Treatment of gas units in RTTOV v11 and new coefficient files for RTTOV v11.3

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Introduction

This document provides details on how RTTOV v11.2 and earlier treated gas units and how this has been improved in RTTOV v11.3 and illustrates the differences for various instruments. New IR and MW coefficient files have been generated for the release of RTTOV v11.3 and the differences between the old and new coefficient files are described.

Status of RTTOV v11.1 and v11.2

Several issues were discovered which affect versions of RTTOV prior to v11.3:

- there were inconsistencies between IR and MW instruments in the assumed units for gas abundances in the input profile;
- inconsistencies were found within RTTOV itself in the assumed gas units for certain calculations although the impact of these is not significant in practice;
- bugs related to gas unit conversions were discovered within the MW coefficient generation code;
- a bug related to the 2m water vapour variable was discovered in the IR coefficient generation.

The situation for RTTOV v11.2 and earlier is as follows:

IR coefficients

The optical depth regression assumed the predictors were calculated in units of ppmv over dry air. Therefore the input units to RTTOV should be ppmv over dry air. Strictly speaking the calculation of atmospheric density (used to determine the geometry of the radiation path) and the calculation of Rayleigh single-scattering for visible/near-IR simulations both assumed input gas units of ppmv over moist air, but the impact of these inconsistencies when supplying gases in units of ppmv over dry air is negligible in practice.

In addition a bug was recently discovered in the IR coefficient file generation which affects all v7 and v8 predictor coefficients generated since RTTOV v11.1. This is related to the 2m water vapour variable and it results in errors in the prediction of optical depths due to water vapour in the lower atmosphere.

MW coefficients

The optical depth regression assumed the predictors were calculated in units of ppmv over moist air. Therefore the input units to RTTOV should be ppmv over moist air. All calculations within RTTOV which apply to MW simulations are consistent with this assumption. However some inconsistencies in the treatment of gas units were discovered within the MW coefficient generation code which have now been fixed.

Changes for RTTOV v11.3

It is expected that the optical depth regression should be superior for trace gases other than water vapour if the predictors are calculated using gas abundances in units of ppmv over dry air because the number of gas molecules (of species other than water vapour) is more directly related to the abundance expressed with respect to dry air than moist air. To obtain consistency between the IR and MW, all MW coefficients have been regenerated using predictors calculated with ppmv over dry air and with bug fixes applied within the MW coefficient generation code. In addition there have been some updates to the oxygen line parameters and the 183GHz line half-width.

In addition all v7 and v8 predictor IR coefficient files have been regenerated to correct the 2m water vapour bug. The v9 predictor coefficient files for VIS+IR sensor channels, v9predictor all-trace-gas hyperspectral sounder files, and SSU coefficient files are unaffected by the bug and so have not been regenerated.

RTTOV v11.3 provides four options for the input gas units:

- **2 => ppmv over moist air.**
- **1 => kg/kg over moist air.**
- **0 => compatibility mode** (default): this treats the gas units as in RTTOV v11.2 and earlier. For IR instruments the input units should be ppmv over dry air.
  For MW instrument coefficient files generated before September 2015 the input units should be ppmv over moist air.
- **-1 => ppmv over dry air**: used by coefficient generation software, but this is a valid option.

The gas units are specified in the profiles structure: *profiles(:)%gas_units*. Where multiple profiles are passed into RTTOV in one call all profiles must have the same value for *gas_units*. The units also apply to the 2m water vapour value in *profiles(:)%s2m%q*.

For *gas_units* = -1, 1 and 2, RTTOV v11.3 provides complete consistency in the treatment of gas units internally and between the IR coefficients and the new MW coefficients. For the AD and K models the output gas adjoints and Jacobians are in the same units as the input gas profiles.

It is recommended that where possible users upgrade to RTTOV v11.3 and that the new coefficient files are used in preference to the existing ones.

The compatibility mode (default) ensures that when using the same coefficient files and input profiles the simulated radiances will not change between RTTOV v11.2 and v11.3 (other bug fixes notwithstanding). Therefore no differences in RTTOV outputs will be observed due to this change when updating from v11.2 to v11.3 unless the value of *profiles(:)%gas_units* is modified and/or the new coefficient files are used.

For RTTOV v12 the compatibility mode will be removed and any value of *gas_units* less than or equal to zero will indicate ppmv over dry air.

Summary of coefficient file changes

IR

In v11.2 and earlier:

- Input gas profiles should have units of ppmv over dry air.

For v11.3:

- Input gas units selected by user.
- Bug related to 2m water vapour fixed in IR coefficient generation (applies to v7 and v8 predictor IR files only).

MW

In v11.2 and earlier:

- Input gas profiles should have units of ppmv over moist air.

For v11.3:

- Input gas units selected by user.
- Optical depth predictors are calculated using water vapour in units of ppmv over dry air to be consistent with IR (if using the new MW coefficients with v11.2 or earlier, input gas profiles should have units of ppmv over dry air, though this is not recommended).
- Bugs fixed in gas unit conversions within MW coefficient generation.
- Coefficients incorporate updates to the oxygen line parameters and the 183GHz line half-width.

Examples of impacts of changes

Impacts in the IR – gas units

Figures 1-4 below show statistics of the differences in IASI and HIRS simulations when RTTOV is run in compatibility mode for a set of profiles passed in ppmv over moist air and the same profiles passed in ppmv over dry air. The plots show the mean, RMS and maximum absolute differences calculated over the diverse 83 profile set used for training RTTOV and over an independent 52 diverse profile set. The simulations were run for a zenith angle of 0º. They give an indication of the errors that may result from running RTTOV v11.2 with units of ppmv over moist air rather than ppmv over dry air for IR instruments.

The largest differences are observed in the window regions. In sounding channels, the small change in water vapour burden (due to the change in units) has only a small effect on the height of the weighting function. However for surface-sensitive channels a small impact on the total atmospheric transmittance can change the top of atmosphere radiance significantly as it modifies the comparatively large surface emission term.

The IASI simulations used the Metop-A v9 predictor 101L coefficient file with all variable trace gases (diverse 83 set) and variable ozone and CO2 (diverse 52 set).

The HIRS simulations used the NOAA-19 v8 predictor 54L coefficient file with ozone and CO2 as variable trace gases.

Impacts in the IR – old vs new coefficient files

Figures 5-7 below show statistics of the differences in IASI simulations between the old and new coefficient files. The new files include the fix to the 2m water vapour bug. Simulations were run the for the independent 52 diverse profile set for a zenith angle of 0º. The three figures show results for the v7 predictor 54L and 101L files and the v8 predictor 101L file. Figures 8 and 9 show the same for NOAA-19 HIRS v7 and v8 predictor 54L coefficient files.

For IASI there are relatively large maximum differences in some channels: these are worst case impacts. Comparisons over the diverse 83 profile training set and over the US76 standard atmospheres show much smaller maximum differences.

Impacts in the MW – old vs new coefficient files

Figure 10 below shows statistics of the differences in ATMS simulations for the old and new coefficient files. The plot shows the mean, RMS and maximum absolute differences calculated over the independent 52 diverse profile set. The simulations were run for a zenith angle of 0º. They give an indication of the differences that may be expected between the old and new MW coefficient files due to the bug fixes in the coefficient generation and the updated spectroscopy.

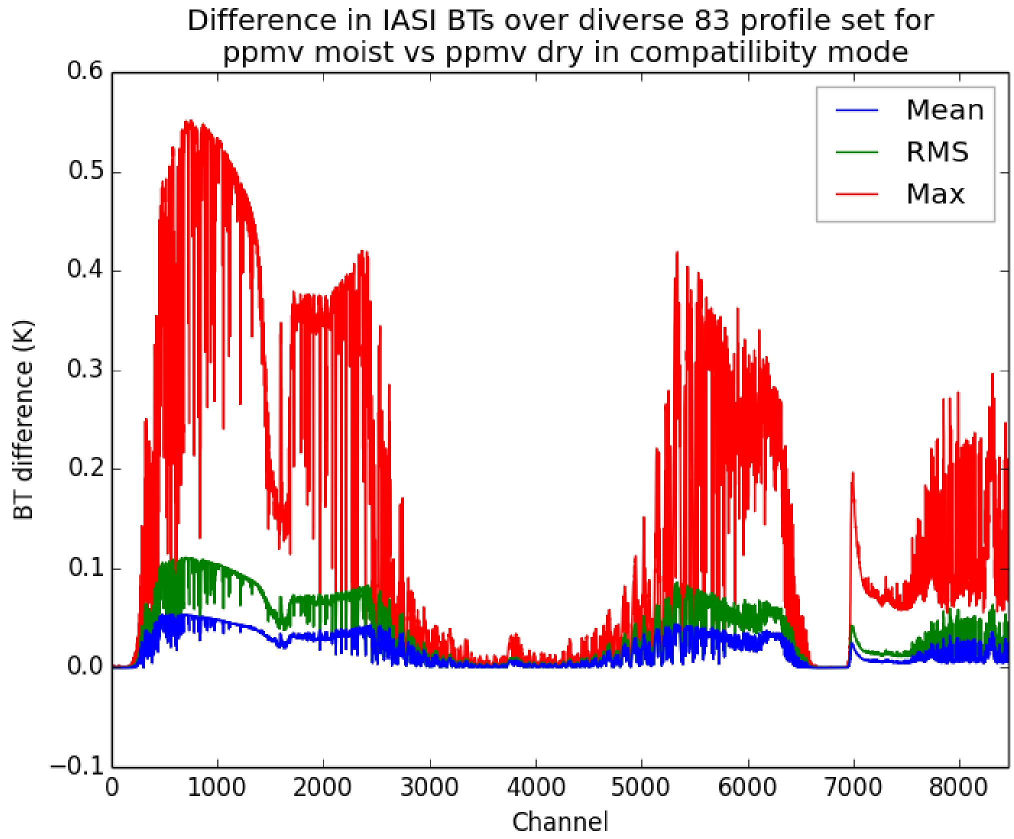


Figure 1

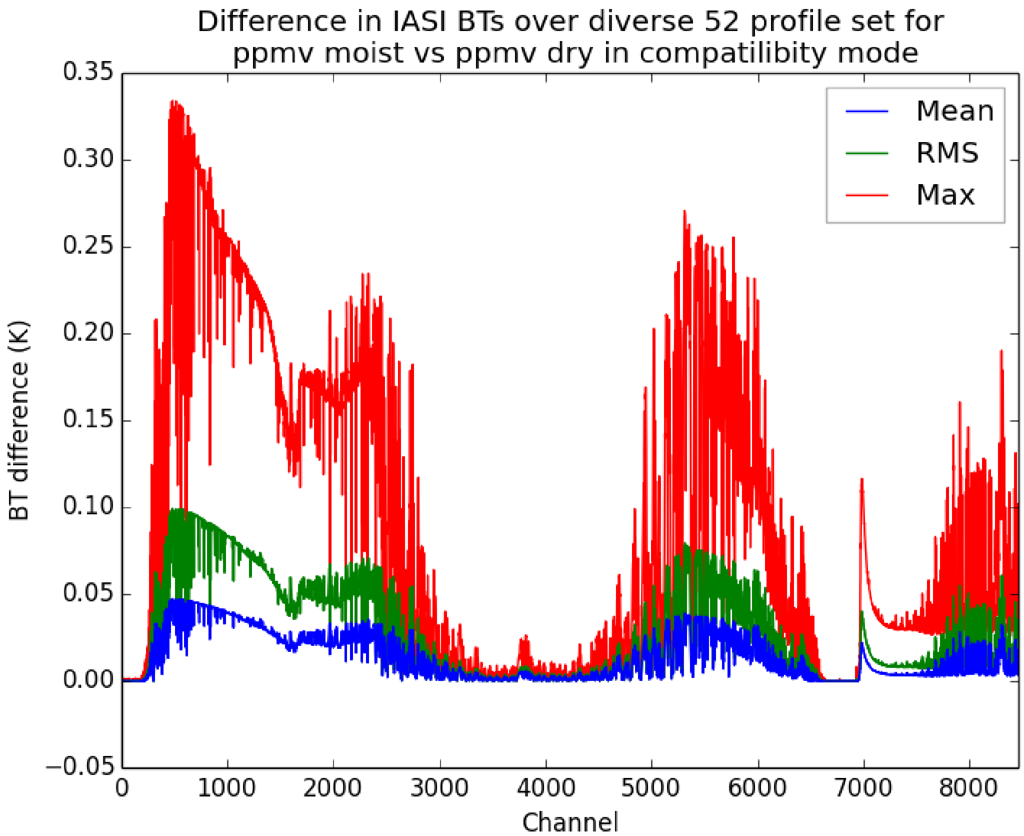
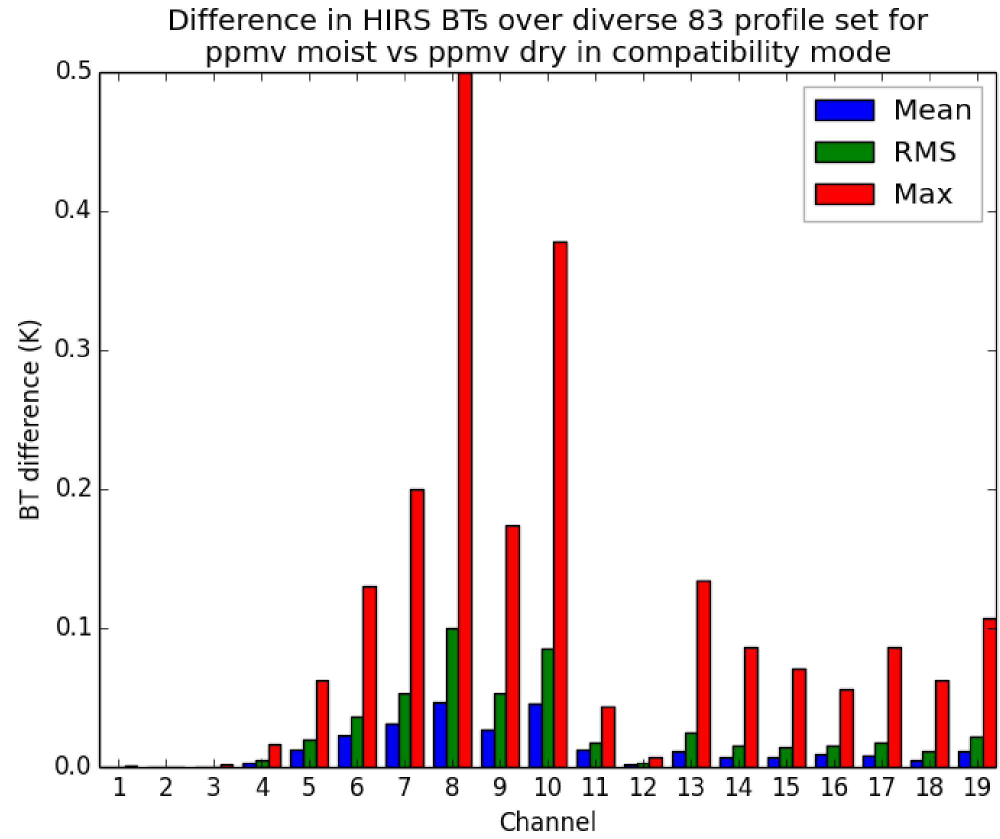


Figure 2



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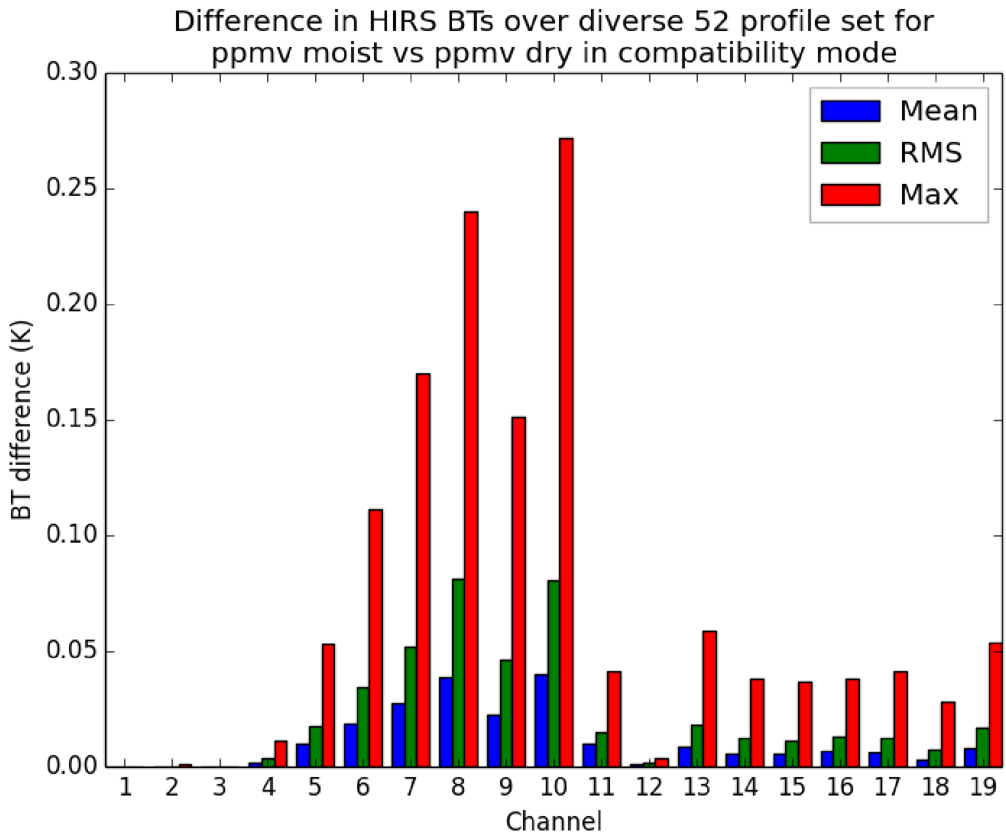

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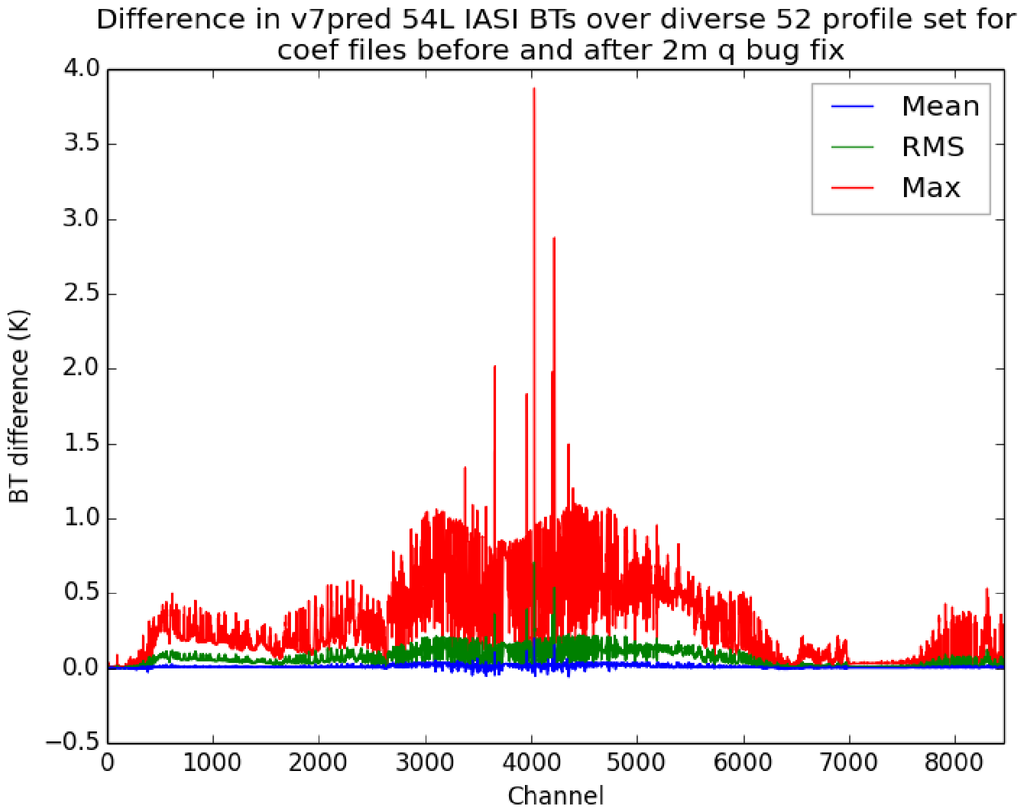

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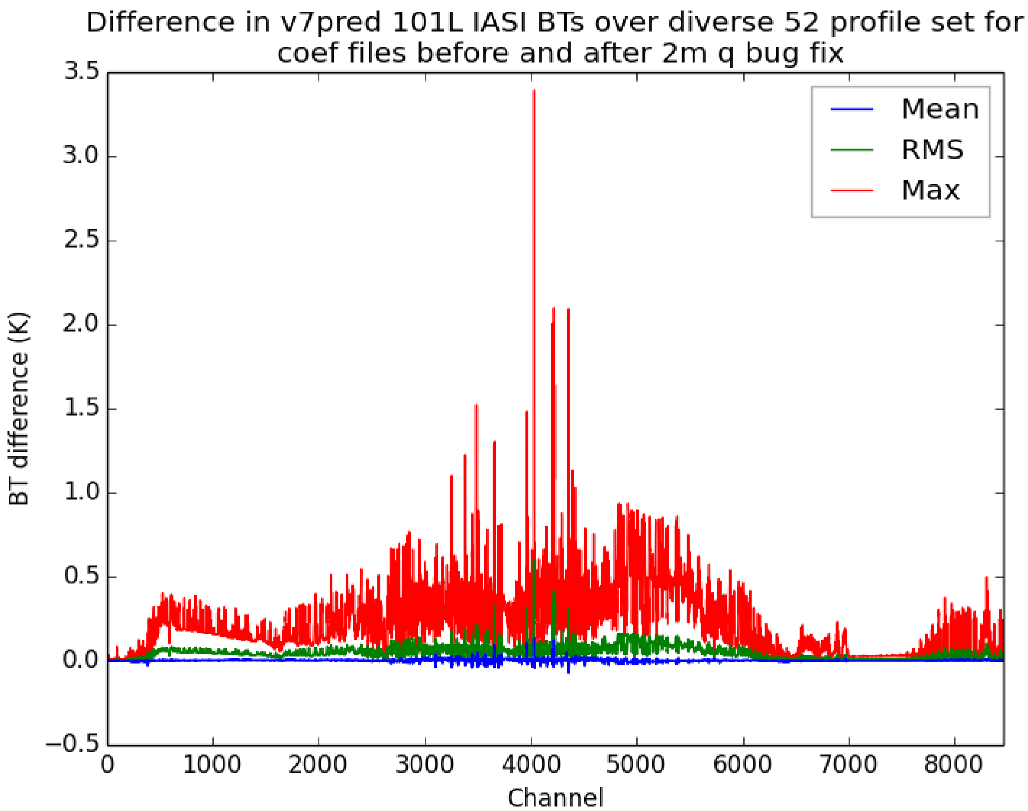

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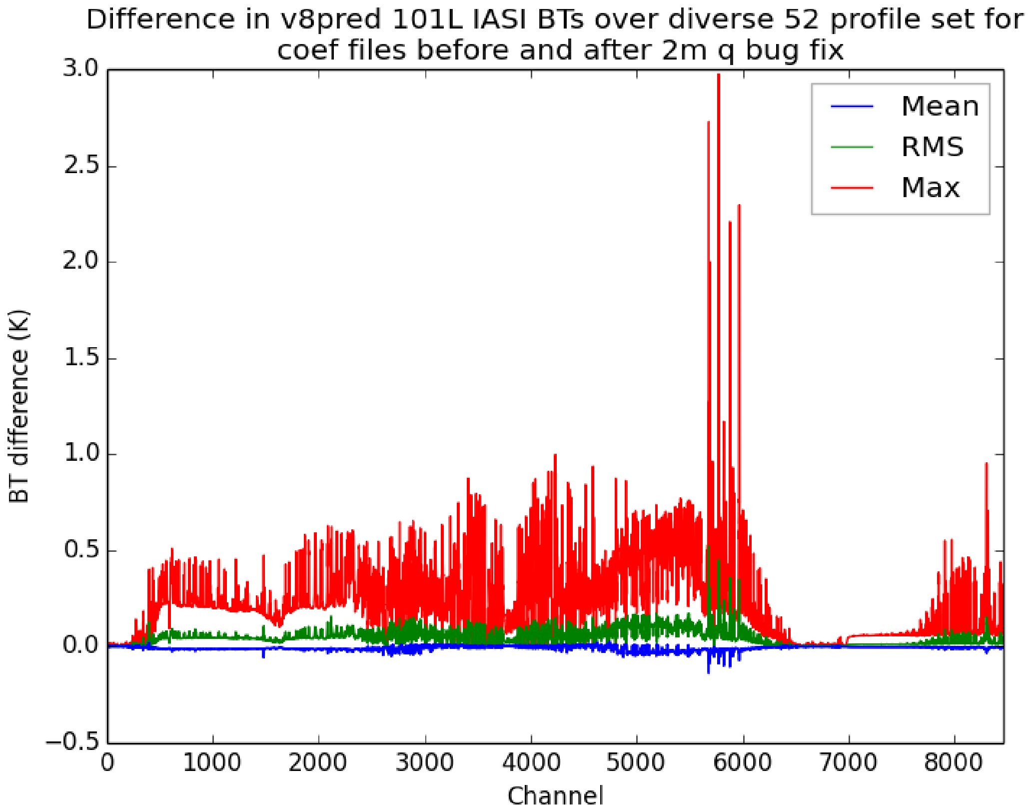

Figure 7

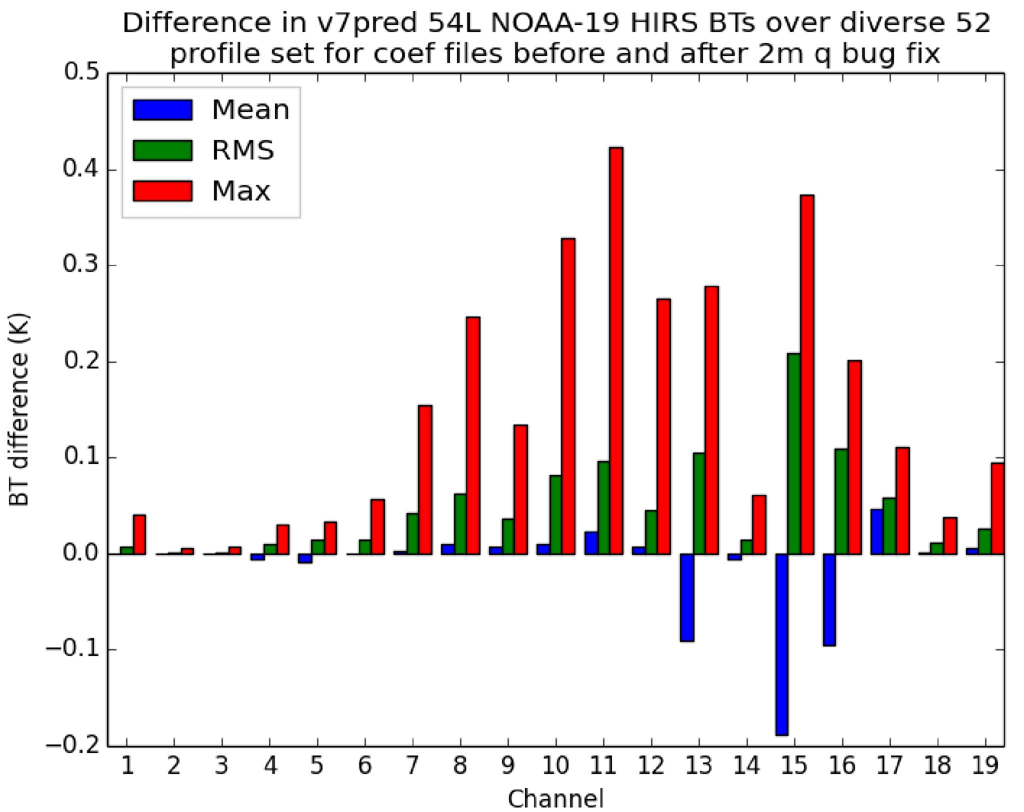

Figure 8

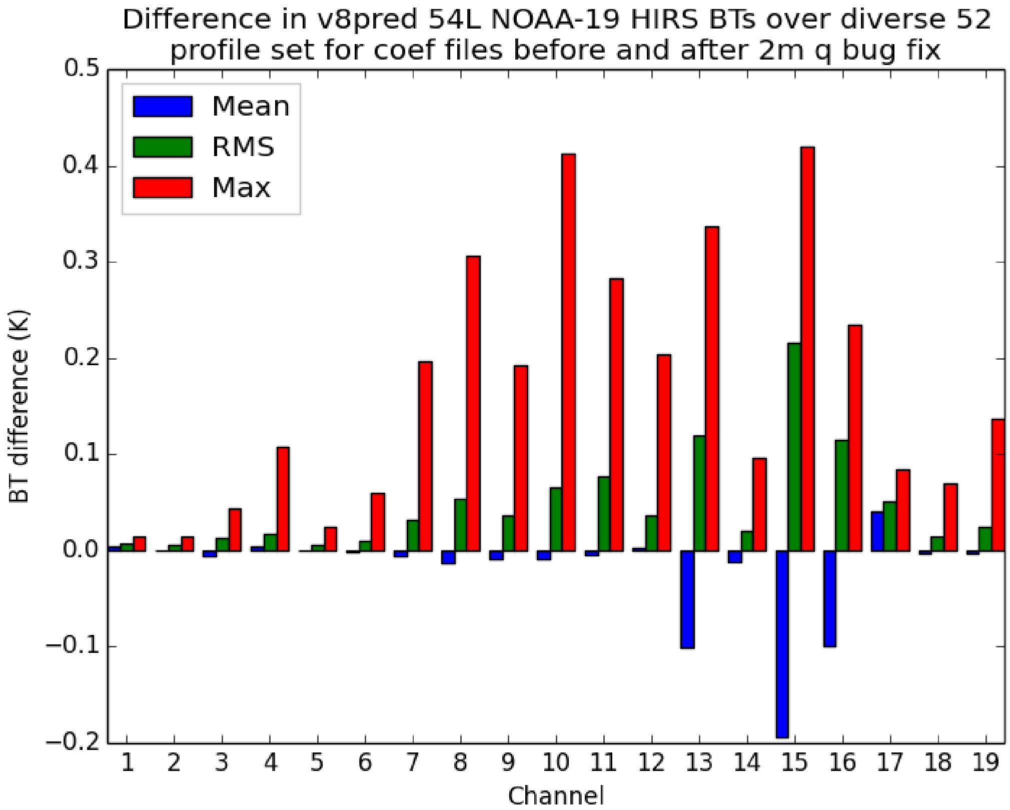

Figure 9

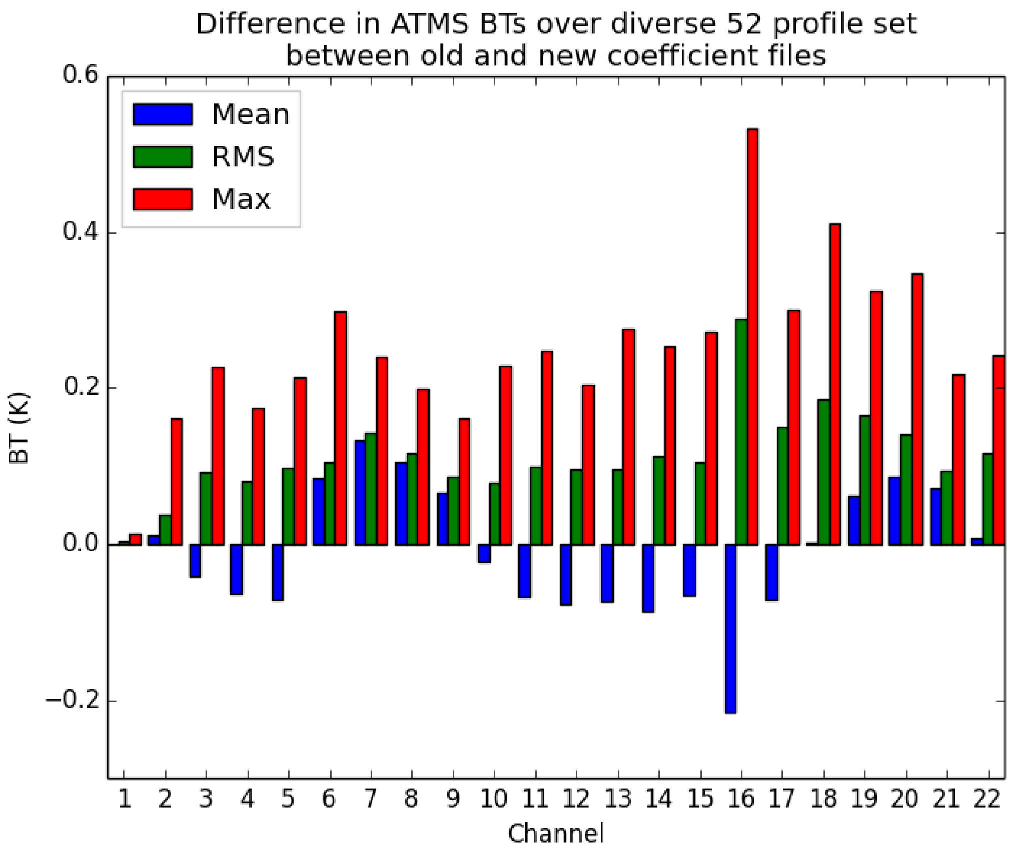

Figure 10