

QAtools Shiny-App User Guide

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1 Introduction

1.1 General scope

This manual describes a “Shiny app” named “QAtools” that is intended to facilitate the review of data from new flights of the NSF/NCAR/EOL/RAF research aircraft. (NSF=National Science Foundation; NCAR=National Center for Atmospheric Research; EOL=Earth Observing Laboratory; RAF=Research Aviation Facility), presently a C-130 and a Gulfstream V. The objective of this tool is to support quality assurance during research projects and during subsequent processing of data from those projects. The underlying scripts read the netCDF data archives produced by the processing program “nimbus”, which reads the data files recorded by the data systems on the research aircraft and converts the digital information to engineering-unit output. Nimbus is described here. The QAtools app can also help analyze past projects. (For a list of recent projects, see at this EOL web page; data requests can be made via links on that page.) However, the data archive used here is a different one, mostly matching that available on EOL storage under “/scr/raf_data”. These files often contain variables not present in the final production files, including housekeeping and redundant measurements, so they provide additional information for the assessment of data quality. That working repository is duplicated in part on the server that supports QAtools, and new files must be transferred to that cloned repository.

1.2 What is a “Shiny app”?

A “Shiny app” is an interactive web application based on the “shiny” package for R. The routines and data files reside on a server and can be accessed either locally or remotely as a web page. See <https://shiny.rstudio.com> for complete information. A very cursory tutorial is also included in the QAtools package, as described below. The QAtools Shiny app is accessed at this URL (temporarily installed on the RAF ground station, so this address may change in the future): <https://128.117.84.138:3838/QAtools>. This is presently inside the UCAR firewall so if you are outside you need to use VPN. When the ground station is at a remote location for a field project, the URL will be different.

1.3 The reference repository

The code for this Shiny app resides on GitHub at <https://github.com/WilliamCooper/QAtools.git>. However, a complete installation requires downloading several other GitHub repositories also, as described in Appendix A.3 to this User Guide. The “Ranadu” package (available at this URL) is used extensively and is installed on the Shiny server. Other required R scripts are also on GitHub. See the appendix for details. The code is also present on EOL file space in directories under ~cooperw/RStudio/, notably QAtools. There is no Shiny server there, but it can still be used as a Shiny app from a local directory. If you duplicate the files under ~cooperw/RStudio/ to user space where you have write permission, you can run this as a normal Shiny app on barolo.

2 Outline of the General Structure

The basic structure of QAtools features multiple layers of tabs, each supporting a different analysis tool. The top level includes these tabs:

Guide. This tab duplicates the summary information in the paragraphs below, for quick reference.

Background information. This section includes two main topics, the “Suggested checks” tab that provides guidance on a possible sequence for using this tool for various variables, and the remaining tabs that contain tutorial or training material. The latter will not be part of normal use of this tool but may be of interest because they develop some recommendations that are not conventional.

Past Projects: This tab provides access to compilations of measurements from past projects that can aid in the assessment of problems. For example, the flight-dependent and project-dependent comparisons between ATX and AT_A, QCXC and QC_A, and PSXC and PS_A will give some guidance regarding what tolerance is expected, and differences among available INS outputs can help determine what range to expect in future projects. The available tests also include comparisons between measured profiles and those expected from the hydrostatic equation. The latter provides for independent prediction of pressure from temperature or temperature from pressure, and so is a useful test based on independent measurements.

Tools: Some tools for calculating new variables, for fitting, and for transfer of measurements to other analysis programs are provided by secondary tabs under this tab. The first supports calculation of a new variable to be added (temporarily) to a data file so that it can be used with other analysis tools in QAtools. This tool can be used with the “ShiftInTime” function to generate new variables with different time shifts, or to apply filters to variables. There is also a “lm fit” tab that supports fitting of functional relationships (e.g., polynomials) to data in the netCDF files, e.g., as is needed to determine empirical coefficients for representing angle of attack in terms of BDIFR or the static pressure correction in terms of the measured pressure and dynamic pressure. The last tab on the right supports examination of measurements in external programs like ncplot, Xanadu, python, etc. An advantage is that the working file with any added variables but without undesired variables can be transferred to those other programs.

Review: Review plots have been generated automatically for some recent projects using an R script. The implementation here supports those same plots, but with the added capability to work interactively by, for example, selecting subsets in time or adding new variables to the plots. This is a core capability of QAtools and will often be the best starting point for review of data from a flight. Indications of problems then can be explored using other parts of QAtools.

Known Problems: This tab includes several checks for common problems. There is a tab to help search for dewpoint-overshooting problems, one to use periods when in cloud to test for agreement between the temperature and measured dew point, one to search for variables that are outside normal ranges or are frozen or have spikes, and one to assess if the cavity pressure in the dewpoint instruments has changed from that expected on the basis of earlier projects.

Special Processing: This last tab supports processing runs to add some variables to the archive files that represent processing with a Kalman filter (for wind), alternate calculation of the vertical

wind based on a new representation of the angle of attack that has been discussed and evaluated but not yet implemented in routine processing, a third tab to represent recalculation of the alternate AKRD representation, and a tab to add variables representing the elevation of the surface below the aircraft and the altitude of the aircraft above the surface to the standard files. These are not intended for routine processing, for which there are stand-alone scripts; rather, they are intended to allow inspection of the results to determine if such separate processing is desirable.

3 Suggested Usage (emphasizing the “Review” tab)

3.1 First-pass review

Overview

The suggested starting point for quality review is the “Review” tab (the fifth tab in the main window). This is an interactive interface to a set of plots that cover a standard set of variables. Cycling through these plots can check quickly for unusual behavior so that potential problems can be identified and then investigated further by other means. The default tab in the lower right panel is “plot” but there are other choices also, as described in more detail below.

Normal use

Once the project and flight have been defined (as described below), normal use will consist of these steps:

1. Cycle through the available plots using the “plot” numeric-input slot and note potential problems that may need further investigation. The plot number can be changed in three ways:
 - (a) Select the displayed number by sliding the mouse cursor over it, then type the new number.
 - (b) Place the cursor in the entry slot, then use the up-and-down arrow keys to increment the number. This is often the best choice because the cursor can be left in the entry slot while you step through the plots.
 - (c) There are small arrows in the entry slot that also can be used in the same way.
2. Alternately, if you want to proceed to plots for a specific type of variable, like the wind, you can use the “plot class” menu to jump to those plots. Most plot classes contain multiple plots, so this is a way to find the plots pertaining to a particular class of variable. Once at the first plot in the class, the methods in the item above can be used to step through that class.
3. You may want to refine a particular plot in the following ways:

- (a) Select a subset time interval. This can be done by “brushing” the left-mouse button over the desired time interval in the lower right-panel plot; i.e., hold it down while moving over the desired time range. To reset, use the F4 key. Alternate ways of selecting the time interval are discussed under the “time range, restrictions” section below.
- (b) Apply restrictions, for example by only considering temperature measurements when the airspeed is above some threshold to avoid approach and during-takeoff measurements. This is described in the “time range, restrictions” section below.
- (c) Add or remove variables from the plot. You can do this by CNTL-left-mouse clicking the variable name in the left-panel “variables” menu to add or remove it, or by left-mouse clicking on a variable to select it only. The available variables for each plot are defined in a configuration file for the project. If you want to add some other variable to the plot, use the “add var” dropdown menu near the top right of the window. If you want to plot something else, you can also use the “extras” plots at the end of the plot sequence, which support plotting of any variable in the netCDF file.

There are detailed descriptions of the standard plots in Appendix A.1 and a description of how to set up the plots for a new project is included in Appendix A.2.

Additional details regarding use of the “Review” tab

The following discusses all the controls available in the “Review” tab. Many of these won’t be needed during normal use.

1. The top panel, extending across the display below the top tabs, has two options controlled by the buttons at the left side:
 - (a) “project, flight, and plot” causes controls to be displayed for selecting the project, the flight, and the plot number. The project is selected using the drop-down menu at the top left of the sub-panel, and the flight and plot number are determined by numeric entries into the “Flight” and “plot” entry slots. To change the latter two, select the entry and then type a new entry or use the other methods described in the first item under “normal use” above. There are checkboxes that allow selection of research flights, test flights, or ferry flights (respectively, “rf”, “tf”, “ff”). A suffix may also be selected: ‘none’ for normal files, ‘Y’ for files with revised vertical wind, “KF” for results from the Kalman-filter processor, and “HRT” for 25-Hz files. The suffix “H” is also accepted. There are also buttons for the following functions:
 - i. “save config” to save any reconfigured plots where, for example, you have changed the displayed variables. Use this with consideration for other users because the change is saved in the configuration file for the project and so will affect everyone using this tool.

- ii. “PDF” and “PNG” buttons that save all the plots in PDF or PNG format. The plots observe the selected time interval but only apply the “restrictions” if the “apply restrictions” checkbox in the sidebar is selected. It takes about a minute to generate either set of plots and the app will not respond until finished. When running on a Shiny Server, these will be written to the “RStudio/QAtools” directory on the computer hosting that server. In the case of the “PDF” button, they are displayed in a new browser window where they can be downloaded and saved. For the PNG button, they are saved in the directory “RStudio/QAtools/PNG” which is not normally accessible, although if running from the groundstation those files are in the /home/ads file directory. For single downloads, the displayed files in the “Plot” display can be saved by right-clicking on the image and selecting “save image as ...”.
 - iii. The “R” button saves the R code used to generate the plot. This may be useful if it is desirable to tailor the plot in some way for specific uses beyond data review.
 - iv. The “quick” button displays a list of all available variables and provides a pop-up time plot of the variable(s) selected.
- (b) “time range, restrictions” provides a slider control that can be used to select subset time intervals. The selection applies to all plots, not just the time-series plots. The two ends of the slider can be moved by left-mouse-clicking on them and holding the click to slide them. There is a “rst” button that resets the display to the full range. The “F4” key also resets the time range. Four additional numeric-input slots at the right side of this panel can define limiting values for the minimum airspeed, the maximum absolute value of the roll, the minimum altitude, and the maximum rate of climb of the aircraft. These restrictions are only imposed when the “apply restrictions” checkbox in the middle of the left panel is selected. They can be used to eliminate turns, periods near takeoff and landing, low-level flight, and rapid climbs and descents.
2. The next section of the plot, below the preceding panels, is divided into two parts:
- (a) The sidebar control panel, containing the “plot class” menu that can be used to jump to particular sequences in the plots, the “apply restrictions” checkbox that applies the restrictions defined in 1(b) above, a “variables” menu that permits changing the plotted variables, and a set of buttons at the bottom that activate other programs but should not be used and will not work for the shiny-server version of this program.
 - (b) The main display panel, the right-bottom panel, shows the selected plot. At the top of this panel are another series of tabs, “plot”, “stats”, “histograms”, “soundings”, and “listing”. The “plot” tab is the default and the tab that will be used during normal use. The other tabs show the same variables in the main plot but in other formats, which may be useful for special cases. All these obey the restrictions imposed by the time range and, if “apply restrictions” is selected, by the defined restrictions.

General expectations for the plots

Appendix A.1 provides more detail regarding the expected appearance of the plots.

3.2 Background -> Suggested checks

The next suggested step is to go to the “Background” tab and select the “suggested checks” tab. This provides some recommended steps for variable-dependent tests that won’t be repeated here. Suggestions are available under tabs labeled “PSXC/QCXC”, “ATX”, “humidity”, “INS performance”, “WIC”, “WD/WS”, and “LWC and particles”. Many of these suggestions relate to comparisons to expected performance as seen in past projects and use the “Past Projects” tab, while others relate to the “Known Problems” tab. Items under these tabs will likely continue to develop as new tests are constructed.

4 Detailed Descriptions of Other Key Tabs

4.1 The “Past Projects” tab

General intent

This tab provides a series of functions that support comparisons to expected behavior of measurements based on past projects. For example, throughout the history of the GV the “PS_A” measurement of ambient pressure has shown a consistent relationship to the best values of the research-system measurement PSXC, so checking that the same relationship applies to a new project is a good test of the validity of the measurement PSXC. Similar comparisons can be made to several other measurements using the tabs in this section. Each tab is described in some detail in the following sections. These descriptions will likely be easier to follow if you look at an example while reading them. A good suggested flight to view is CSET flight 7.

PSXC

There are two lower-level tabs under this one:

1. “Compare to PS_A”: This tab generates two plots for the selected project and flight (or, if the “ALL?” checkbox is checked, for all flights in the project:
 - (a) The left plot is a histogram of the difference between the measured pressure PSXC and the pressure determined from PS_A by a fit to historical data. In this case, the fit for the GV is
$$\text{PSFIT} = c_0 + \text{PS_A} * (c_1 + c_3 * \text{PS_A}) + c_2 * \text{QC_A}$$

where $c_{\{0-3\}} = \{-2.624, 1.00631, 0.016021, -4.6658e-06\}$. This gives a fit to past measurements that has a standard deviation from those measurements of only about 0.2 hPa, which is smaller than the uncertainty limit for this measurement, so this is a stringent test. The mean and standard deviation shown above the left plot will usually be about 0.2 hPa or smaller for good measurements. There is an analogous but different fit for the two pressure variables from the C-130 (PSFDC and PSFC).

- (b) The right plot shows mean and standard deviation for the difference between PSFIT and PSXC for bins in PSXC, and so tests for altitude dependence in the representation of PSXC. The numbers along the right side of the plot show the number of 1-Hz measurements used for each bin in PSXC. Where the numbers are small, the results may be unreliable because they may result only from rapid climb or descent through those levels. For the C-130, the points with error bars show PSFDC and the green line shows PSFC.

There is a “Help info” button that will pop-up a description of what to expect for these two plots and will show an example. Dismiss that pop-up using the “Dismiss” button or by clicking anywhere in the main window.

2. “hydrostatic-eq check”: The hydrostatic equation expresses a relationship between changes in pressure, temperature, and height, so with low-uncertainty measurements of height from a GPS receiver that equation can be used to predict pressure from temperature or temperature from pressure during climbs and descents. In this case, the prediction is for pressure under the assumption that the temperature (ATX) is correct. That leads to the plotted lines vs. altitude that show the difference between the measured pressure and that predicted from integration of the hydrostatic equation. The blue line is the prediction, and the two red lines show limits that would result if the temperature is adjusted by $\pm 0.5^\circ\text{C}$. An offset often arises at low level, conjectured to arise from the slow time response of the temperature sensor during rapid climb, and this often produces an offset of 2 hPa or so in the integrated pressure. Once above the lowest levels, the offset should remain reasonably constant. The “All?” checkbox does not apply to the hydrostatic-equation check because only the first climb is used for the calculation. Here also, there is a “Help info” button that provides an example of expected behavior and some guidance regarding how to interpret this plot.

QCXC

The displays here are analogous to the “Compare to PS_A” plots above, but for QCXC as compared to QC_A. No comparison to a hydrostatic-equation prediction is possible for QCXC, so there is only one pair of plots generated under this tab. See the “help info” button.

ATX

Under the “ATX” tab, there are three lower-level tabs:

1. “Prediction from AT_A”: The relationship between AT_A and the best research temperature has been reasonably consistent in recent projects, although there are some significant differences (esp. at low temperature). This relationship has led to a regression prediction of ATX from AT_A that can be used to check if the recent consistency continues to hold for new projects. The two plots generated under this tab are a histogram of the difference between the predicted and measured ATX and a plot showing that difference in bins of PSXC, to check for an altitude dependence. As for the above histograms, the numbers at the right side of the plot show the numbers of 1-Hz measurements in each bin, and bins with a small number of measurements may have anomalous errors arising from rapid climb or descent through those levels. As for other items in the “Past Projects” tab, the “Help info” button provides guidance regarding interpretation of this plot and a sample plot, so that information is not repeated in this User Guide.
2. “Comparisons among ATs”: Because there are usually redundant measurements of temperature available, it is possible to check for problems by searching for disagreements among those measurements. CTRL-left-mouse click on the displayed variable menu to select two to compare. [XXX multiple pairs do not display correctly yet.] The plot shows the mean and standard deviation of the difference in bins of temperature to illustrate how the differences vary across the range of measurements. Difference significantly larger than 0.3°C , the expected uncertainty in temperature, may be indications that the discrepancy should be investigated further. Two exceptions are the “normal” tendency of AT_A or AT_A2 to be higher than ATX at low temperature and the tendency of ATH2 to be systematically about 0.5°C lower than ATH1 and temperatures around -60, perhaps because the recovery factor is not represented correctly for ATH2.
3. “hydrostatic-eq check”: This test is like the hydrostatic-equation prediction of pressure from temperature above, except that the pressure is assumed to be correct and the temperature vs height is deduced by integrating the hydrostatic equation. Whereas a profile is required to predict pressure from temperature, the temperature at individual points can be predicted from the change in pressure with height, so entire flights or entire projects can be used for these plots. See the “Help info” button for more information on the data restrictions used and the specific form of the hydrostatic equation. Difference exceeding the claimed temperature uncertainty of about 0.3°C may be indications that further study is needed. For example, this plot for ORCAS suggests a systematic error of up to 2°C at the lowest temperatures (with ATX too high), so this suggests further investigation of this possibility.

INS/IRU comparisons

The two lower-level tabs under this tab show histograms (with mean and standard deviation) for the difference between pitch and roll measurements from redundant INS units and for the difference in heading. [XXX problem to be fixed with heading] These are potentially useful for determining project-dependent offsets to use in the “Configuration.R” file for the “Review” tab. Offsets may

vary among projects, but the standard deviations should remain small compared to 0.05° , the expected uncertainty limit quoted for the inertial navigation systems. Larger numbers may indicate deterioration of performance for one of the units being compared.

Maneuver study

This tab has several lower-level tabs:

1. “search for maneuvers”: This tab has a series of checkboxes for the various types of maneuver and a “search” button to search for maneuvers. *For existing projects, this search should not be used in most cases because sets of maneuvers have already been compiled and edited, and using this search button will overwrite the existing set of maneuvers.* If you click this button, a warning will ask if you really want to overwrite the existing file. Normally this should be done only for new projects. The search covers all available flights for the selected project, including test and ferry flights, and will take a few minutes. A notice “search in progress” will appear at the bottom right of the display window, and you should wait for that message to disappear before continuing.
2. “Speed Run”: Under this tab, the available speed runs for the selected project will be displayed at the top left. Select one of the checkboxes to see that speed run (if any are displayed). Three plot formats are available:
 - (a) “recovery factor”: This plot shows the measured recovery temperature RTX as a function of $V^2/(2c_p)$ so that the slope corresponds to the recovery factor for the temperature sensor. The fitted slope is listed at the top of the plot, as the second fit coefficient. The response time of the temperature sensor often produces two distinct lines, one while the airspeed is increasing and another for decreasing airspeed. The “set delay” slider makes it possible to delay the RTX measurement, and introducing a delay of around –1500– –2500 ms often reduces the scatter in this plot (as reflected in the displayed value for the “rms”). For good speed runs, values around 0.99 for the recovery factor are expected for RTH1.
 - (b) “angle of attack”: The second plot that can be selected using the “type of plot” drop-down menu shows the angle of attack (AKRD) along with the value AOAREF expected if there is zero wind. A fit represented by $AOAREF = c_0 + c_1(ADIFR/QCF)$ has the coefficients shown at the top of the plot. Typical values of these coefficients vary among projects but are often about 4.4 and 21. If AKRD and AOAREF differ significantly, either conditions are poor for the speed run (perhaps with real vertical wind on nonuniformity of temperature) or the empirical representation of AKRD may need re-evaluation.
 - (c) “airspeed dependence”: The last plot supports display of variables as functions of airspeed during the speed run. Portions while the airspeed is increasing are shown as green dots, while portions with decreasing airspeed are shown as red dots. This display

is often the best way to determine the time constant of sensors, because for linearly increasing or decreasing airspeed the offset is equal to the time constant. Introducing a delay to minimize the difference between the two sets of dots in the plot (as represented by the rms) is a good way to determine that time constant. This often indicates a time constant for RTH1 of about 2.3 s, although that may vary with the air density at the flight altitude. The dropdown menu “other variable” provides choices of other measurements so that the same can be used with any airspeed-dependent measurement.

You can click the “Info” button to see more information about speed runs and the use of this tab.

3. “Pitch”: The pitch maneuver is used primarily to test the immunity of the vertical-wind measurement to aircraft vertical motion. The displayed plot shows three time-series lines, for PITCH, ROC (rate of climb), and WIC. The blue line indicating PITCH can be used to determine where the pitch-maneuver lies in the displayed time interval. During that maneuver, it is desirable that there be no correlation between ROC and WIC as would be expected if the aircraft motion does not affect the measurement of vertical wind.
 - (a) A time-slider control can be used to set two time intervals, one for the “environment” (which is best set to include times near the pitch maneuver when the pitch and vertical wind are steady) and a second for “pitches” that should be set to include only the pitch maneuver. (These can be set by “brushing” along the time-series plot with the appropriate choice, environment or pitches, selected.) An additional cyan line is plotted along the bottom of the plot to indicate the region selected for the pitches. The reason for these selections is that the standard deviation of WIC in the region selected as the environment (excluding the “pitches” region) can be compared to the standard deviation during the pitches. If there is no effect of the aircraft motion, it is expected that these will be equal. Both are listed at the top of the plot. In addition, a “transmission” expressed in percent is calculated by finding the maximum value of the correlation coefficient between WIC and ROC when various delays are imposed, determining from that the standard deviation is WIC that can be attributed to correlation with WIC, and calling “transmission” 100 times the ratio of that standard deviation to the standard deviation in ROC. Transmission then represents the percentage of the imposed aircraft motion that enters the measurement of vertical wind while compensating for possible delays between the signals. Desirable results are to have the RMS in WIC be smaller than 10% of the RMS in ROC, to have transmission <10%, and to have the standard deviation of WIC during maneuvers not be much larger than the same standard deviation in the environment.
 - (b) In addition, this tab includes two sliders to control the time shift imposed on PITCH and ROC. It is often possible to reduce transmission significantly by adding these adjustments. When that is the case, it may be useful to investigate the time shifts further, but there are many other ways to determine the time shift. (See, for example, the technical note on the Kalman filter.)

Some additional information can be viewed by clicking on the “Info” button.

4. “Yaw”: The yaw tab acts like the “Pitch” tab, so the preceding instructions apply to this display also.
5. “Circle”: The “Info” button under this tab provides extensive discussion and references for the circle maneuver, so that won’t be repeated here. Instead, this item will focus on usage of the tab:
 - (a) Select a checkbox under the “select circle maneuver” menu (if any are shown). If there are none, that indicates that no circle maneuvers were flown during the selected project.
 - (b) There are three plots that can be selected using the dropdown menu named “plot”:
 - i. “track”: This plot displays the flight track in a reference frame that drifts with the wind, so the display should appear as circles if the maneuver was flown well. The normal flight track includes dashed portions that are outside the period of the flight maneuver and solid-green portions that are the selected flight maneuver. The “set interval” slider can be used to refine the selected times. At the top of the plot two measurements of average wind for the maneuver are listed, one obtained from the measurements and the second determined only from the drift in the flight track. These two values should be in good agreement, at least within 0.3 m/s in wind speed. (The agreement in direction will usually be within 1° if the wind speed is at least 10 m/s.)
 - ii. “WS fit”: This plot shows the variation in measured wind speed as a function of the angle between the heading and the mean wind direction. This plot is discussed in some detail in the NCAR Technical Note on “Uncertainty in Measurements of Wind from the NSF/NCAR GV Research Aircraft.” The “set interval” slider does not affect this plot because the algorithm used selects and right-turn and left-turn segments of the plot that are used. Prior to constructing the plot, time shifts of varying amounts are applied to the heading and the time shift giving the minimum offset between mean values of wind speed for the right-turn vs left-turn portions of the maneuver is used to construct the plot. This time shift is listed at the top of the plot. The measurements of airspeed, binned into intervals in the angle ξ , are the points with error bars, shown separately for right-turn and left-turn portions of the flight track. The orange lines are sinusoidal fits to those measurements. From these measurements, it is possible to estimate the airspeed error and another error that is the heading offset modified by a contribution from the sideslip offset. The results are listed at the top of the plot, and the annotation at the bottom right indicates the standard deviations in measured windspeed before and after application of this correction. For reference, the standard deviation in airspeed without correction is also listed. For good maneuvers and good performance of the wind-measuring system, it is reasonable to expect that the indicated correction to airspeed should be within about 0.3 m/s, the estimated uncertainty in measured wind components. Because this result relies on steady wind speed during the maneuver, it may be

necessary to consider several maneuvers before making adjustments to the measurements. Interpretation of the angle offset obtained using this procedure requires an additional test, as described with the next plot.

- iii. “SSRD offset”: Offsets in the heading and in sideslip affect the measured wind in almost the same way during level flight, so an additional step is required to separate these effects. As explained in the text displayed when the “Info” button is pressed, these have different effects in turns and that can be used to separate the two offsets. The estimated offset in sideslip from these measurements is shown as a histogram in this plot. Individual measurements have substantial uncertainty, but the mean of the measurements often can be determined with a standard deviation of about 0.02° . Once the offset in sideslip is determined, the offset in heading can also be found by using the results shown in the previous plot. The heading offset so determined is also listed in the annotation at the top of the plot, along with the sideslip offset that was used in processing and the one that this analysis suggests. (For this plot, the “set interval” slider has no effect because the measurements to be used are selected automatically from the appropriate parts of the full flight track.)
- (c) There are two other controls available in this tab, but they should not be needed during normal use. The “save times” button saves the times selected for this maneuver, and the “delete” button removes the maneuver from the database. These both affect the central database used by all users, so please avoid use of these unless it is necessary. (If the database is modified inadvertently, there is always the GitHub repository from which it can be restored.)
- 6. “Reverse Heading”: The sidebar control panel for this maneuver is similar to that for the circle maneuver. As for that maneuver, the “Info” button provides an extensive discussion of the usefulness of this maneuver and explains the individual plots that are available. This explanation therefore won’t be repeated here.

4.2 The “Known Problems” tab

Scope

Only a few known problems are dealt with in this version. Others will likely be developed in the future as appropriate problems are recognized. Each of the lowest-level tabs is discussed in one of the sections below. All share the top-panel entry slots for “Project” (a dropdown menu of those available) and for “Flight” (a numeric entry assumed to refer to a research flight unless the “test flight” checkbox is selected).

The DP overshoot/SS tab

This tab supports some rather complex operations not documented elsewhere, so this manual section is more involved than most.

The chilled-mirror instruments depend on maintaining the mirror temperature in equilibrium with the dewpoint, so lags in heating or cooling the mirror can cause the measurement to lag behind the right value and then to overshoot when reaching the right value. This is common during descents when the dewpoint increases rapidly, but it also occurs at other times as well. The purpose of the “DP overshoot/SS” tab is to identify such regions and possibly tag them for further action, which may include setting the measurement to be missing (i.e., the missing value flag -32767) or adding a data-quality flag to the output indicating that the measurement is suspect. The QAtools Shiny app does not add such flags to the archive, but it records time periods that might need such flags. Four types of time-interval candidates are identified: (i) overshoot; (ii) supersaturation; (iii) out-of-balance; and (iv) miscellaneous analyst-identified intervals. Sets of such intervals can be saved as R data.frames, easily converted to EXCEL spreadsheets, that have names like DQFCsetrf03.Rdata and are saved in a subdirectory named “Problems”. In separate processing, these can be used to modify the archived data files, perhaps by adding a data-quality variable or by setting time periods for specific variables to be missing.

The first release of QAtools only provides these tests for DPL. A future change will add similar capability for DPR, but at least for the GV it has been more common for DPR to be unusable so this extension has been postponed.

Instructions: (available also in a pop-up display activated by the “Info” button)

Once a project and flight are selected, a plot will be generated that has these variables:

MIRRTMP_DPL The left-chilled-mirror temperature. (This tab focusses on DPL because, at least for the GV, DPR is so often questionable that it is seldom useful to consider it. Eventually this tab will include a DPL/DPR selection menu.)

DPERR This variable is an estimate of the error in MIRRTMP_DPL based on its second derivative, as described below, and is a useful predictor of overshoot events.

ATX The temperature, provided for reference. (Normally, the mirror temperature should not exceed the temperature.)

CBAL A running-mean value of the BALANCE variable provided by the instrument, indicating times when the mirror temperature is not in balance with the equilibrium vapor pressure.

DPLQUAL This variable is calculated to be an automatically generated indicator of periods when the data quality of the measurement is questionable and should be flagged.

MT_DPL This variable is only shown if the “add VCSEL prediction” button is selected. It is a prediction of what the mirror temperature should be, and it is calculated including compensation for the pressure in the chilled-mirror sensing cavity. The calculation of this variable takes about a minute, and after clicking the button you should wait for the in-progress message at the bottom right of the window to disappear before proceeding. When the VCSEL performs well, departures between this variable and the measured mirror temperature are good indicators of mirror-temperature problems.

If no processing has yet been saved for a particular flight, the displayed plot will show these variables for the full flight. If previous processing has been saved, a set of candidates will be listed in the bottom-left panel, and these can be edited. The initial processing steps differ for these two cases:

- Case 1: No previously saved data-quality file. In this case, the list in the bottom-left panel will include only “none”. The first step then is to generate a list of candidate time intervals where there may be problems. This list will appear when you click the “search” button. These events are candidates for overshooting or unrealistic supersaturation. Additional events will be generated if you click the “auto Flag” button; these are regions flagged on the basis of indications from the instrument that it is not in balance with the existing water-vapor pressure in the instrument cavity.
- Case 2: A previously saved data-quality file exists for this flight. In that case, a list of candidates will appear in the bottom-left pane. Only candidates previously identified as appropriate to include in the data-quality file and listed with “Y” just right of the indicator button in the list will be saved, however. If you want to see additional candidates and perform the full review again, you can select the “search” button. New candidates added by the search button by default have “N” as the to-be-saved indicator, so you can distinguish newly added events from previously saved events. Usually it is not necessary to repeat the “auto flag” process unless previous processing has rejected an interval, and by default auto-flagged intervals have “Y” as the to-be-saved indicator so they will usually already be in the data-quality file.

In either Case 1 or Case 2, you can then proceed to review the candidate events. You can create a list with “Y” indicating events to save in the data-quality file and “N” indicating events to discard. You can proceed using these actions:

1. To change all indicators to “Y”, click the “accept all” button.
2. To review a specific event, by click on its radio button. The display will change to a time interval spanning the event but focused on it. A title line will indicate the type of potentially erroneous event (i.e., “overshoot”, “supersaturation”, “balance” or “other”). Modify the event using one or more of the following:
 - (a) There are two time slider controls, one controlling the full period displayed and a second controlling the subset interval to be flagged as questionable. Usually you will not need to change the first, but the second may need fine adjustment. The easiest way to set this interval is to “brush” over the desired time interval (i.e., hold down the left mouse button while sliding the cursor over the desired interval). You can reset this interval to the full displayed interval using the “reset this slider” button, with the “brush affects which slider?” menu set to “data-quality flag...”, or you can move the delimiters on the second time slider (perhaps using the left/right arrows after clicking on the slider delimiters for fine adjustment). When you adjust the data-quality-flag time interval, the “Y/N” indicator is automatically set to “Y”.

- (b) Use the “reject” button to reset the indicator to “N”. The display will automatically move to the next candidate if any remain in the list.
 - (c) Use the “accept” button to accept the event as displayed and move to the next event (if any remain).
 - (d) Use the “next” button to move to the next event without making any changes to the existing event. This has the same effect as clicking on the next radio button.
3. To add a user-generated event to the data.frame, use the “define new” button. You need to use both time sliders in this case, the top one to define an appropriate display interval for the event and the bottom or data-quality one to define the limits of the interval containing data to be flagged.
4. When the displayed “Y/N” indicators are set appropriately, click the “save” button. **Unless you do, nothing will be saved and you will need to start over when you return to this flight.** Changing the project or flight number also replaces the working list with an appropriate one for the new flight. You can save repeatedly because each save overwrites what was saved previously, so it’s useful to save frequently while working through the candidate list.

Additional Details:

1. *The format of the data-quality data frame*

The variable names in the data-quality data.frame are named {Start, End, dqStart, dqEnd, Use, Flag, Type}. They are respectively the start and end times for the interval to display (usually about 2 min before and after the event, the start and end times of the candidate interval with questionable measurements, a logical variable (always TRUE in the saved file) indicating if the event should be saved, a flag indicating the severity of the evidence of an error, and the type of event.

This is some additional information on the event types, which can be one of these four:

- (a) Overshoot candidates, identified by an algorithm discussed below that is based on the second derivative of the measured mirror temperature.
- (b) Supersaturation candidates identified from regions where the dewpoint exceeds the temperature by more than 4°C. This fairly large tolerance was selected because otherwise an unmanageable list was produced in some cases. This tolerance may be adjusted in the future.
- (c) Out-of-balance candidates, identified from the “BALNC” variable provided by the chilled-mirror instruments that is an indicator of times when the instrument detects significant departure from the correct (in balance) mirror temperature on the basis of a departure from the ice or water thickness expected on the mirror.
- (d) Analyst-defined events that provide a flexible means of adding events not otherwise identified to the data.frame.

2. Calculation of the VCSEL prediction (MT_DPL)

The expected mirror temperature for a dewpoint sensor can be calculated from the VCSEL-measured vapor pressure ($e_{VXL}=EW_VXL$) as follows:

$$r = \frac{\varepsilon e_{VXL}}{p - e_{VXL}} = \frac{\varepsilon e_{CAV}}{p_{CAV} - e_{CAV}} \quad (1)$$

where r is the mixing ratio, p the ambient pressure, ε the ratio of the molecular weight of water to that of dry air, e_{CAV} the vapor pressure in the sensing cavity of the dewpoint sensor, and p_{CAV} the pressure in that cavity. Solving for e_{CAV} gives the expected result that

$$e_{CAV} = \frac{e_{VXL} p_{CAV}}{p} \quad (2)$$

To find the mirror temperature T_m at which the water vapor pressure will be in equilibrium with the ice coating on the mirror, the “enhancement factor” $f(p, T_{DP})$ that accounts for the effect of total air pressure on the value of vapor pressure in equilibrium with the mirror temperature must be included. If T_{DP} is the dewpoint temperature in the cavity, then the dewpoint temperature in the cavity can be found from

$$e_s(T_m) f(p_{CAV}, T_m) = e_{CAV} \quad (3)$$

Then the expected mirror temperature T_m is determined by solving

$$e_s(T_m) f(p_{CAV}, T_m) = e_{VXL} \frac{p_{CAV}}{p} \quad (4)$$

for T_m , where $e_s(T_m)$ is the equilibrium vapor pressure that corresponds to the temperature T_m . The enhancement factor is given in the technical note on processing algorithms, Eq. (26), and the formula for $e_s(T)$, based on the Murphy-Koop equations, is also specified there.

3. Predicting overshoot cases

The control circuit for the dewpoint sensor attempts to maintain a constant ice thickness by increasing or decreasing the mirror temperature via thermoelectric coolers. If the mirror temperature is T_m and the target temperature is T_m^* , the heating or cooling can be modeled as proportional to the difference but with a maximum heating or cooling rate and the possibility of heating past the target temperature, perhaps with a second-order equation of the form

$$\frac{dT_m(t)}{dt} = -\alpha \int_0^t (\Delta T(t') \exp(-\frac{t-t'}{\tau})) dt' \quad (5)$$

where $\Delta T = T_m - T_m^*$. In addition, there will be a limit on the maximum rate of heating or cooling. A reasonable simulation of the overshooting problem at high temperature was obtained with $\alpha = 0.14^\circ\text{C s}^{-1}$ and $\tau = 30$ s, as shown by the green line in Fig. 1, which is a simulation of the actual mirror temperature (red line) on the basis of the mirror temperature predicted from the VCSEL measurements (blue line).

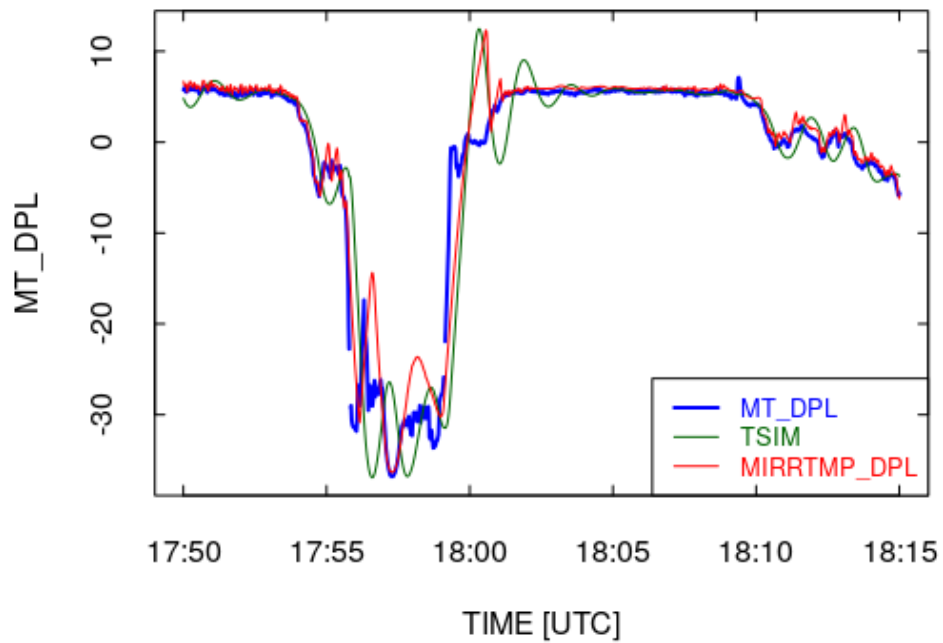


Figure 1: An overshooting example from ORCAS flight 7, 17:50:00–18:15:00 UTC. The line MT_DPL is the prediction from the VCSEL measurements of the expected mirror temperature of the dewpoint sensor, the TSIM line is the simulation, and the MIRRTMP_DPL line is the actual measurement.

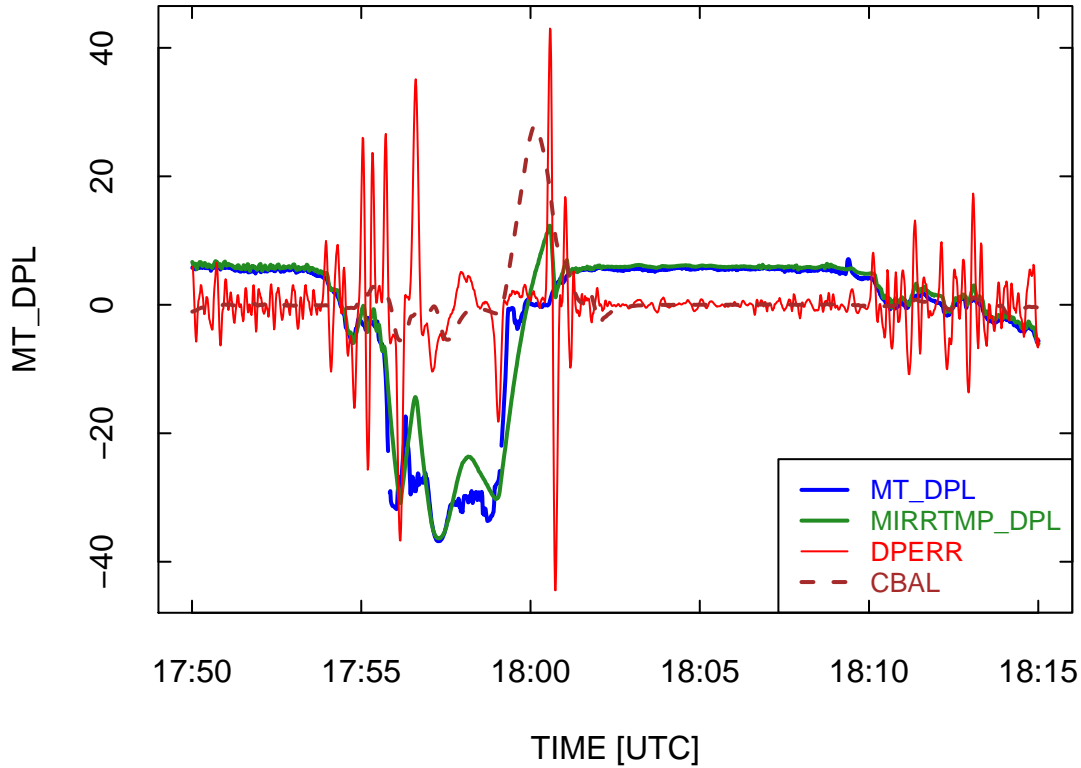


Figure 2: Adding an error estimate DPERR based on (6) and 1-min rolling-mean BALNC (CBAL, dashed brown line) to the previous figure.

Equation (5) can then be used to search for periods where overshoot is expected. Differentiated, this equation leads to the prediction that the measured mirror temperature will be in error by

$$\Delta T(t) = -\frac{\tau}{a} \frac{d^2 T_m(t)}{dt^2} \quad (6)$$

so times where the negative second derivative of the measurement is large are likely cases of overshooting. However, using this to identify overshooting reveals some cases that appear to be valid cases of overshooting but do not seem appropriate to eliminate from the data archives. These might be useful to identify someday with a data-quality flag if that is implemented in the future.

4. The BALNC variable

The measurement DP_DPL is accompanied by a variable BALNC_DPL that represents the

degree to which the mirror temperature departs from its equilibrium value. This provides another means of identifying regions of erroneous measurements of either sign. Periods with extended imbalance tend to develop large errors, so a running mean of the BALNC variable is a useful indicator of times when errors are likely. It may be useful to provide a data-quality flag that identifies such periods. Figure 2 shows an example, where the 60-s running mean of BALNC, divided by 500 for scaling is shown as the brown line. Exploration of this variable suggests that it may be useful to include four data-quality levels: 0 for $\text{abs}(\text{CBAL}) < 4$, 1 for $4 < \text{abs}(\text{CBAL}) < 10$, 2 for $\text{abs}(\text{CBAL}) > 10$, and 3 for data-QC-reviewer-identified problems.

5. *Search for dewpoint-frostpoint transition*

```
## Warning: Ignoring unknown aesthetics: x
## Warning: Ignoring unknown aesthetics: x
```

The standard calculation of humidity from the dewpoint sensors assumes that the instruments maintain the mirror at the dewpoint temperature for measurements above 0°C but measure the frost point for measurements below 0°C. If that is not true, a transition might be expected during climbs and descents as the change from water to ice occurs at some temperature below 0°C during climbs. The predicted DPL mirror temperature from the VCSEL hygrometer (MT_DPL) provides a means of testing if there is evidence of such a transition. For this purpose, measurements were stratified into categories with the dewpoint increasing or decreasing, and then the plot shown in Fig. 3 was constructed to show the difference as a function of mirror temperature. There appears to be an indication of an anomaly near 0°C for both increasing and decreasing mirror temperature. For decreasing mirror temperature (typically from measurements during climb), one might expect an offset to arise from a need to freeze the water on the mirror, which in this case would release latent heat of fusion, delaying cool, and cause the measurement to be too high. This might account for the blue bar just below 0°C in the figure. However, the case of increasing mirror temperature (red bars) shows an offset just above 0°C that cannot be attributed to the reverse effect, because for increasing mirror temperature the melting of ice on the mirror will require additional heat and delay the response of the mirror temperature, leading to a positive error instead. The cause of the negative anomaly during climbs, if real, is not clear.

This study suggests that there may often be an extra anomaly in the measurement of dewpoint from the dewpoint hygrometers just after climb through the 0°C level, and that it may be fairly large, 4–6°C. However, the effect of the difference between dewpoint and frostpoint for measurements during climb, expected to be only about 1°C at –10°C dewpoint, is marginal to detect in this way; either appears to be consistent with the observations in the region from –10–0°C.

To refine this estimate, it is useful to screen the measurements for overshooting and supersaturation, because these often occur in the region of interest and can affect the analysis. This was done for flight 7 of ORCAS and the comparison made between the predicted value

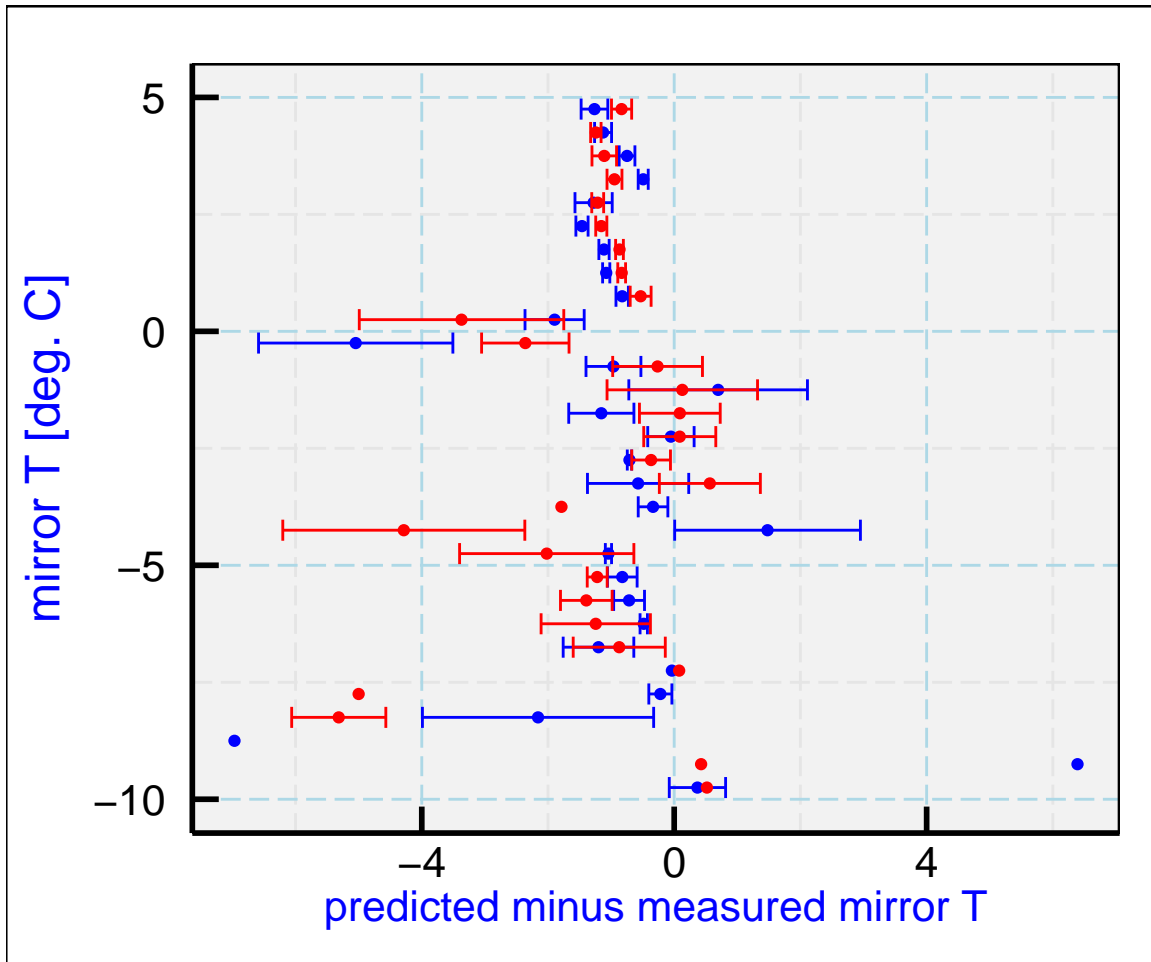


Figure 3: Comparison of the predicted mirror temperature for the DPL sensor, based on the humidity measured by the VCSEL, to the actual measured mirror temperature, for ORCAS flight 7. Blue bars show results for decreasing mirror temperature and red bars are results for increasing mirror temperature.

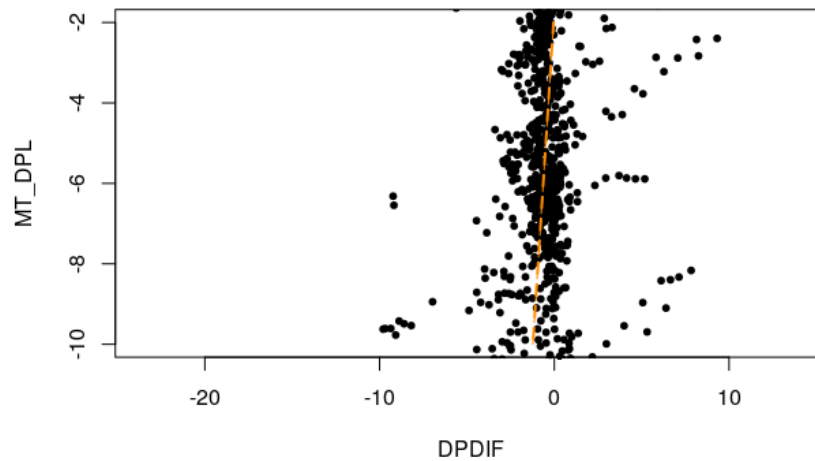


Figure 4: The difference between the predicted mirror temperature (MT_DPL) and measured mirror temperature (MIRRTMP_DPL) for measurements in a climb (with decreasing dewpoint) and after editing the measurements extensively to avoid overshooting and other erroneous measurements from the DPL dewpoint instrument. The regression fit is $DPDIF=0.25+0.15*MT_DPL$, while the slope expected if the mirror surface remains supercooled water is about -0.1.

and measured value of DPL mirror temperature, with the result in Fig. 4.(blue line). The regression-determined slope has the wrong sign to account for an erroneous measurement above a water-covered mirror here, but there is enough scatter in the measurements even after editing to remove suspicious values that it appears not possible to determine if the mirror coating is supercooled water or ice in the temperature range a few degrees below 0°C.

6. *An Example with an Added Data-Quality Variable*

The dewpoint measurement is one where it would be particularly useful to add a data-quality indicator instead of setting the measurements to be missing. This could be automated based on the running mean of the variable BALNC, with suggested thresholds in absolute magnitude at 2000 and 5000. A third level could be assigned for those identified by a reviewer as likely bad.

An example processed in the recommended way, without user intervention, is available: /scr/raf_data/ORCAS/ORCASrf07WAC.nc. The data-quality flag is called DPL_QUAL: 0 => good, 1 => out-of-balance, 2 => seriously out of balance, 3 => analyst-added flag. There are none of the latter category in this file.

The “in-cloud check” tab

The “Info” button under this tab provides instructions regarding use. This information is duplicated here, partly because it is not convenient to print the pop-up display activated by this button.

This section of the QA tool looks for in-cloud measurements using some supplied criteria and then, for measurements meeting those criteria, checks for expected relationships. The key check is the comparison between temperature and dewpoint, because these are expected to be almost the same for most in-cloud conditions. A separate document explores the expected difference in terms of the quasi-steady supersaturation and the expected relaxation time to this value of humidity, and also checks for possible effects of cloud water on the temperature sensor; see this note. However, for the purpose of data review, it is reasonable to expect close correspondence (within less than 0.5°C) between the temperature and dewpoint, except for cases where the liquid water content reaches large values (1 g m^{-3} or more).

Relationships that are reasonable to expect for in-cloud measurements include the following:

- The dewpoint and temperature should be almost the same. The slow response of the chilled-mirror hygrometers affects this comparison, so it is only feasible when the VCSEL hygrometer provides the measurements of humidity (i.e., $\text{DPXC}=\text{DP_VXL}$). In addition, the temperature sensors respond more slowly than desirable (typically 1-2 s), so some adjustment might be appropriate for this response time. In the document referenced above, the humidity measurement was filtered to match the observed response of the temperature sensor, but in the case of the QA tool provided here the only compensation is that it is possible to use measurements only from periods when the sensor has been in cloud for some defined period, typically 3 s.
- Conserved thermodynamic properties obey linear mixing relationships in many cases that reflect the extent to which the cloud properties are affected by entrainment. Examples are the “Paluch diagram” or the “Betts mixing diagram” provided by the Ranadu Shiny app and not duplicated here. Linear mixing lines in such diagrams are reassuring indicators that the sensors are working properly.
- Entrainment is associated with dilution and evaporative cooling, so regions with lower values of conserved thermodynamic properties like wet-equivalent potential temperature or total water mixing ratio are likely to have associated smaller or negative vertical wind. These relationships are not expected to hold for whole-project or even whole-flight data sets but are likely in single cloud passes.

Many other tests can be developed as part of this QA tool, but for now are left to future developments. The focus here is on the temperature-dewpoint comparison.

Instructions for the “in-cloud check” tab:

- At the top of the “in-cloud check” tab there are four numeric-entry windows that allow the user to specify the desired criteria for a measurement to be considered “in cloud”:

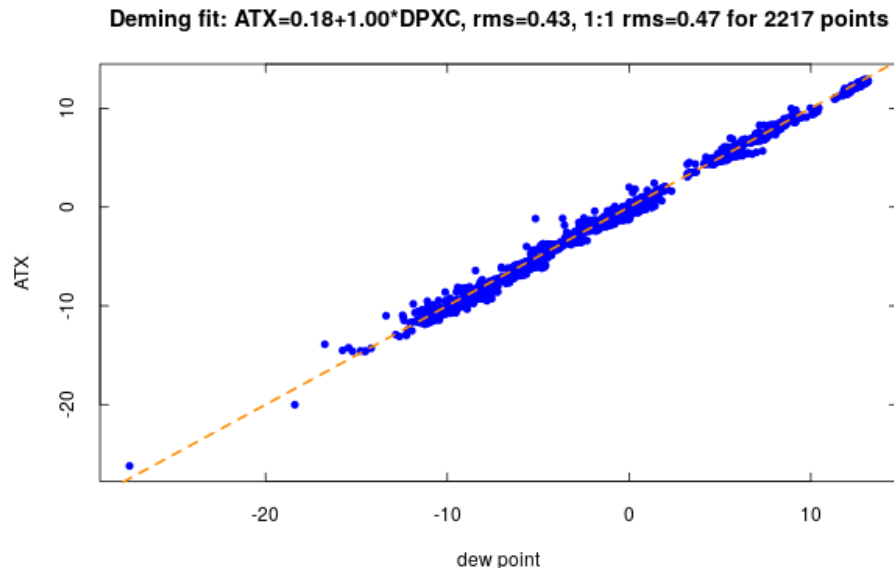
- *CONCD*: The minimum droplet concentration as measured by the CDP. Reasonable values are perhaps 10 in maritime conditions and 100 in continental conditions.
 - *PLWCD*: The minimum liquid water content as measured by the CDP. Reasonable values are perhaps 0.1, although higher values might be explored to search for effects of wetting on the temperature sensor.
 - *seconds*: The required number of seconds preceding a measurement when other criteria for being in-cloud must be met. For example, an entry of 2 means that only measurements that meet the other criteria and for which the preceding 2 s of measurements also meet the criteria will be included. A good starting value is 2.
 - *sigma to remove*: There are often some obvious outlier points that distort fits. Specifying 3 on this line, for example, will remove points that have residuals from the initial best-fit line of 3 or more standard deviations. A value of 2 or 3 appears to be a good starting point.
- *The main plots*: The main plots appear in two windows at the right-side bottom:
 1. The first one is by default a scatterplot showing temperature (ATX) vs dewpoint (DPXC) for all the points in the selected flight that meet the in-cloud criteria. If there are no such points, a message announcing this appears in place of the scatterplot. The orange dashed line in the scatterplot is a 1:1 line (not the best-fit line). At the top of the scatterplot, the intercept and slope for a “Deming fit” (see this note) are listed along with two RMS values, the first relative to the best-fit Deming line and the second relative to the 1:1 line. The number of points entering the plot is also listed. This plot can be replaced by a histogram of the difference between ATX and DPXC by selecting “histogram” from the drop-down menu under “plot type”. The title of the histogram includes the mean and standard deviation of the difference.
 2. The second-panel plot below the first can show either the CDP concentration, CDP liquid water content, vertical wind, or the pair of variables {ATX,DPXC}. These variables can be selected from the drop-down menu under “plot variable”. For this plot, the in-cloud regions are displayed as heavy red lines. In addition, the time interval can be specified for both this and the top plot by dragging the indicators on the “time range” slider or by “brushing” (holding down the left mouse button and dragging) over the desired time interval in the bottom plot. Once a restricted range is selected, you can return to the unlimited range using the “reset time” button near the top left of the display. Don’t confuse this with the “reset flag” because that has another function explained below. The “F4” key also resets the time interval. For convenient stepping through a flight, you can specify an interval like 1 h near the start of the flight and then use the “next” button to step forward by the specified interval or the “previous” button to step backward.
 - *Using all flights*. There is an additional checkbox named “All flights for this project” that will combine all in-cloud measurements from all flights on a specified project. However,

that will often include some periods of bad data that compromise the composite results. To exclude particular times, see the next item.

- *Excluding data.* Sometimes there are periods where the comparison is obviously bad and where, to obtain composite results without those bad periods, it would be useful to exclude some measurements. This section describes how to exclude some intervals and save those results for later use if desired:
 1. First, select the time interval to be excluded. This can be an entire flight or subsets of a flight, but it must be done with the “All flights for this project” checkbox unchecked. For example, you could “brush” the time interval in the bottom time-history plot to select an interval and see the values in both displayed plots. If you decide you want to exclude that interval, click the “flag interval as bad” button. It will be added to the “list of rejected times” at the bottom of the left panel.
 2. If you want to change the excluded event, select the radio button on the left side of the entry and then click “reset flag” to reset the entry.
 3. If you want to save your entries for use another time, click “save” near to middle-top of the display. The rejected times will be saved as a data.frame “BadCloudEvents” in a file “BadCloudEvents.Rdata” and this will be loaded automatically on the next run. This data.frame has the information required to blank-out or quality-flag the data later if desired. The Rdata file can be renamed to preserve it or it can be deleted to start over.

It is particularly useful to exclude bad periods in cases where all-project plots are constructed, because in those cases all the selected reject events will be excluded from the composite plot.

- *An example:* The following figure is an example constructed using all flights from the OR-CAS project, with some data exclusions to avoid outlying points:



The “out-of-range, frozen, spikes” tab

General description:

The starting point for this review section is a list of “raw” variables from a project archive. The variables are selected only if they have no “Dependencies” attributes and so are the original basic measurements. Other variables may depend on these, and in that case any data-quality flags applied to these variables should propagate to the derived variables. The starting-point data.frame is named `frozenRange` and is saved in the file `frozenRange.Rdata`. This is loaded at the start of each run. It was originally constructed using the routine `checkRange.R`. It contains the names of the raw variables, the lower and upper limits of the expected range, the “long_name” attribute from the netCDF files, and two additional flags named “keep” and “Raw”. The first, when FALSE, allows a variable to be ignored in searches for problems, and the second (perhaps poorly named) is FALSE if the variable is primarily a housekeeping variable and TRUE if it is better interpreted as a basic measurement. The range limits and flags can be changed during use and the `frozenRange` data.frame can be saved with the new values. For this reason, a starting-point reference is also stored as `frozenRangeRef.Rdata` so it can be restored if necessary.

The raw variables are reviewed for four problems:

1. measurements outside the specified range of expected values;
2. measurements that appear to be “frozen” – unchanging for a specified time (default 60 s);
3. measurements that appear to be “spikes” – with values more than a specified number of standard deviations (default 3) from a low-pass-filtered version of the signal; and

4. measurements that appear to be “jumps” because their value changes in one measurement interval by more than a specified percentage of the expected range (default 20%).

The results can be saved in a “BAD” data.frame that specifies flagged variables and time intervals for the four problems. This must be saved or it will be lost when the processing run ends. The information it contains can be used later to set data-quality flags or set intervals to the missing-value flag. Three levels of BAD flags are used: (1) for program-flagged questionable variables, (2) for more-serious program-flagged intervals, and (3) for reviewer-flagged intervals. At present, no level-2 flags are generated, but this may be a later enhancement.

More details:

The specific tests are these:

1. *Out-of-range variables.* The expected range limits stored in the frozenRange data.frame are used. These can be changed by changing the “min” and “max” entries, and if desired the modified frozenRange data.frame can be saved using the “save limits” action button.
2. *Frozen variables.* Intervals are flagged if the variable is unchanged (to machine-precision tolerance) for a specified period of time, controlled by the “seconds for frozen” entry window. The implementation uses the “rle” (run-length-encoding) function in base R for efficient searching.
3. *Spikes.* Spikes are identified by first applying a low-pass Butterworth filter to the variable with a bandpass limit determined from the time interval used for the frozen-variable test. To avoid end effects and phase delays, the series is first extended by the specified time interval on each end and then forward and backward filters are applied and averaged. The standard deviation of the filtered variable is calculated, and any original measurements that lie more than a specified multiple of that standard deviation from the filtered value are flagged. The default test is 3, but this can be changed by changing the entry in the “sd for spike” entry window.
4. *Jumps.* Jumps are identified by single-time-interval changes of more than a specified fraction of the expected range for the variable. The specified limits (“min” and “max”) and the percentage change (“% range for jump”) can be changed to adjust this test.

Instructions for using the “out-of-range, frozen, spikes” tab:

This QA function is accessed by selecting the “out-of-range/frozen/spikes” tab under the “known problems” tab in the main window. The project and flight number should be specified in the top entry windows. At start-up, the program will display a time-series plot in the bottom-right window that shows the first variable. This plot shows, as dashed red lines, the specified limits, and any points outside the limits are flagged with green dots. Portions of the time series identified as frozen are plotted as magenta lines, and spikes and jumps are shown as black or orange dots, respectively. In addition, any identified problems will be listed below the plot. Two selection menus control these displays:

1. "plot type" controls the type of plot displayed, which is either a time-series plot as described above or a histogram of values for the selected variable.
2. "list type" selects the list type to display below the plot, and this selection also is used to control the type of search that occurs when the "search" button is clicked. No lists is displayed when the "out-of-range" item is selected, to avoid a very long list.

Details regarding other controls and displays:

In addition, the information in the following table is displayed:

Window label	Contents	Comments
raw variable	Sequence number in frozenRange	
min	Lower limit for this variable	
max	Upper limit for this variable	
[unnamed]below "raw variable"	Variable name	Display only; changes are ignored
[unnamed] right of variable name	Variable long_name	From netCDF file
housekeeping?	Should variable be regarded as housekeeping? (from frozenRange)	If checked, searches can ignore this variable
keep	Should variable to included in searches if other tests are met?	If unchecked, searches will skip this variable.

In addition, these entries control searches for problems:

Window label	Contents	Comments
seconds for frozen	For frozen test, duration without change	Default 60
sd for spike	Limiting multiple of standard deviation used for spike test	Default 3
% range for jump	Limit at which change is considered a jump	Default 20%

The app then has these action buttons:

- reset time: If the time range has been limited to a portion of the flight, either through movement of the time-slider buttons or via the "brush" function, this button resets the time to the full duration of the flight.
- search: Search through variables and make a list of variables with a specified problem. The search target is determined by the "list type" selection box, so that for example of "frozen" is selected then the search will produce a list of variables with at least one identified "frozen"

problem. The result is a list of checkboxes at the bottom left that can be selected to review the variables identified with problems. Any variable with "keep" unchecked will be skipped during the search, and if the "include housekeeping in searches" checkbox is unchecked then any variable with the "housekeeping" checkbox checked will also be skipped.

- flag interval as bad: To use this button, first a time interval should be selected that contains the measurements to be flagged. When this button is clicked, the displayed interval is added to the "BAD" data.frame with the flag variable set to 3, to indicate that a reviewer has entered this manually. Be sure to restrict the time interval before using this button; otherwise, the entire flight may be flagged erroneously as bad.
- add list to BAD: When this button is clicked, the single list specified by "list type", for the displayed variable only, is added to the "BAD" data.frame. This data.frame is not saved, however, until the "save BAD" button described below is clicked.
- add all lists to BAD: This button acts like the preceding button except that all four lists are added to the BAD data.frame. This saves the results for one variable only.
- save limits: Use this button to save the frozenRange data.frame to the file frozenRange.Rdata. This data.frame is read at the start of a run, so that will preserve any changes to limits or flags that have been made.
- save BAD: The BAD data.frame is saved only when this button is clicked. As for the frozen-Range data.frame, BAD is read at the start of a run and added to during processing, so it is possible to construct the resulting BAD data.frame using several uses of the app, adding to the results each time. If the BAD data.frame is not saved, any changes made will be lost when the app is stopped.

Suggested sequence:

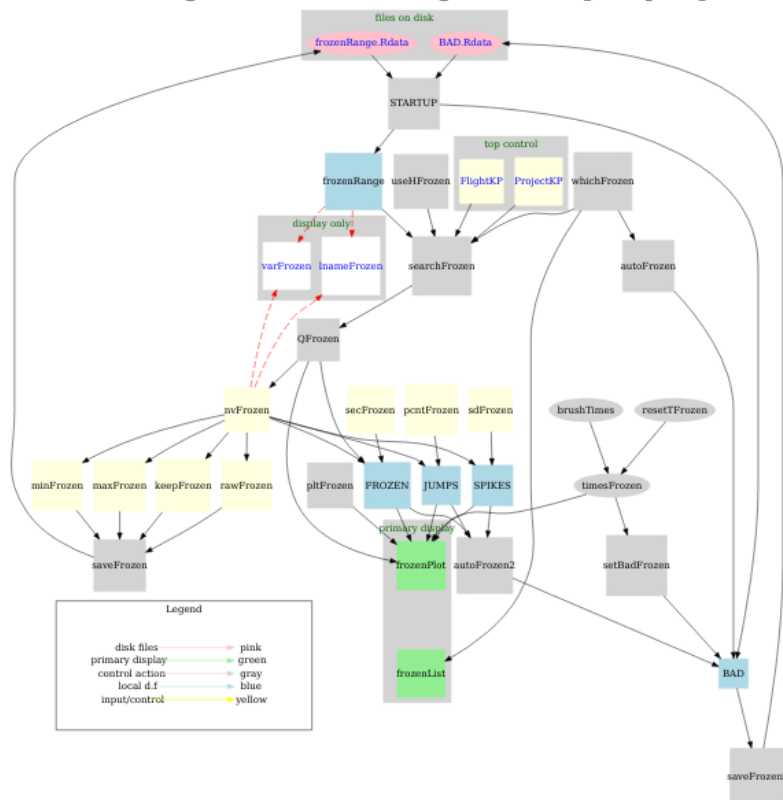
1. Start with the "include housekeeping in searches" checkbox unchecked. Click the "search" button to get a list of candidate events to examine, starting with the default "frozen" entry in the "list type" menu.
2. For each radio button in the list at the bottom left:
 - (a) See the bottom-right list and the magenta portions of lines.
 - (b) If useful, adjust the "seconds for frozen" entry.
 - (c) Note that, for frozen, sometimes discrete available values lead to "frozen" entries that are not really a problem. GGOIDHT is often such an example.
 - (d) If the "frozen" events appear serious, click "add list to BAD" to add them to the current list. Remember that this only adds them to local variables; to save the BAD data.frame to a file, click "save BAD".
3. Select the "out-of-range" List Type. Click "search". For each radio button that appears:

- (a) See the green dots indicating out-of-range points. (They may be overlapped with orange "jump" dots.)
 - (b) Adjust the "min" and "max" entries if needed; save them if you desire to reuse new limits.
 - (c) If the out-of-range events appear serious and appropriate to flag, click "add list to BAD".
4. Select the "spikes" List Type, and click "search". Then, for each radio button that appears:
 - (a) See the black dots indicating spikes and the list of spikes that appears below the plot. The black dots may be overlapped by orange dots, but they are larger so should still give a black halo to the orange dots.
 - (b) Adjust the "sd for spike" entry if needed. You can also adjust the "seconds for frozen" entry because it determines the Butterworth-filter time constant.
 - (c) If the "spike" events appear appropriate to flag, click "add list to BAD". Remember that this only adds then to a local data.frame, so if you want to preserve these results you should click the "save BAD" button.
5. Select the "jumps" List Type and click "search". For each radio button that appears:
 - (a) See the orange dots indicating jumps, and the list of jump times below the plot.
 - (b) Adjust the "% range for jump" entry if needed.
 - (c) If the "jump" events appear appropriate to flag, click "add list to BAD".
6. When finished, if you want to preserve your work, click "save BAD". Also, if you have made changes to the limits ("min" and "max") or the "housekeeping" or "keep" flags, you may want to save the new limits and flags by clicking the "save limits" button.

You may want to repeat this process with the "include housekeeping in searches" checkbox checked, to see the housekeeping events. This will produce many more events to examine, but it may help you identify problems in primary variables that are flagged by problems with the housekeeping events. To see even more events, you can step the "raw variable" number through all the primary variables. This will display everything, even the variables for which "keep" is FALSE. It may be useful also to step through variables with the "plot type" set to "histogram".

Because the interactions among various controls are more complex for this tab than for most, a detailed control diagram is included below, and a similar tabulation of the controls is saved in a spreadsheet file named Frozen.csv.

Control Diagram for out-of-range/frozen/spike/jump tab



The “check DP cavity P” tab

This tab can be used to test if the cavity pressures in the chilled-mirror dewpoint instruments are appropriate. Instructions and a description are included in the left panel of the display.

4.3 The “Special” tab

Non-standard processing routines are provided under this tab for three processing scripts:

1. A Kalman-filter processor that combines GPS-provided and INS-provided information to improve the measurements of wind.
2. A special processing script that calculates new vertical-wind measurements using a complementary-filter empirical representation of the angle of attack.
3. A processor that adds variables representing surface elevation below the aircraft and height-above-terrain.
4. (the tab indicating “Comp filter AKRD” is not yet functional)

In each case, the purpose is to support evaluation of the results, not to implement a processing step that would add these variables to a final archive file. If these processing steps appear useful, that may be encouragement to provide similar processing for the production data archives. The modified netCDF files are saved in the QAtools data directory with identifying names, so they can be retrieved from there and examined further with standard visualization tools like ncplot.

Because there is extensive documentation with each of these tabs (including an accepted but not-yet-published NCAR technical note describing the Kalman-filter processor, that information is not duplicated here. See the reference material provided under the tabs for these scripts for further instructions regarding use. Using these may be slow: It may require an hour to run the Kalman-filter processor on a full project, and if the terrain-height information has not been downloaded previously this can also take 10s of minutes for a new-project download from the NASA-provided data archive.

4.4 More tools

Some components of QAtools have not yet been described in this User Guide. In many cases, use of these components is straightforward and adequately documented in the component itself (for example, for the tool supporting calculation of new variables and addition of those variables to the dataset being used). Others, like the interface to ncplot, will not work in the version supported by the shiny-server but will work when using the RStudio-supported user interface. One component that may be of some interest is the Shiny app version of Ranadu, which can be accessed under the “tools” tab or independently via `HOSTNAME::3838/Ranadu` where `HOSTNAME` is the IP address of the ground station supporting the shiny server. That tools provides a variety of additional plot capabilities and has its own manual which provides rather complete information and guidance regarding use. It will probably receive little use for quality assessment, but it may prove useful in later data-analysis projects.

A Appendices

A.1 The Standard Plots in the “Review” Tab

It may be useful to look at plots from past projects, like these [link XXX] from CSET, when reading the following descriptions. Still better, run the QAtools Shiny app, select the Review tab, and look at something like CSET flight 7 while reading these descriptions.

1. Track plot: A plan-view display of the flight track with some appropriate geographic features (including country and state boundaries). The plot includes wind barbs plotted in the direction *toward which* the wind blows. The standard variables are LATC and LONC, and the wind flag has length 1% of the plot size for each m/s of wind speed. This is only intended for general orientation as context for using the remaining plots. Better flight tracks are available using the kml files produced during normal processing.

2. Time-height plot: The geometric and the pressure altitude of the aircraft as functions of time. A third variable is included based on independent calculation of the pressure altitude; this is a remnant from a time when there was some question about the pressure altitude. The added variable PRZ will normally be exactly equal to PALT. It is common to have differences between the pressure and geometric altitude of 1000 m or more, and in baroclinic conditions it is common for the geometric altitude to vary significantly while the pressure altitude stays constant during flight segments at fixed flight levels (determined by pressure).
3. Time series of temperature measurements: Plot 3 is a time-series plot of the available temperature measurements. It is common for the research temperatures to be in agreement to at least within 0.5C and for the avionics temperatures to be higher, esp. at the lowest temperatures, by as much as 1C. The next plot provides a better way to see these comparisons.
4. Comparisons of temperature measurements: Plot 4 shows pairwise comparisons of the temperature measurements, normally organized to show each temperature vs the selected reference temperature for the project. The black dots are scatterplot symbols for the two measurements, and a regression-fit line is shown with fit coefficients at the top of each plot. The red lines show the difference between temperatures plotted against the reference temperature, so they indicate when there is a temperature-dependent difference in calibration. For example, the comparison of AT_A to the reference research temperature often shows that AT_A is higher at low temperature but in reasonable agreement elsewhere. The scale for the red lines is shown on the right ordinate axis, with dashed lines showing the +/-1C limits. Differences that fall outside these lines are often indicators of problems needing investigation.¹
5. Time-series dewpoint measurements: The available dewpoint measurements usually include the two chilled-mirror sensors DP_DPL and DP_DPR and the dewpoint derived from the VCSEL, DPVXL. The chilled-mirror sensors often show problems arising from inability to sense the lowest dewpoints, slow response, and overshooting effects especially during descents. The VCSEL-provided measurement is often the most reliable. Also shown in this plot is the temperature measurement, which serves as a reference expected to be an upper limit for the dewpoint. Times when the dewpoint exceeds the temperature are indicators of a potential problem, often arising from overshoot. The next plot provides an additional indicator of differences among the measurements.
6. Scatterplot comparison of dewpoint measurements: Plot 6 shows each dewpoint measurement plotted against the selected reference for the project (usually DPVXL). The orange lines denote differences of +/-5C, so significant portions of measurements outside this range indicate potential problems needing further investigation. It is common for the chilled-mirror measurements to differ from the VCSEL-provided measurement at low dewpoint and during rapid descents.

¹ A common deviation is for the two elements in a multiple-sensor probe to differ increasingly at low temperature. This is thought to (possibly) be the result of flow separation at high Mach number and relatively high angle of attack, which would change the recovery factor. This conjecture needs further investigation but produces a common pattern in these comparisons.

7. Comparison of pressures in the chilled-mirror sensing cavities: Recent measurements from the dewpoint sensors have been corrected for the pressure measured in the sensing cavity, and the corrections are quite important. This plot checks the measured pressures in the cavities by comparing them to empirical predictions based on recent projects. Also plotted for reference is the static pressure measurement PSXC. Only pairwise comparison are significant (e.g., CAVP_DPR vs CAVPF_DPR, the latter the empirical prediction), and differences before takeoff and after landing are not significant because they extrapolate the empirical formulas beyond their region of validity. Departures more than usual (10–20 hPa) are indicators of potential problems with the pressure measurements.
8. Comparison of water-vapor-pressure measurements: Another indicator of consistency is shown in Plot 8, where the vapor-pressure measurements, mixing ratios, and relative humidities are shown as time series. For the vapor-pressure measurements, the vapor pressure corresponding to the measured temperature is also shown (as the cyan line) to provide an expected upper limit and a possible reference value when in warm cloud. Significant super-saturation is an indicator of a potential problem, and significant departures from saturation in warm cloud can also indicate a calibration problem with either temperature or water vapor pressure.
9. Ambient-pressure measurements: It is expected that the total pressure measurement PSXC will be in reasonable agreement (0.5 hPa) with the avionics-based pressure PS_A. The difference between PSF and PSFC/PSXC will normally be smaller than a few hPa. The brown line plots PS_A-PSXC relative to the right-side axis, with ± 2 hPa limits shown as dashed lines. The delay and filtering of PS_A will often cause it to differ significantly from PSXC during climbs and descents, but the difference should be small during level flight, where PS_A is often slightly higher than PSXC.
10. Dynamic-pressure measurements: Plot 10 is a similar plot for dynamic pressure. The top panel compares QCR and QCF; the mean difference is often only a fraction of a hPa. The bottom plot compares QC_A and QCFC; like the comparison for ambient pressure, the dynamic pressures often differ significantly during climbs and descents but should be in reasonable agreement (0.5 hPa) during level flight. The difference is again plotted as the brown line in the lower panel, with ± 2 hPa limits shown as the dashed brown lines.
11. Airspeed and Mach number: Alternate tests of the dynamic pressure are provided by Plot 11, which shows the calculated airspeeds and Mach numbers. The top panel also shows the difference between TAS_A and TASX as the red line; it is plotted relative to 200 m/s and amplified so that ± 1 m/s is represented by the dashed red lines. In level flight this difference is usually within the limits shown by the dashed lines.
12. Total pressure: The total pressure is the sum of the ambient pressure and the dynamic pressure. Pitot tubes on the research aircraft deliver reliable values for the total pressure even when there is a static-defect error affecting the individual components, so comparing these pressures from the research pitot tube and the avionics sensors is a stringent test of performance of the pitot tube pressures. These are plotted as PtotF and PtotAvionics, respectively,

and should agree within about ± 0.5 hPa. The red line in this plot shows the difference amplified by a factor of 20 and plotted relative to 500 hPa. The dashed red lines indicate ± 1 hPa limits. A cyan line shown in this plot relative to those amplified limits and centered on 500 hPa shows the difference between the static-pressure correction (or PCOR) reflected in the measurements as PSFC-PSF and that expected from the standard formula as given in the Processing Algorithms technical note. This is a check and should normally be zero.

13. Wind measurements: The three panels in Plot 13 show the horizontal wind direction (WDC), horizontal wind speed (WSC), and the vertical wind (WIC). For the first two, the INS-calculated wind (IWD and IWS) are also shown. These are not as complete as the standard wind measurements because they don't include adjustment to the GPS-provided values of aircraft motion or some parts of the gust components, but they provide an approximate reference that is usually close to the values WDC and WSC. The flight-average vertical wind is shown at the top of the third panel; it should usually be within about ± 0.1 m/s of zero. Applying restrictions (especially to eliminate turns) may improve the agreement.
14. Wind horizontal components: Another view of horizontal wind is provided by Plot 14, which shows the easterly and northerly components of the measured wind (UIC and VIC) and also the INS-provided corresponding measurements IUX and IVY. The differences can be significant, especially in periods with transient changes in direction, because of the weaknesses in the INS-provided measurements, but the measurements should be in approximate agreement in steady flight.
15. Schuler oscillation test: The ground-speed measurements from inertial navigation systems undergo sinusoidal variations called Schuler oscillations. Comparing INS-provided ground-speeds like VEW and VNS to the corresponding measurements from a GPS receiver (GGVEW and GGVNS) will reveal these oscillations with 84 min periods. These differences are shown as red lines in Plot 15, with ± 1 m/s limits shown as dashed red lines. Normal INS operation will keep the magnitude of these errors within about 1 or 2 m/s. Larger errors may call into question the reliability of INS measurements of other variables also, including pitch which is also affected by the Schuler oscillation.
16. Complementary-filter test: Standard processing for horizontal wind uses a complementary filter to combine the good high-frequency response from the INS and the good low-frequency accuracy of the GPS to produce the final wind components. The correction applied by the complementary filter can be seen in Plot 16, where the differences between VEW and VEW and between VNSC and VNS are plotted. These differences mostly reflect the Schuler oscillation in the INS-provided measurements, but the plot is slightly different from the preceding plot because that plot reverences GGVEW in place of VEW. The new information in this plot is that provided by the green traces, which show $DVEWG = VEW - GGVEW$ and $DVNSG = VNS - GGVNS$. The complementary filter, applied as a single-pass filter, does not remove the Schuler oscillation completely, and any remnant suggesting poor performance of the complementary filter will be evident in these variables, but these long-period variations

should be small (ca. 0.1 m/s). High-frequency spikes in these green lines may indicate timing differences between the components entering the wind calculation that need adjustment. These may occur especially in turns or climbs and descents, so the influence of these may be tested by selecting the “apply restrictions” checkbox.

17. Relative-wind angles: The relative-wind angles of attack and sideslip (AKRD/ATTACK and SSRD/SSLIP) are determined by fits to flight periods where it is assumed that horizontal wind fluctuations and vertical wind are negligible, as described in the technical note on Processing Algorithms [ref: XXX]. For vertical wind, the reference is $AOAREF = PITCH - (ROC/TASX) * 180/\pi$. Plot 17 compares this to AKRD. The values should match in regions where the vertical wind is zero, so extended periods of disagreement likely indicate a problem with the empirical representation of angle of attack. The pitch is also plotted in the top panel; this should match AKRD during periods of level flight when the vertical wind is negligible, but it will differ significantly in climbs and descents. The formula used for sideslip is $SSREF = THDG - \text{atan2}(GGVEW-u, GGVNS-v) * (180/\pi)$ where u and v are the respective east and north components of the horizontal wind. These should agree reasonably (ca. 0.1°) during periods when the horizontal wind is steady, but there may be significant differences in turns so it is useful to activate the “apply restrictions” checkbox for this comparison. If there are additional INSs represented in the data file, these variables can be added by CNTL-left-clicking on them in the “variables” menu.
18. INS comparisons: There is usually more than one INS in the aircraft, so the duplicate measurements from these systems can provide an indication of data quality. There are often offsets arising from differences in installation, and those can sometimes change between projects. Typical offsets are used for each project once they are known, but these may need to be changed in the configuration file for the project. Plot 18 compares the pitch, roll, and heading measurements from different INSs. In each panel, the red trace shows a magnified plot of the difference, with respect to the right-side ordinate axis, with $\pm 0.05^\circ$ dashed red reference lines indicating normal tolerances. The offset being used is also included in the title, and if there are consistent different offsets these values should be changed in the configuration file (Configure.R), which has a separate section for each project. Inconsistency from flight to flight or larger-than-expected variations during a flight may indicate a problem with an INS unit.
19. Additional INS tests: The top panel in Plot 19 shows a comparison of the vertical acceleration measured by the standard INS (ACINS) and other units present (e.g., ACINS_IRS2). These will usually be in very good agreement ($< 0.01 \text{ m/s}^2$ mean difference). The middle panel compares the INS-provided rate-of-climb measurement (VSPD) to the similar variable from the avionics system (VSPD_A); these will also usually match with low tolerance ($< 0.01 \text{ m/s}$ mean difference), and the mean values for the duration of the flight will usually be very small ($< 0.01 \text{ m/s}$) if calculated from takeoff to landing at the same airport. The third panel compares the altitude provided by the avionics system (ALT_A) to that from the GPS receiver. These will normally match well, but they will differ from those provided by the INSs because the latter (ALT, ALT_IRS2) are updated to match pressure altitude instead

of geometric altitude. You can add additional variables by CNTL-left-mouse clicking on variables to add (or subtract).

20. Radiation measurements: If present, remotely sensed surface temperature (RSTB) is plotted in the top panel of Plot 20 and upwelling and downwelling IR radiation variables (IRBC and IRTC) are plotted in the bottom panel.
21. Aerosol and hydrometeor concentrations: The top panel of Plot 21 shows the aerosol particle concentrations as time series. The variables plotted include (if present) the CN concentration CONCN, the PCASP concentration CONCP, and the UHSAS concentration in three variables, CONCU, CONCU100 (larger than $0.1\ \mu\text{m}$), and CONCU500 (larger than $0.5\ \mu\text{m}$). The bottom panel includes hydrometeor size distributions. A 60-s smoothing filter is applied to these time series to reduce the noise that is otherwise present in the 1 Hz measurements. Reasonable aerosol concentrations will usually have CONCN highest followed by CONCU, CONCU100, and CONCU500; the latter will often barely appear at the bottom of the plot. Reasonable cloud-droplet concentrations will usually be in the range from a few 10s to several 100s cm^{-3} , and reasonable 2D concentrations will usually be in the $0.1\text{--}100\text{s/L}$ or $10^{-4}\text{--}10^{-1}\ \text{cm}^{-3}$ range.
22. UHSAS housekeeping variables: The UHSAS produces many housekeeping variables, some of which are shown in this plot. Consult an expert (e.g., Mike Reeves) for interpretations of these variables. (That's because I don't understand them well enough to interpret them with confidence, although I have tried in the legends.)
23. Mean diameters: Mean diameters are shown in three panels, the top one for aerosol spectrometers (UHSAS, PCASP), the middle one for cloud droplets (CDP, FSSPs, although the 2DC mean diameter DBAR1DC is also shown for reference but with an inappropriate scale), and the bottom one for precipitation (DBAR1DC with a more appropriate scale). 60-s smoothing is applied to the traces in the top two panels. All are shown with units of μm . Reasonable CDP mean diameters can fall anywhere in the range shown in the middle panel, but large values often arise from false measurements produced by large particles. Mean diameters from the 2DC should only be larger than $100\ \mu\text{m}$ in regions containing drizzle or rain or ice particles.
24. Liquid water content:
 - (a) The top panel in Plot 24 shows time-series plots of the measurements of liquid water content. The best indications of cloud-water content are from the CDP and from the CSIRO/King probe (PLWCD and PLWCC). In regions with real unfrozen liquid water, these measurements should agree, but they often differ by a factor of two or more, probably as a result of incorrect calibration of the sizing in the CDP. If FSSPs (SP100s) are present, the liquid water content from them is also represented in the top panel. In addition, the "RICE" variable indicating the presence of supercooled water is also plotted. This is not a direct measurement of liquid water content, but in the presence of

supercooled water this trace will display a sawtooth pattern as ice accumulates on the sensor and is then removed by heating.

- (b) The middle panel shows the power (PLWC) used to maintain constant temperature in the CSIRO/King hot-wire probe. Normal operation outside cloud will usually require 10–15 W, but this depends on what temperature is maintained by the probe. In water cloud, the power will increase because additional power is required to evaporate the water striking the sensor, and the resulting calculation of cloud water content is that shown in the top panel (PLWCC). If the power ranges outside these limits, the algorithm providing liquid water content may need revision to adjust for a different wire temperature.
 - (c) The bottom panel shows the liquid water content that would be obtained if all 2D images are interpreted as rain drops with the maximum dimension of the image. This is seldom the case, so this is usually a significant overestimate of condensed water content, but it provides an indicator of periods when there is significant ice or precipitation.
25. CDP housekeeping: The CDP provides housekeeping variables that are indicators of the quality of the measurements. These are shown in Plot 25:
- (a) (top panel) The depth-of-field acceptance fraction. This is expected to be around 20–30% in cases where the CDP is measuring cloud droplets. Low values may occur in regions with ice particles, or they may indicate a problem with the optical adjustment of the CDP.
 - (b) (middle panel) The average transit time. Typical values are often around 0.5 μ s. It may be useful to apply restrictions to eliminate before-takeoff times if they are present.
 - (c) (bottom panel) The CDP laser power. When operating well, this will usually be above the dashed red line.
26. Skew-T thermodynamic diagram: This plot provides general context by showing atmospheric stratification. It may be useful to select a restricted time period, for example by changing to Plot 2 (time-height), selecting a climb by “brushing”, then changing back to this plot to see only that climb. You can change back to the full-flight time range using the F4 key. [XXX Need to change the title and add the time range]
27. Potential temperatures: Plot 27 shows time-series plots of the potential temperatures (top panel) and the adiabatic equivalent potential temperatures (bottom panel). This is included primarily to provide for easy time-range selection by “brushing” for use with the next plot.
28. Potential-temperature stratification: This plot show the potential temperatures as functions of pressure, to indicate stratification. Mixed layers will have approximately constant potential temperature, and increasing potential temperature with decreasing pressure indicates stability.
29. CDP/FSSP size distributions: Plot 29 begins a series of examples of the cloud-droplet size distributions. These are plotted in 1-s panels and are only shown when the concentration

is some bin exceeds 1. The units are $\text{cm}^{-3}\mu\text{m}^{-1}$. The times and total concentrations are shown at the top of each plot. Eight panels are shown on each of four plots, if there are that many seconds meeting the display test. To select other starting times, use the “time range, restrictions” time slider or “brush” on a plot like Plot 21, resetting using the F4 key.

30. (see 29)

31. (see 29)

32. (see 29)

33. UHSAS/PCASP size distributions: These plots are analogous to those for the CDP discussed as Plot 29, except that they show aerosol size distributions. The units are $\text{cm}^{-3}\mu\text{m}^{-1}$, and plots are generated only when CONCU exceeds 50 cm^{-3} .

34. (see 33)

35. (see 33)

36. (see 33)

37. 2DC size distributions: These plots are analogous to those for the CDP discussed as Plot 29 above, except that they are generated from the “1D” representation of the 2DC size distributions. The units are $\text{L}^{-1}\mu\text{m}^{-1}$, and plots are generated only when CONC1DC exceeds $0.1/\text{L}$.

38. (see 37)

39. (see 37)

40. (see 37)

41. Air chemistry: This and the following plot are reserved for air chemistry, esp. CO and O3.

42. (see 41)

43. Extra time series: This and the following plot are skeleton time-series plots that can be changed to show any of the measurements in the data file. Use CNTL-left-mouse clicks to add or subtract variables. Sometimes there will be a few-second delay caused by fetching variables from the data file that were not used previously.

44. (see 43)

45. Extra scatterplot: This is a skeleton plot for display of scatterplots. If two variables are selected, the plot will show a single scatterplot; if more variables are selected, the plot will show all possible pairs of variables.

A.2 Enabling a New Project

There are a few steps that need to be taken when this Shiny app is used for a new project:

1. The netCDF files produced for data evaluation need to be at the location searched by the Shiny app. On the raf-groundstation2, this is /home/ads/Data, so data files must be placed in an appropriate project subdirectory like “SOCRATES” and should have path names like “/home/ads/Data/SOCRATES/SOCRATESrf01.nc”. Underscores (e.g., SOCRATES_rf01.nc) will not work in the present structure. so if names like this are used to produce preliminary netCDF files then links to those files with the expected form will have to be created.
2. There is a character vector named “PJ” in the global.R file that contains all the project directories that will be searched for data files. A new project should be added to this list of projects, probably best as the first entry so the start-up default is that project.
3. QAtools searches for available projects at start-up by looking for directories that contain a “rf01.nc” file in the project directory. If there are only test flights, it may be helpful to create a link with a name including rf01 to tf01. This problem should be removed in a future version, but the naming conventions are deeply embedded in these tools so that won’t be done for a while.
4. A file named “Configuration.R”, residing in the QAtools directory, contains information regarding which measurements are available for each project. A section will need to be added to this file for a new project. The existing projects show the general format needed for this addition. For the shiny-server version, this edited file needs to reside in the location “/home/ads/RStudio/QAtools/Configuration.R” and should be owned by the “ads” user.

It may be useful to download revisions to the Shiny app from the repository on GitHub, which should always be up-to-date. The appropriate repository location is saved in the .git directory under the QAtools directory, so to update go to “/home/ads/RStudio/QAtools” and, as user “ads”, type “git pull”. This will update the directory to match the GitHub version.

A.3 Installation Instructions

This appendix covers installation of the QAtools Shiny app in a user directory. After this installation, the user can run this for his/her own use, but it will not be available to others. To make it available for delivery from a web site, the shiny-server must be installed on that web site and the local code must be transferred to the program space served by the web server. Instructions for installation of the shiny-server are available from this web site and are straightforward, so they aren’t included here.

To be consistent with the basic structure used elsewhere, this is best done by creating an “RStudio” directory under the user’s home directory and then creating the following as additional subdirectories under “RStudio”. The first step is to be sure that “R” and “rstudio” are installed and working.

For instructions regarding how to install these and create the following directories, see the “Background” -> “RSessions (tutorial)” -> “Getting Started” section on a working QAtools session or, if one is not available, see the RSessions project on barolo (e.g., log in to barolo.eol.ucar.edu:8787 and go to the “RSessions” project). If all else fails, you can go to the GitHub repository and download the manuals for the Ranadu Shiny app or the Ranadu Manual at these locations: RanaduShiny-Manual or RanaduManual. Both include detailed instructions for initial set-up.

The following table lists packages that are expected by QAtools. These should be installed, e.g., by using the RStudio “Packages” -> “Install” -> “CRAN” tabs.

Package	Required by:
shiny	QAtools
knitr	(misc – generating documents)
ncdf4	Ranadu
maps	“ “
ggplot2	“ “
ggthemes	“ “
graphics	“ “
grid	“ “
nleqslv	“ “
zoo	“ “
fields	“ “
stats	“ “
signal	“ “
reshape2	“ “ and KalmanFilter
plyr	“ “
numDeriv	KalmanFilter

The repositories listed in the following table need to be transferred to a user’s workspace. QAtools relies on functions provided by the R package “Ranadu”. Installing that first will indicate some other packages that are needed if they are not available, so the RStudio interface can be used to add those packages in your local R installation.

The repositories that should be copied to local user workspace under “RStudio” are these, where GitHub addresses should be preceded by <https://github.com/WilliamCooper/>

Directory Name	GitHub address	Provides:
Ranadu	Ranadu.git	utility functions for using netCDF aircraft-data files
QAtools	QAtools.git	this Shiny app for data-quality review
RSessions	RSessions.git	(optional) tutorial regarding using R and Ranadu
KalmanFilter	KalmanFilter.git	(optional) apply Kalman-filter corrections to wind
HeightOfTerrain	HeightOfTerrain.git	(optional) add height-of-terrain variable

In each case, the sequence using RStudio is:

1. File -> New Project -> Version Control -> Git

2. Provide the repository name from the above table (prepending “<https://github.com/WilliamCooper>” without the quote marks), the Project directory name, and “~/RStudio” for where to put the new subdirectory.
3. Click “Create Project”. The system will create the new directory and download the appropriate code.

For Ranadu, you will need to build the package/srv/shiny-server. In RStudio, select “Build” -> “Build and Reload”. If an error message indicates that some required packages are missing from your installation, use the “Packages” -> “Install” -> “CRAN” procedure to download and install the needed packages. This process is not required for the other project directories.

Once all these directories are downloaded, go to the “QAtools” project (e.g., use the RStudio dropdown menu at the top right of the window or the “Open Project” -> “RStudio” -> “QAtools” -> “QAtools.Rproj” menu sequence in the RStudio user interface. In the bottom-left RStudio window (the “console” window that accepts R commands), type “library(shiny)” and the “runApp()”. The application should start and appear in your local web browser. If the new window doesn’t appear, you may need use this procedure: Select the “Files” tab in the bottom-right pane of the RStudio interface, click on “server.R”, then use the dropdown menu that appears near the right side of the top-left pane (the small arrow to the right of the “Run App” button) to select “Run External”.

A.4 More tutorial information

There is a general tutorial on using R and in particular the Ranadu package, hosted at this web address: <https://ncar-eol.shinyapps.io/RSessions> . There is also a summary regarding spectral analysis at this URL: <https://ncar-eol.shinyapps.io/RSessions> .

Reproducibility:

PROJECT: QAtoolsUserGuide
ARCHIVE PACKAGE: QAtoolsUserGuide.zip
CONTAINS: attachment list below
PROGRAM: QAtoolsUserGuide.Rnw
ORIGINAL DATA: /scr/raf_data/
WORKFLOW: WorkflowQAtoolsUserGuide.pdf
GIT: <https://github.com/WilliamCooper/QAtools.git>

Attachments: QAtoolsUserGuide.Rnw
QAtoolsUserGuide.pdf
SessionInfo