

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

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

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

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

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

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 follows:

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

where $T_{\mathrm{RS_{Lau}}}$ is the temperature measured with a radiosonde above Lauder and $\widehat{T}_{\mathrm{RS_{Lau}}}$ 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:

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

with the partial derivatives:

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

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

and

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

respectively, and therefore:

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

The uncertainty on inferred RS temperatures ($\widehat{T}_{\mathrm{RS_{Lau}}}$) is estimated as follows:

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

In Eq. (22), $\sigma_{T_{\mathrm{Diur_{Lau}}}}$ and $\sigma_{T_{\mathrm{Diur_{Inv}}}}$ 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 ($\sigma_{T_{\mathrm{SASBE}(t)}}$), at the 1σ level, is calculated for every temperature value in the SASBE and is shown as black uncertainty bars in the top panels of Figs. 4–9.

4 Results

The temperature SASBE for Lauder is available in hourly resolution for 1997 to 2012 at 16 vertical levels. 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 h (temperature) or ± 12 h (pressure). In this study, the uncertainty added by the interpolation is not taken into account.

As an example, Fig. 4 show the hourly temperature SASBE at 925 hPa, and its individual components, for 6 to 9 December 2010. Panel 4a shows the SASBE temperature (black line) and its associated 1σ 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

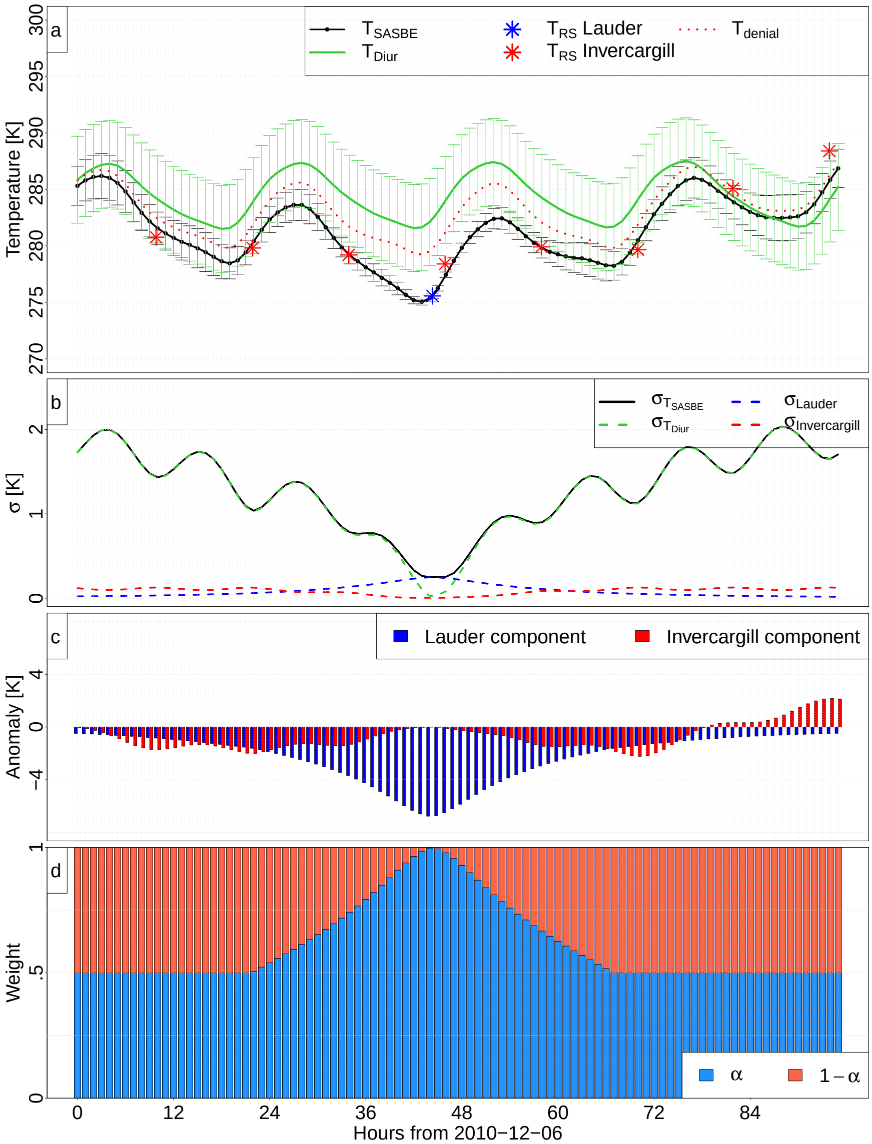


Figure 4. Temperature SASBE at 925 hPa and its individual components for 6 to 9 December 2010. **(a)** Temperature SASBE (black line), diurnal cycle (green line), denial study (i.e. pretending no measurements exist at Lauder, dotted red line), and radiosonde temperature measurement if available (Invercargill: red star; Lauder: blue star). **(b)** 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 ($\sigma_{T_{\mathrm{SASBE}}(t)}$) is shown as black line. **(c)** Weighted Lauder radiosonde temperature anomaly ($\sum_{i=1}^{N}\phi\cdot w\cdot T^{*}_{i_{\mathrm{Lau}}}(t)$, blue bars) and weighted estimated Lauder temperature anomaly ($\sum_{j=1}^{M}\phi\cdot w_j\cdot \widehat{T}^{*}_{j_{\mathrm{Lau}}}(t)$, red bars). **(d)** 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.

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 Sect. 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). Typically two radiosondes are launched daily from Invercargill at about 10:00 and 22:00 UTC (i.e. eight launches during the 4 days plotted), while typically one radiosonde is launched from Lauder each week.

Panel 4b 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 in-

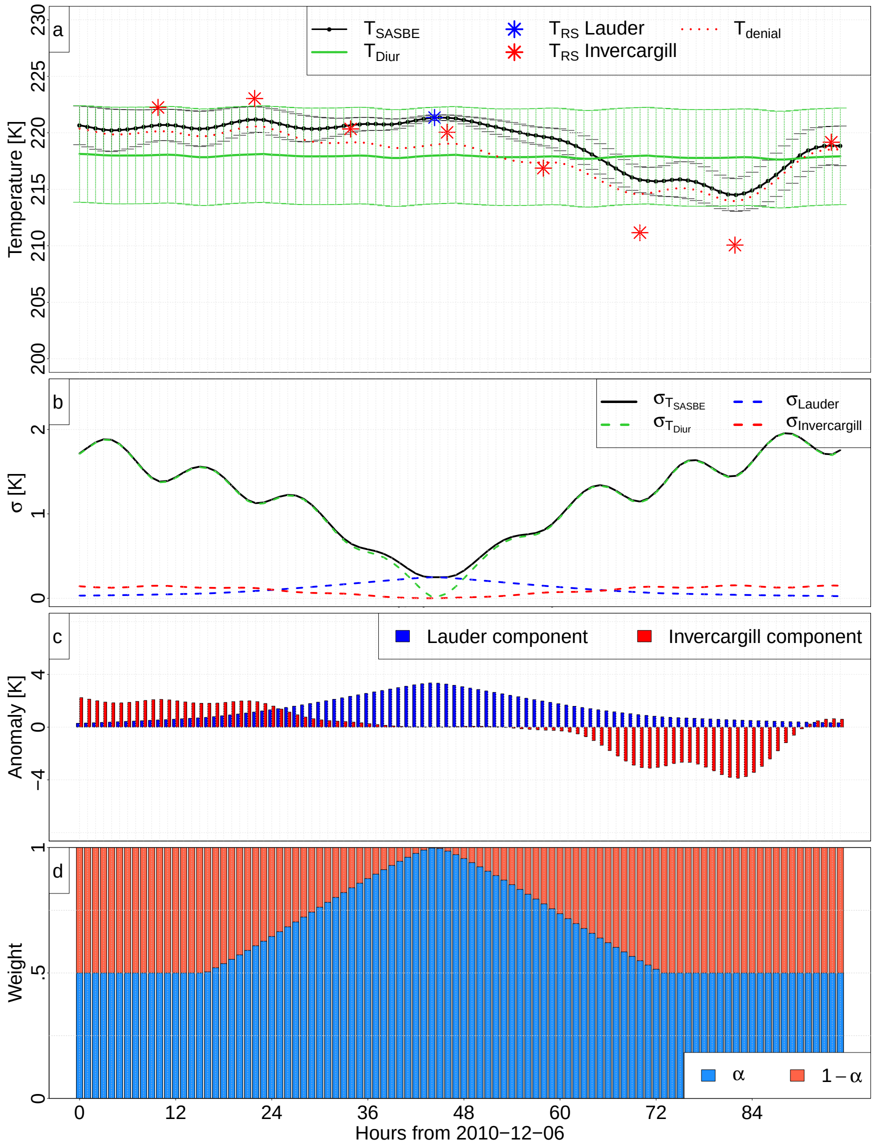


Figure 5. As in Fig. 4, but at 150 hPa.

fluence the SASBE and therefore increase the uncertainty. Panel 4c shows the weighted contribution from the Lauder radiosonde anomalies $\left(\sum_{i=1}^{N}\phi \cdot w \cdot T^{*}_{i_{\mathrm{Lau}}}(t)\right)$ in blue and the weighted contribution from the estimated Lauder anomalies $\left(\sum_{j=1}^{M}\phi \cdot w_j \cdot \widehat{T}^{*}_{j\mathrm{Lau}}(t)\right)$ in red. The bottom panel shows the weights ϕ and $(1-\phi)$ which are given to the Lauder anomalies and estimated Lauder anomalies, respectively. As the autocorrelation of temperature anomalies decays slower in the stratosphere, the influence of the temperature measured in Lauder decreases more slowly at 70 hPa level (see Fig. 6) than at the 925 hPa level.

Figures 5 and 6 show the temperature SASBE for the same time frame at the 150 and 70 hPa level, respectively.

It can be seen in Figs. 4 and 5 that using the Invercargill measurements as a proxy for the temperature above Lauder is an improvement compared to using climatology, i.e. the diurnal cycle, only. 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 those instances. However at the 70 hPa level the fit to the radiosonde measurement in Lauder is slightly worse using Invercargill measurements as a proxy.

Figures 7 to 9 show the SASBE at 4 days during the austral winter at 925, 150, and 70 hPa, respectively. The diurnal temperature cycle is less pronounced in austral winter as can

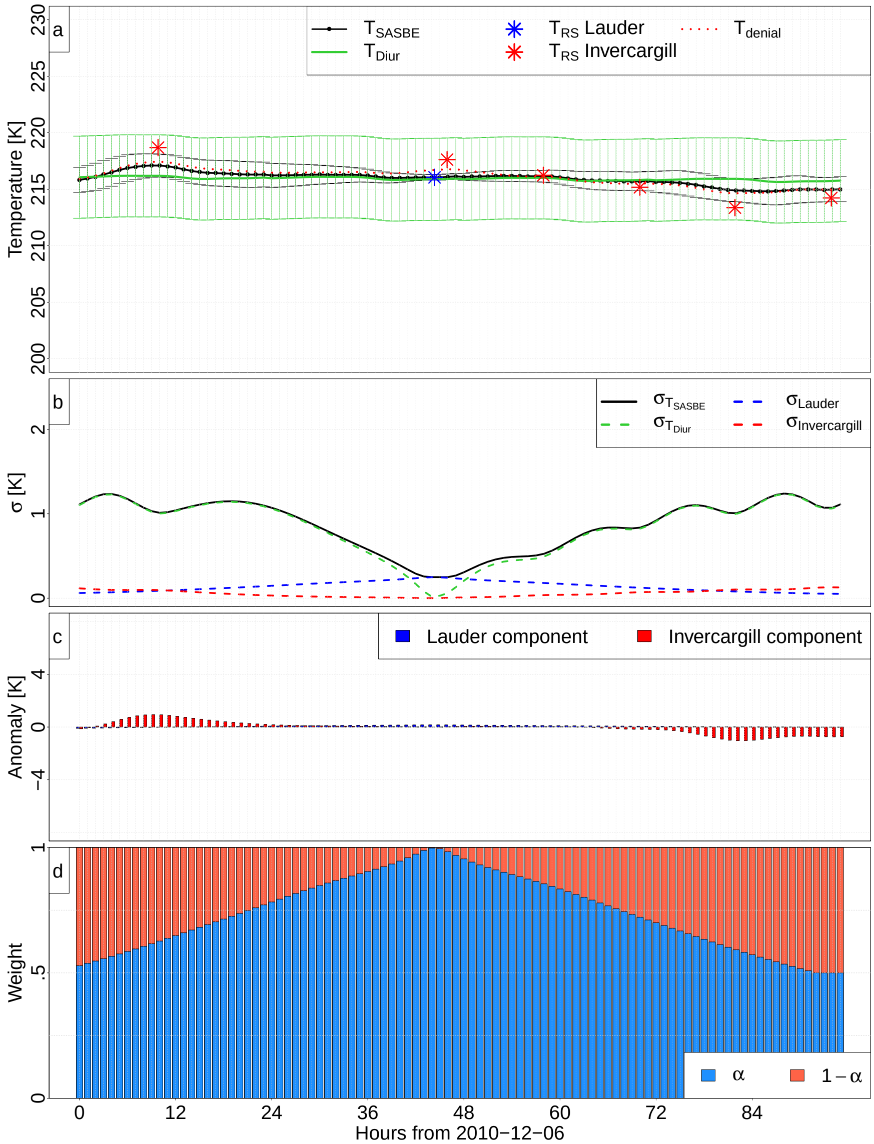


Figure 6. As in Fig. 4, but at 70 hPa.

be seen by comparing Fig. 7 with Fig. 4. For the Lauder radiosonde launch at 16 July 2003, the fit to the radiosonde is improved by using Invercargill measurements as a proxy at the 925 hPa level and at the 150 hPa level, however, the fit is slightly diminished at 70 hPa.

To evaluate if using Invercargill measurements as part of the SASBE is valuable, in general, it is tested whether using estimates of temperature anomalies above Lauder which are based on measurements from Invercargill improves the SASBE in comparison to using merely the ERA5 diurnal cycle. This is tested by analysing the yearly mean absolute residuals between the Lauder radiosonde measurements and (i) the diurnal cycle (green) and (ii) the diurnal cycle plus inferred Lauder temperature anomalies (denial study, red); see Fig. 10. At most pressure levels, and for all years, the residuals are distinctly smaller when using the estimated temperature anomalies. This means that using the Invercargill radiosondes plus a transfer algorithm improves the SASBE compared to using the diurnal cycle alone. At the 20 and 10 hPa level, improvements are only visible during certain years as most radiosondes from Invercargill do not reach these pressure levels.

5 Summary and discussion

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

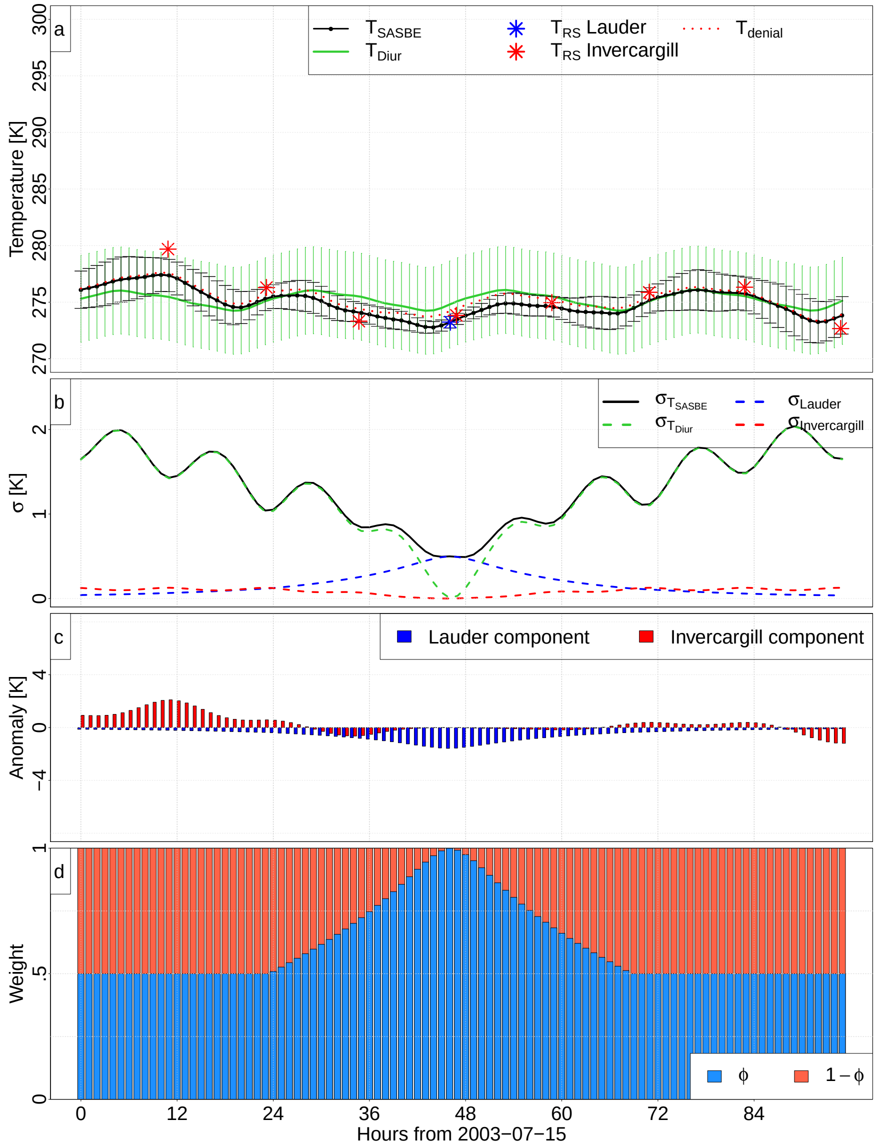


Figure 7. As in Fig. 4, but for 4 days in July 2003 at 925 hPa.

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. The described method is likely to be applicable to other ECVs that have a large spatio-temporal scale, such as ozone above the boundary layer. However, for ECVs that vary rapidly over distance and time, such as water vapour, the described method is unlikely to provide useful results. Therefore, prior to applying the method, the correlation between the time series of a chosen variable at both locations should be evaluated.

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 between data that are used to train the regression model, and the maximum weight given to

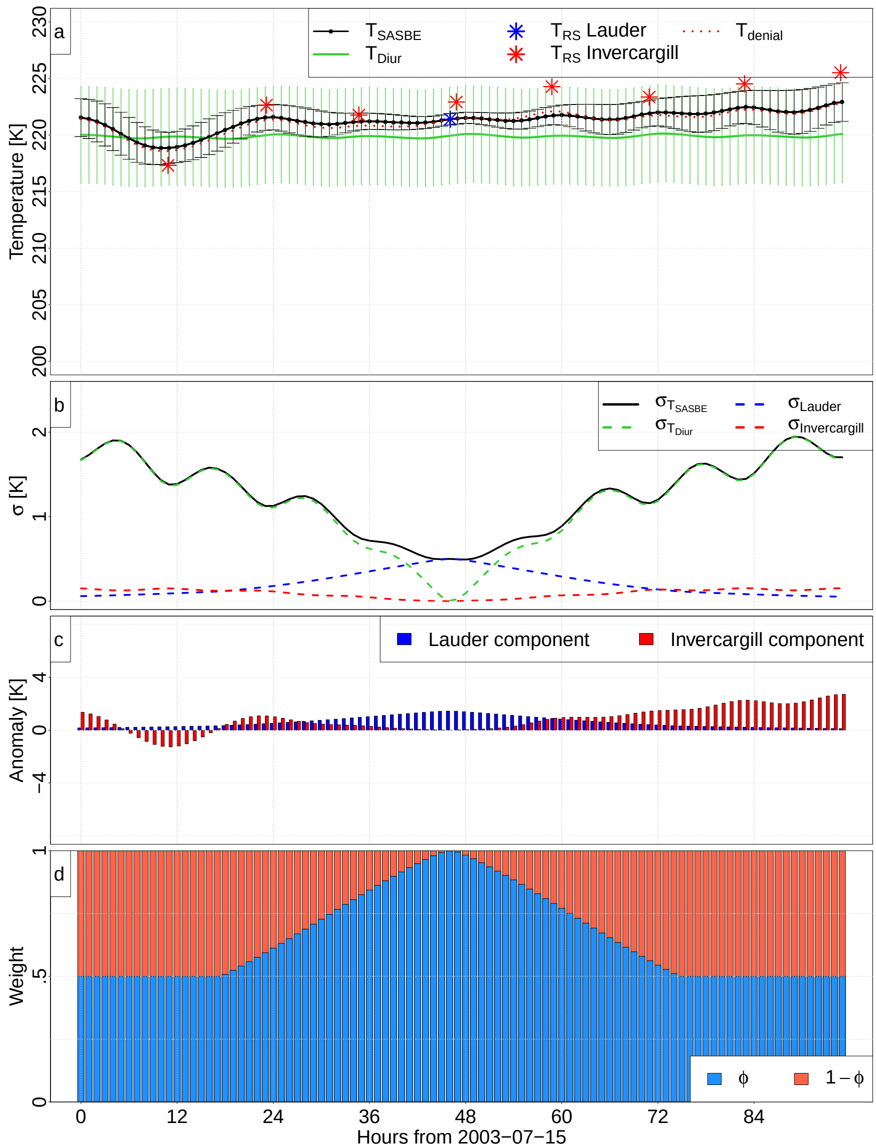


Figure 8. As in Fig. 4, but for 4 days in July 2003 at 150 hPa.

the estimated anomalies. Furthermore, different options for the calculation of the weights might be possible.

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 pro-

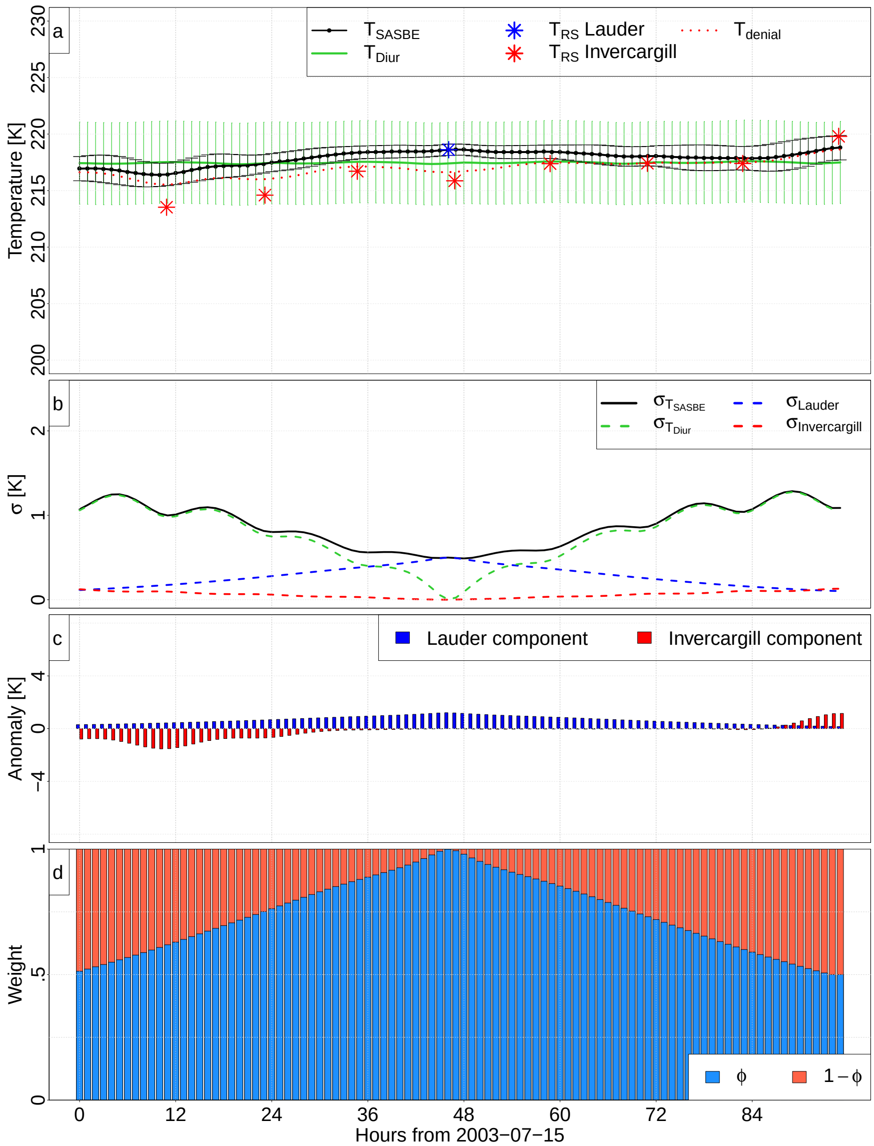


Figure 9. As in Fig. 4, but for 4 days in July 2003 at 70 hPa.

vide such a radiance space validation as it has been described in Tradowsky et al. (2016) and Tradowsky (2018). 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. hundreds 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 of 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

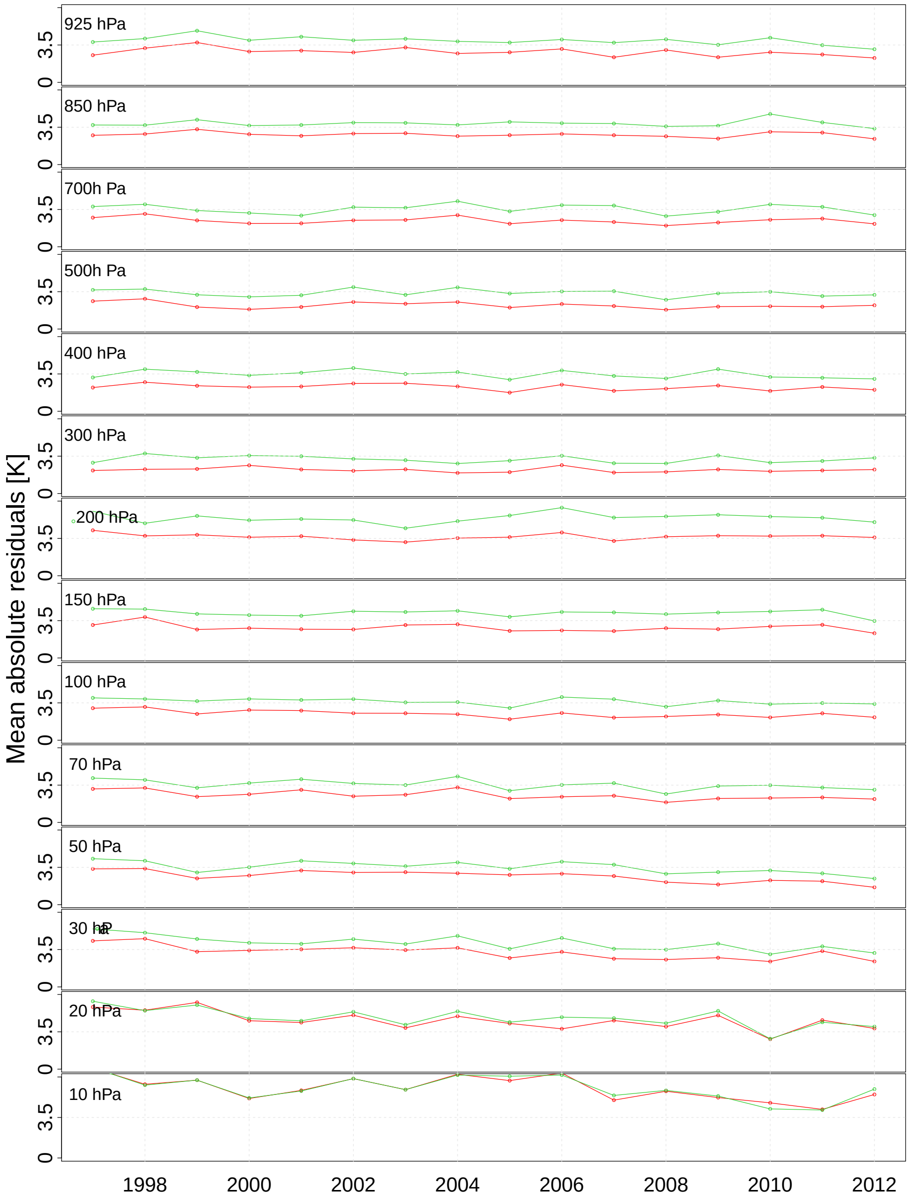


Figure 10. Yearly mean of absolute residuals between the Lauder radiosonde measurements and both (i) the diurnal cycle (green) and (ii) the denial study (red).

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, to the best of our knowledge, Lauder radiosonde measurements have not been assimilated into ERA5, at least not prior to 2017, as they are not part of the Integrated Global Radiosonde Archive (IGRA) and have not been assimilated by ECMWF's operational forecast model prior to 2017 (Bruce Ingleby, personal communication, 2018). At times close to a Lauder radiosonde measurements, the SASBE is primarily determined by the Lauder radiosonde temperature. Thus, the SASBE may be valuable for assessing 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.

6 Code and data availability

The temperature SASBE for Lauder, New Zealand, has been long-term archived and is indexed with a doi, see https://doi.org/10.5281/zenodo.1195779 (Tradowsky et al., 2018). Users should contact the first author of the paper to inform her about the use of the data product. The code used to produce the SASBE has been developed in R and is available on request from the first author.

7 Conclusions

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 introduced 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. GRUAN operates several distributed sites, i.e. Cabauw and De Bilt, The Netherlands, Beltsville and Sterling, US, and Lauder and Invercargill, New Zealand. While the instrumentation might differ at every upper-air sites, the methodology described here can be adapted for other distributed sites. The results of this study show 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. The method presented enhances the value of upper-air observations 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. While the SASBE presented here will not give an accurate estimate of the true temperature at every time step, 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. The uncertainty is an essential part of the SASBE, and users of the data product are urged to be cognisant of the uncertainties when using the temperature SASBE.

Author contributions. JST developed the methodology for the SASBE, wrote the software, and drafted the paper. GEB supervised and supported the development of the methodology and provided detailed comments on the draft paper. RRQ, PJHB, and JF supervised the work and provided comments to the draft paper.

Competing interests. The authors declare that they have no conflict of interest.

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