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WFC3/UVIS: New Full-Well Saturation Map Reference File

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ABSTRACT

This report introduces the implementation of a new 2-dimensional saturation map for use in the calibration pipeline for the WFC3/UVIS detector. These changes were delivered in `calwf3` *v3.7.1 on December 7, 2023 for the reprocessing of all UVIS data in the Mikulski Archive for Space Telescopes (MAST). Similar to recent updates to the* `calacs` *pipeline, a new SATUFILE reference file will be used for flagging pixels in the data quality (DQ) array of calibrated images which exceed the full-well limit. The updated version of* `calwf3` *with the new SATUFILE effectively flags the same saturated pixels as older versions of* `calwf3` *using the previous method that applied a single saturation threshold from the CCDTAB reference file. Since the DQ flags do not change with this version of the SATUFILE, users will not need to retrieve the updated products from MAST. For products that are missing the SATUFILE keyword, the new* `calwf3` *will revert to using the CCDTAB threshold value. In the future, improved pixel flagging will be possible by updating this 2D saturation map reference file.*

1. Introduction

Full-well saturation occurs in a charge-coupled device (CCD) when accumulating charge from a central pixel begins to spill into neighboring pixels. In *WFC3 Instrument Science Report (ISR) 2010-10*, Gilliland et al. found that the depths at which saturation occurs varies spatially over both UVIS CCDs. They found a ~10% variation in the full-well depths over both UVIS 1 and 2, ranging from 63,000-71,000 e^- and 67,000-72,000 e^-, respectively. Figure 1 shows the full-well depth distribution over the two chips as derived by Gilliland et al. (2010).

Saturated pixels in UVIS images are identified by the `calwf3` calibration pipeline in the `DQICORR` step and subsequently flagged in the image data quality (DQ) array of the calibrated flat-fielded (FLT) file, an end product of `calwf3`. Prior to December 7, 2023, a single scalar threshold, based on the average of the full-well values shown in Figure 1, was used to identify saturated pixels for both chips. A bitwise flag value of 256 is then set for the corresponding pixel in the DQ array of the FLT file. For unbinned full-frame images, the threshold value for flagging saturated pixels is ~65,500 e^- at the nominal gain of 1.5 e^-/DN. Note that this is larger than the full-well depth for certain regions of the detector (i.e. the blue region in Figure 1, spanning much of the right side of UVIS 1), so saturation flagging using a single scalar value will miss pixels saturated with charge above the full-well depth but below that threshold. In the same respect, pixels that reach saturation at a greater depth than the threshold value (i.e. the orange region in Figure 1, spanning the right-bottom edge of UVIS 2), may be misflagged as saturated by this approach.

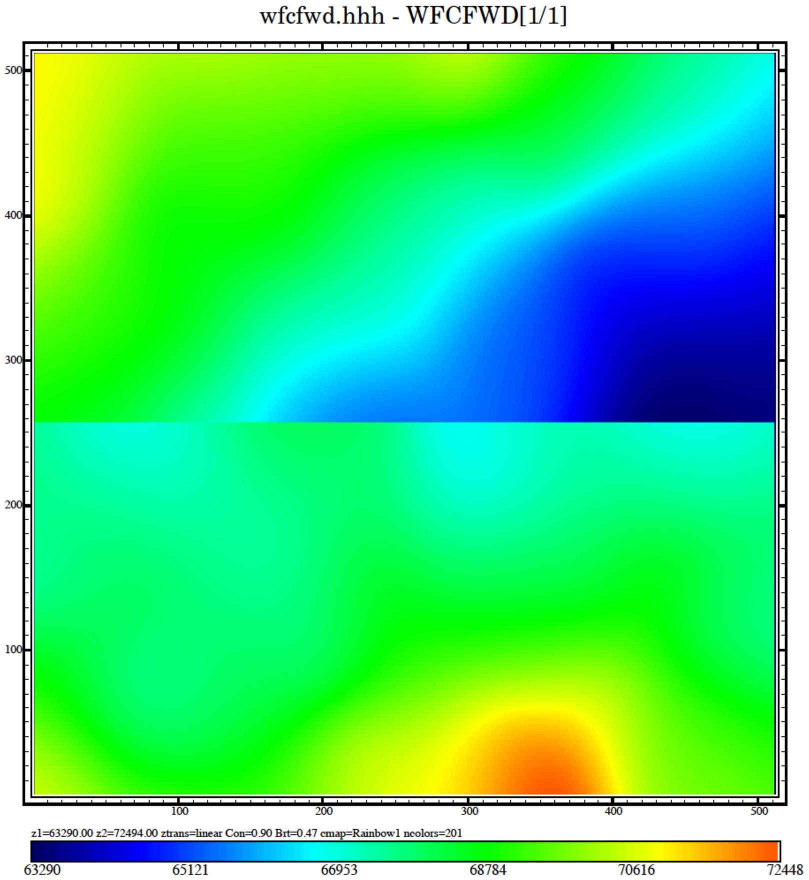

Figure 1. The full-well depth distribution from Gilliland et al. (2010) for UVIS 1 (top) and UVIS 2 (bottom). Prior to December 2023, `calwf3` flagged pixels as saturated when they had a value above ~65,500 electrons. As a result, areas of the CCD where saturation occurs below the threshold may not be flagged while areas with a higher full-well capacity may be unnecessarily flagged.

For `calwf3` to identify and flag saturated pixels of different full-well depths, a 2-dimensional map, rather than a single threshold value, would be needed. This report focuses solely on implementing the necessary infrastructure to enable pixel-to-pixel flagging with a map. Accurately characterizing the full-well saturation levels across the WFC3/UVIS detector, as done in the `calacs` pipeline for the ACS/WFC CCDs (Cohen & Grogin, 2020), is beyond the scope of this particular work.

In this report, we introduce updates to the `calwf3` pipeline (version 3.7.1) that enable a 2-dimensional map to be used for flagging saturated pixels. A new keyword, SATUFILE, now indicates the appropriate reference file to be applied and has been added to `calwf3` and the primary header of WFC3/UVIS FITS files available through MAST. We also detail how the reference files, delivered to CRDS, were constructed and tested.

In Section 2 we give an overview of the changes to the `calwf3` pipeline processes. The format and values for the reference files are discussed in Section 3. Validating the implemented changes to `calwf3` and testing the saturation maps' impact on science data are both discussed in Section 4. In Section 5 we summarize our overall analysis and deliverables, and provide recommendations for WFC3/UVIS users in Section 6.

2. Calwf3 Software Implementation

Figure 2 compares the pipeline processing steps for a single calibrated FLT image using the prior version (3.6.2, left) and new version (3.7.1, right) of `calwf3`. In the prior version, saturated pixels are identified in an initial call to the `DQICORR` function by reading the `SATURATE` values listed in the CCDTAB file. For a commanded gain value (`CCDGAIN`) of 1.5 e^{-}/DN and a commanded bias offset level (`CCDOFST*`) of 3 (corresponding to ~2500 DN), the saturation threshold value is 44,586 DN for 1x1 unbinned and 2x2 binned images, and 45,000 DN for 3x3 binned images, which corresponds to ~65,500 electrons in Figure 1. While not specifically shown in the Data Handbook flow diagram (Figure 3.1, Sahu et al. 2021), the `calwf3` pipeline calls `DQICORR` a second time, after the `BIASCORR` step, to flag 'sink' pixels using the SNCKFILE reference file. Note that this second step is only invoked if both `BLEVCORR` and `BIASCORR` are set to `PERFORM`, as for any observation which opens the UVIS shutter. While calibrated images are not gain corrected after the flat fielding step, the reference files SINKFILE, FLSHFILE, DARKFILE have units of electrons (or electrons/sec), so `calwf3` converts the units of these reference files to DN before applying them to the data.

As of `calwf3` v3.7.1 (implemented in December 2023), the new SATUFILE reference file is also invoked during the second call of `DQICORR`, and under the same conditions as the SNKCFILE. The updated changes to the pipeline are shown on the right panel of Figure 2. A complete history of `calwf3` software changes is available on **Github**[1].

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[1] https://github.com/spacetelescope/hstcal/blob/master/pkg/wfc3/calwf3/History

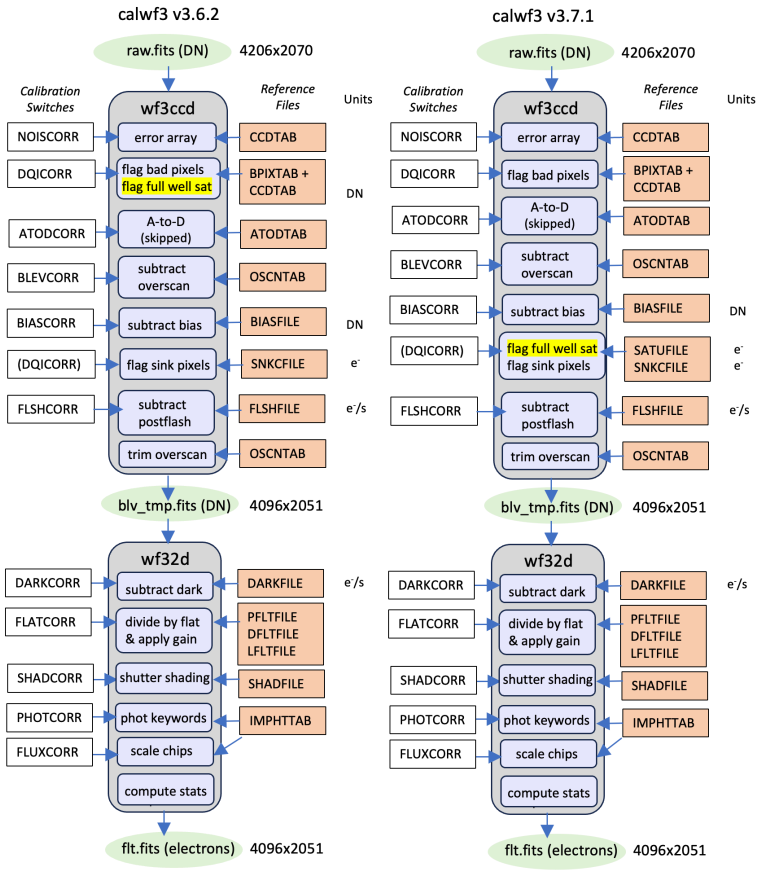

Figure 2. Flow diagram for the UVIS branch of the `calwf3` pipeline which produces a single calibrated FLT file. For simplicity, this diagram excludes the optional CTE correction (`wfcte`) which precedes the `wf3ccd` function and the rarely used `CRCORR` step between `wf3ccd` and `wf32d`. In the left panel, we show an updated version of Figure 3.1 from the WFC3 Data Handbook (Sahu et al. 2022) with more detailed software behavior for `calwf3` v3.6.2. For example, sink pixel flagging is actually performed after BIASCORR in a second call to DQICORR. In the right panel, we show changes implemented in `calwf3` v3.7.1 with saturation flagging now taking place after the flagging of sink pixels.

3. Creating the Reference File

Three saturation map reference files were delivered to CRDS, corresponding to the three on-orbit binning modes available for UVIS external observations: a 1x1 saturation file for unbinned (1x1) and subarray images, a 2x2 saturation file for 2x2 binned images, and a 3x3 saturation file for 3x3 binned images. These maps emulate the single scalar flagging that was previously performed during the first call of `DQICORR` (see section 2), and apply to all UVIS data.

The formatting for each reference file follows the WFC3/UVIS file formats and conventions described in the HST Reference Files Information (HRFI) documentation[2]. There are two maps corresponding to the two 2 CCDs that make up the full UVIS detector array, which are stored

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[2] For more details, see https://newcdbs.stsci.edu/doc/Section11.html

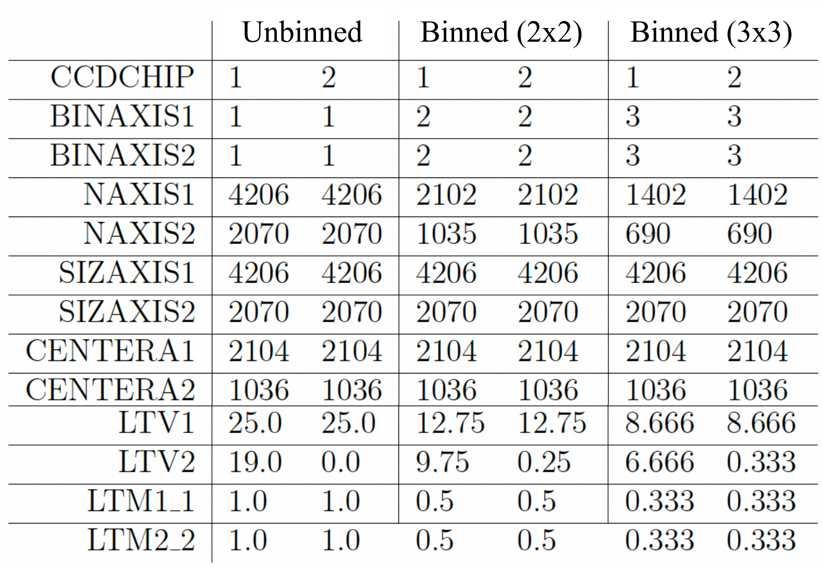
separately in 2 image sets in the saturation FITS file. They are all full-frame to match the format of raw UVIS images.

The saturation reference file is applied after the overscan subtraction step (labeled `BLEVCORR` in Fig. 2), which subtracts the bias level in each CCD amplifier quadrant from the image data. Therefore, to account for this aspect of the data reduction process, each corresponding amplifier quadrant of the saturation maps are also offset by the bias level to ensure correct flagging. Saturation files are also converted from DN to electrons before delivery to CRDS and the BUNIT header keyword is set to 'electrons'.

3.1. **Unbinned Data**

The 1x1 map is a full-framed 2070 x 4206-pixel image with 19 rows of parallel virtual overscan, 30 columns of serial virtual overscan, and 25 columns of serial physical overscan (purple regions in Figure 3). Since full-well saturation flagging of the overscan regions still occurs during the first call of `DQICORR`, the pixels in these regions are set to zeroes in the maps. For more details about the overscan regions of the WFC3/UVIS CCDs see ISR 2003-14 (Bushouse, 2003). In Table 1, we provide a summary of useful image header keywords which define the chip geometry for each UVIS CCD and the corresponding overscan regions for both unbinned and binned images.

Table 1. Image header keywords which define the UVIS chip geometry for unbinned, 2x2, and 3x3 binned data.



	Unbinned		Binned (2x2)		Binned (3x3)	
CCDCHIP	1	2	1	2	1	2
BINAXIS1	1	1	2	2	3	3
BINAXIS2	1	1	2	2	3	3
NAXIS1	4206	4206	2102	2102	1402	1402
NAXIS2	2070	2070	1035	1035	690	690
SIZAXIS1	4206	4206	4206	4206	4206	4206
SIZAXIS2	2070	2070	2070	2070	2070	2070
CENTERA1	2104	2104	2104	2104	2104	2104
CENTERA2	1036	1036	1036	1036	1036	1036
LTV1	25.0	25.0	12.75	12.75	8.666	8.666
LTV2	19.0	0.0	9.75	0.25	6.666	0.333
LTM1_1	1.0	1.0	0.5	0.5	0.333	0.333
LTM2_2	1.0	1.0	0.5	0.5	0.333	0.333

The full-well saturation threshold value from the CCDTAB for 1x1 and 2x2 WFC3/UVIS images is 44586 DN. The commanded CCD bias for each amplifier in DN is recorded in the CCDTAB as `CCDBIAS[A-D]`, and these values are subtracted from the threshold value in their corresponding amplifier quadrants of the saturation map. Finally, the saturation value is multiplied by the average gain of 1.56 e^{-}/DN to convert from DN to electrons. Table 2 lists the original CCDTAB threshold values, the commanded bias levels, the resulting bias-offset saturation thresholds, and the final saturation threshold values in electrons for each amplifier quadrant of the 1x1 and 2x2 saturation maps. Figure 3 shows an image of the final 1x1 saturation maps.

Table 2. Saturation threshold values for each amplifier quadrant from the CCDTAB for the 1x1 and 2x2 saturation maps in DN with the bias removed and converted to electrons using an average gain of 1.56 e^{-}/DN.

Amplifier Quadrant	CCDTAB threshold value (DN)	Commanded bias (DN)	Saturation value with bias offset (DN)	Saturation value (e^{-})
A	44586	2556.4	42029.6	65566
B	44586	2543.8	42042.2	65586
C	44586	2503.3	42082.7	65649
D	44586	2605.7	41980.3	65489

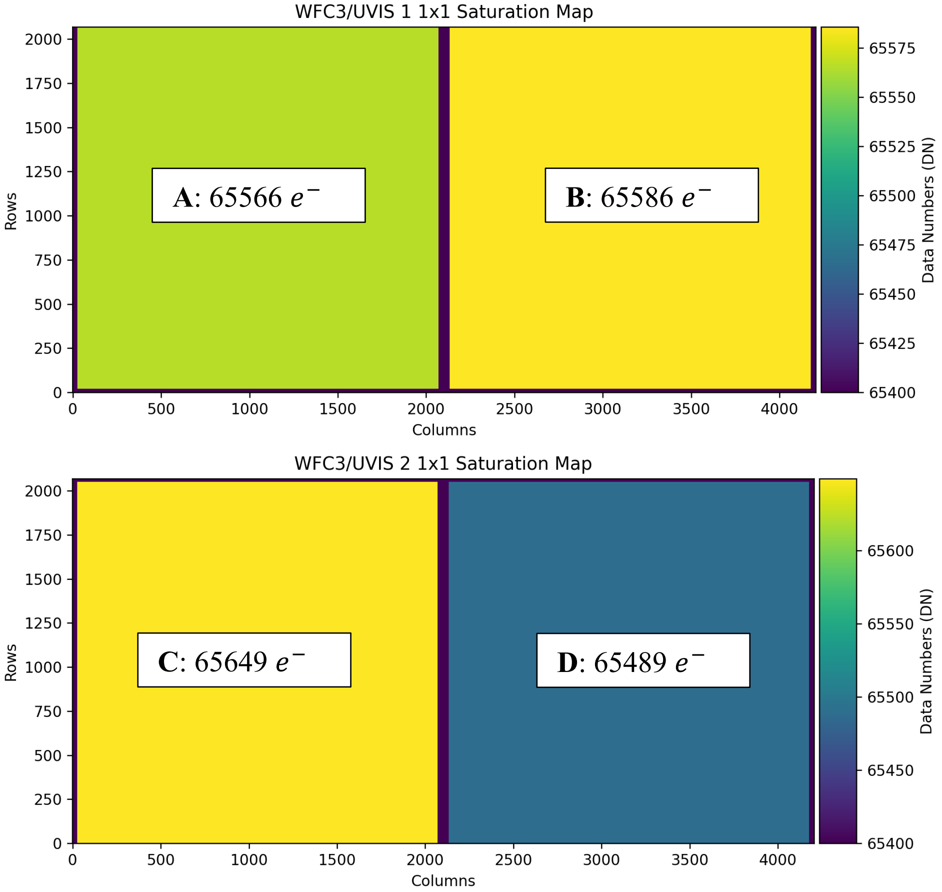


Figure 3. The 1x1 saturation map for UVIS 1 (top) and 2 (bottom). The overscan regions are the purple borders of each amplifier quadrant, and are accordingly set to 0 e^{-} in the saturation map.

3.2. **Binned Data**

When UVIS images are binned, "mixed" rows or columns can occur, wherein a row or column from the overscan region is combined with a row or column in the imaging region (Bushouse, 2003). Because these pixels can no longer provide usable data, we set the value in the corresponding mixed columns/rows of the saturation map to 0 e^{-}. This ensures that the mixed rows/columns are flagged as saturated, to indicate that they should not be used for science. The overscan regions are trimmed from the final image later in the `calwf3` pipeline, but the mixed rows/columns are not, hence the importance of flagging those pixels.

The 2x2 map is a full-framed 1035 x 2102-pixel image with 9 rows of parallel virtual overscan, 14 columns of serial virtual overscan, and 12 columns of serial physical overscan. For 2x2 binned images, in each amplifier quadrant there are two mixed columns (one next to the serial physical overscan and one next to the serial virtual overscan) and one mixed row (adjacent to the parallel virtual overscan). The procedure for determining the saturation threshold values for the 2x2 maps is identical to the 1x1 maps (Table 2). Figure 4 shows an image of the final 2x2 saturation maps.

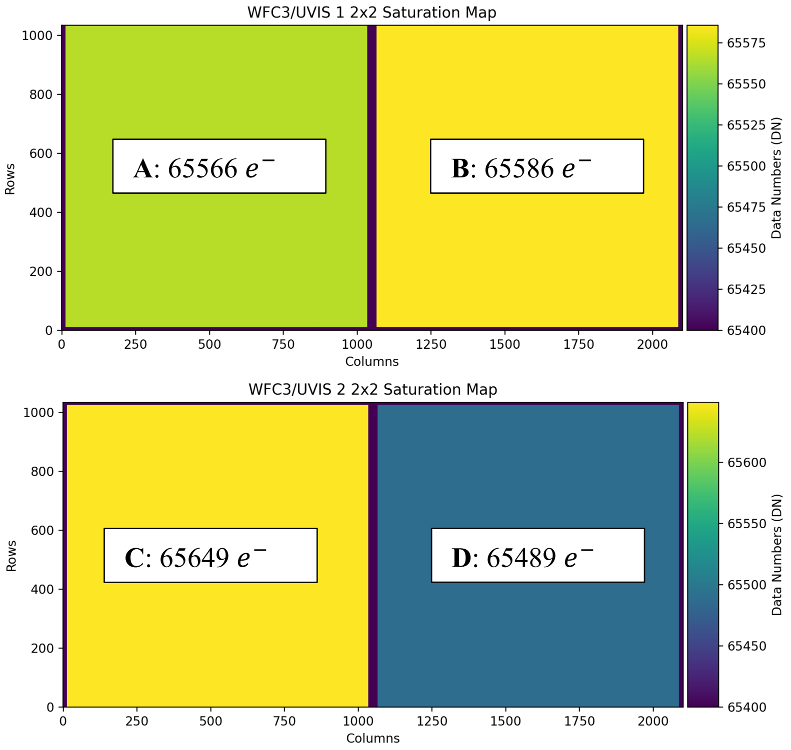


Figure 4. The 2x2 saturation map for UVIS 1 (top) and UVIS 2 (bottom). The overscan and mixed regions are the purple borders of each amplifier quadrant.

The 3x3 map is a full-framed 690 x 1402-pixel image with 6 rows of parallel virtual overscan, 10 columns of serial virtual overscan, and 8 columns of serial physical overscan. For 3x3 binned images, each amplifier quadrant has one mixed column next to the serial physical overscan and one mixed row adjacent to the parallel virtual overscan. The threshold value in the CCDTAB for saturated pixels in 3x3 science images is 45,000 DN. Otherwise the conversion procedure is the same as for the 1x1 and 2x2 maps. Table 3 shows the original threshold values, the commanded bias levels, the resulting bias-offset saturation thresholds, and the final saturation threshold values in electrons for each amplifier quadrant of the 3x3 saturation maps. Figure 5 shows an image of the final 3x3 saturation maps.

Table 3. Conversion of the saturation threshold values per amplifier quadrant for the 3x3 saturation maps.

Amplifier Quadrant	CCDTAB threshold value (DN)	Commanded Bias (DN)	Saturation value with bias offset (DN)	Saturation value (e^-)
A	45000	2556.4	42443.6	66212
B	45000	2543.8	42456.2	66232
C	45000	2503.3	42496.7	66295
D	45000	2605.7	42394.3	66135

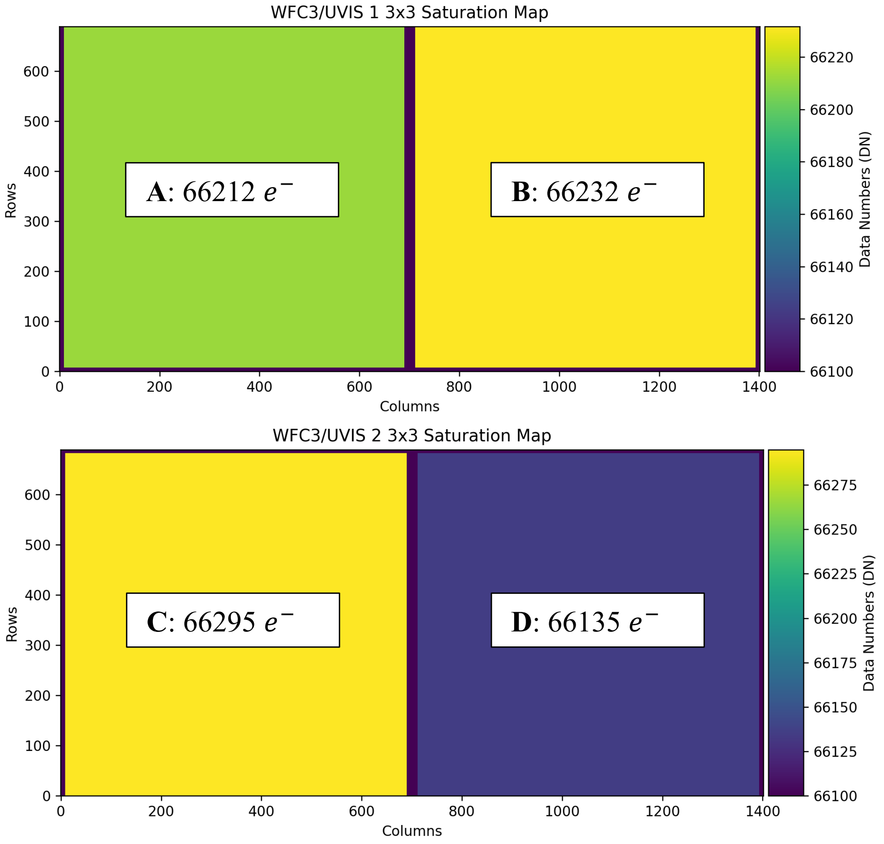


Figure 5. The 3x3 saturation map for UVIS 1 (top) and UVIS 2 (bottom). The overscan and mixed regions are the purple borders of each amplifier quadrant.

4. Validation and Testing

We patch-tested the `calwf3` changes by processing dummy maps and science images through the updated pipeline to confirm it behaves as expected. Figure 6 shows a 1x1 dummy saturation map for UVIS 1 and 2, we filled amplifier quadrants A and C with a value of 100 e^- and amplifier quadrants B and D with a value of 100,000 e^-. This allows us to test both low and high saturation threshold values. In the dummy science image, we placed four evenly spaced horizontal strips across each chip to test for consistency across the amplifier quadrants. From the bottom to top of each chip, the initial values of these strips are 51 e^-, 151 e^-, 100,051 e^-, and 51,999 e^-, as seen in Figure 7. These values are then offset by 51 e^-, when `calwf3` performs the overscan subtraction (`BLEVCORR`) step, yielding final threshold values of 0 e^-, 100 e^-, 100,000 e^-, and 51,948 e^-.

The resulting DQ arrays of the FLT product after processing the dummy science image in `calwf3` with the dummy saturation maps are shown in Figure 8. As expected, regions of the science image in quadrants A and C greater than 100 e^- were flagged as saturated, while the regions in quadrants B and D with values greater than 100,000 e^- were flagged.

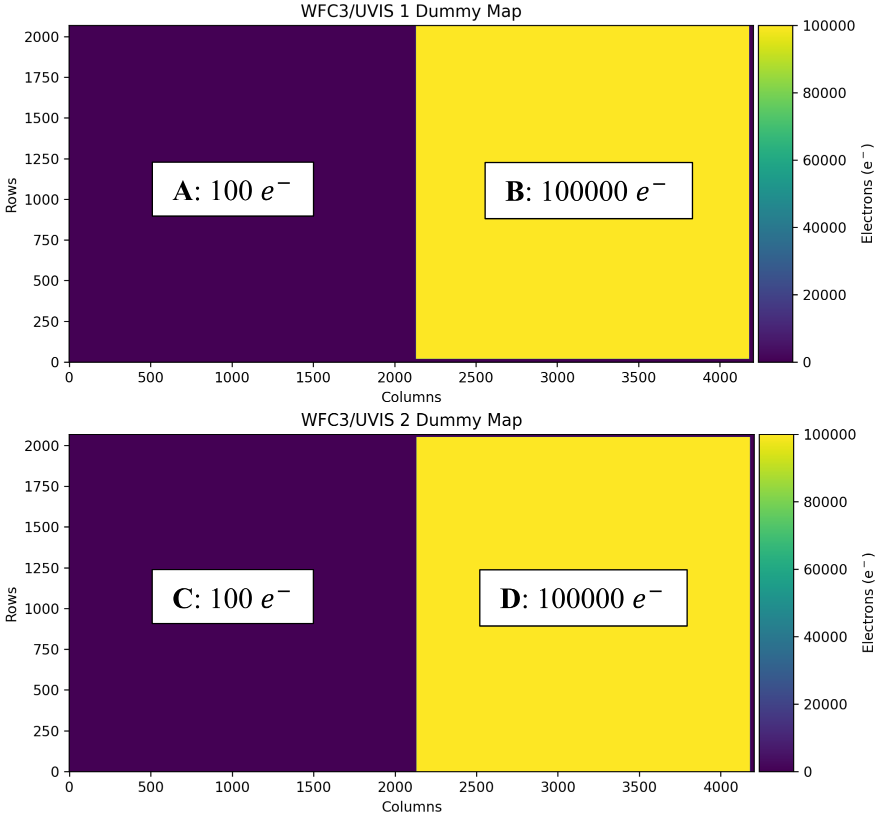


Figure 6. Dummy saturation map for UVIS 1 and 2. The dark, purple regions (quadrants A and C) are set to 100 e^- and the light, yellow regions (quadrants B and D) are set to 100,000 e^-.

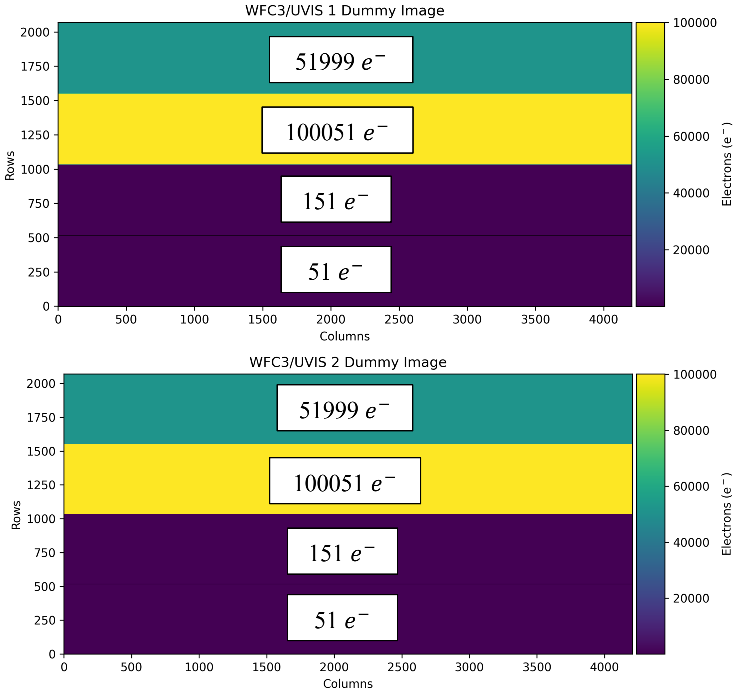


Figure 7. Dummy science image for UVIS 1 and 2. There are four strips of data from bottom to top of each chip set to 51 e^-, 151 e^-, 100,051 e^-, and 51,999 e^-, respectively. They are initialized with these values before overscan subtraction of 51 e^- is applied.

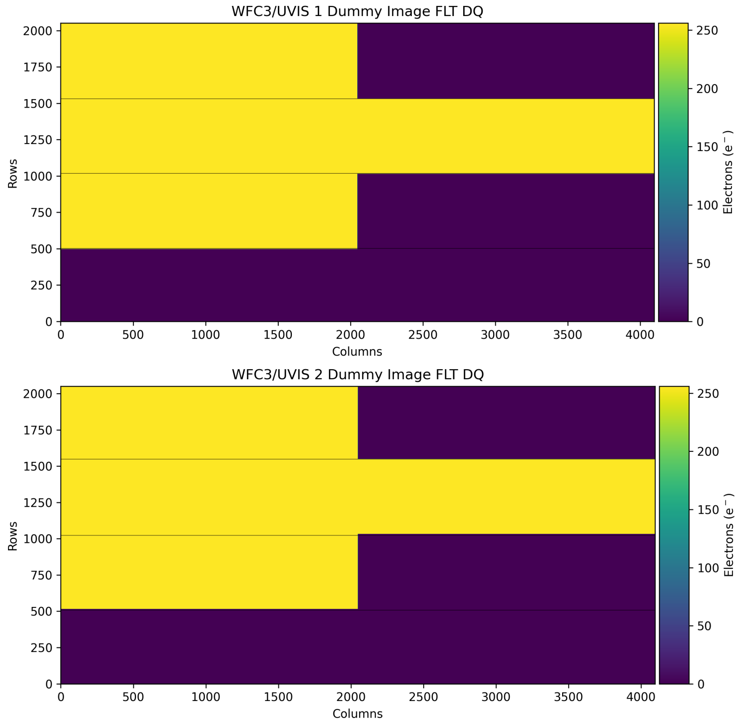


Figure 8. FLT DQ arrays of the dummy science image for UVIS 1 and 2 after applying the dummy saturation maps. The dark, purple regions have not been flagged as saturated pixels. The light, yellow regions have been identified as saturated pixels.

We also evaluate how implementing the newly created amplifier-dependent saturation maps differs from the CCDTAB values in how saturated pixels are flagged in real science images. We performed numerous tests using 1x1, 2x2, & 3x3 full-frame and subarray images containing known saturated sources, with specific examples shown in Figures 9-12. We downloaded the RAW files from MAST, and processed them in `calwf3` v3.6.2 to produce FLT files. We also processed them using `calwf3` v3.7.1, producing new FLT files. We then compared the DQ arrays between the FLT files which were processed with `calwf3` v3.6.2 and thus saturation-flagged with the CCDTAB values, and our newly-created FLT files processed with v3.7.1 and the new saturation reference files.

The top of Figure 9 shows the FLT image of the 1x1 (unbinned) science exposure idhb10esq for UVIS 1. Overplotted are the locations of saturated pixels, identified by both the CCDTAB value and the new 1x1 saturation file. The bottom of Figure 9 shows the zoomed in region of the 2 pixels in UVIS 1 that were flagged by the maps, but not by the CCDTAB. The raw value of the pixel in amplifier quadrant A is ~44585.6 DN which is below the single CCDTAB threshold of 44586 DN. However, this pixel has a value of ~42031.6 DN after overscan subtraction, which is when the saturation map is applied in the updated pipeline. The saturation map threshold for amplifier quadrant A is 42029.6 DN, and therefore this pixel is marked as saturated in the FLT DQ array. The same scenario applies to the second pixel in amplifier quadrant B. For UVIS 1 7,723 saturated pixels were flagged by both the single-value threshold and the amplifier-dependent map, so a difference of two pixels only equates to a ~.03% change from the previous method. Figure 10 shows the saturated pixels flagged in the 2x2 binned image ibl999tfq, where both the SATUFILE maps and the CCDTAB tables flag the same imaging pixels. However, as intended the saturation maps also flag the regions where the mixed rows and columns are located. In the 3x3 binned image iacs02tyq (Figure 11), the pixel flags are again identical with one mixed row now flagged by the saturation reference file. Finally, for the subarray image id6h05ynq in Figure 12, we found no differences in the DQ flagging.

These tests consistently show nearly identical flagging by the SATUFILE maps and the CCDTAB values. Uncertainties of a few pixels can occur near the threshold values for some images while using the maps due to differences between the measured overscan levels in the science image and the constant bias offset in the maps, as described in the 1x1 example. This will have a negligible effect on UVIS data. We validated that the science and error arrays were unaffected in every test case by analyzing data difference statistics, images and histograms.

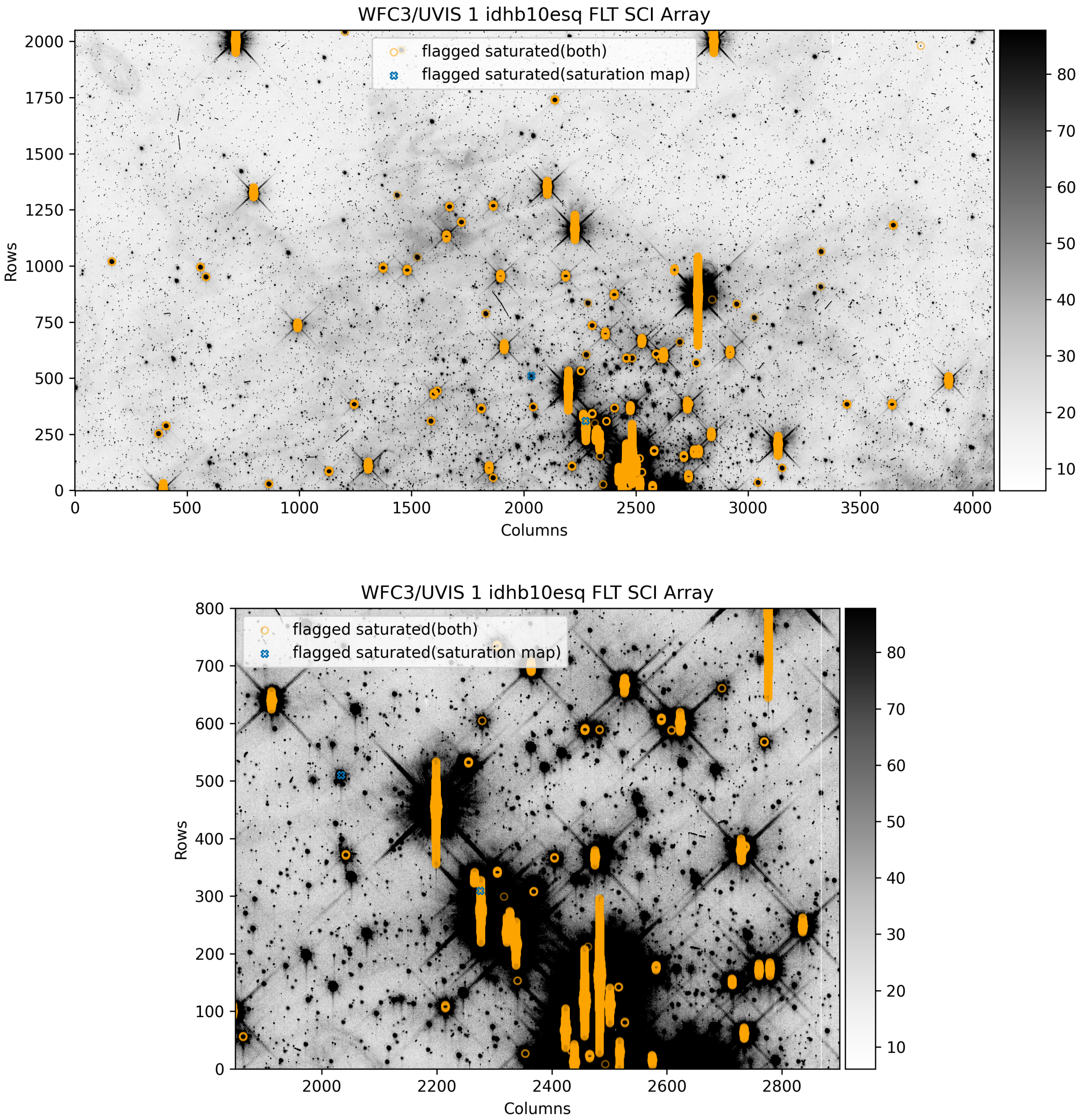


Figure 9. Saturated pixels (orange apertures) identified by both the CCDTAB and saturation maps in the unbinned (1x1) science arrays of dataset idhb10esq for UVIS 1. There are two pixels flagged by only the saturation maps, as indicated by the blue x markers.

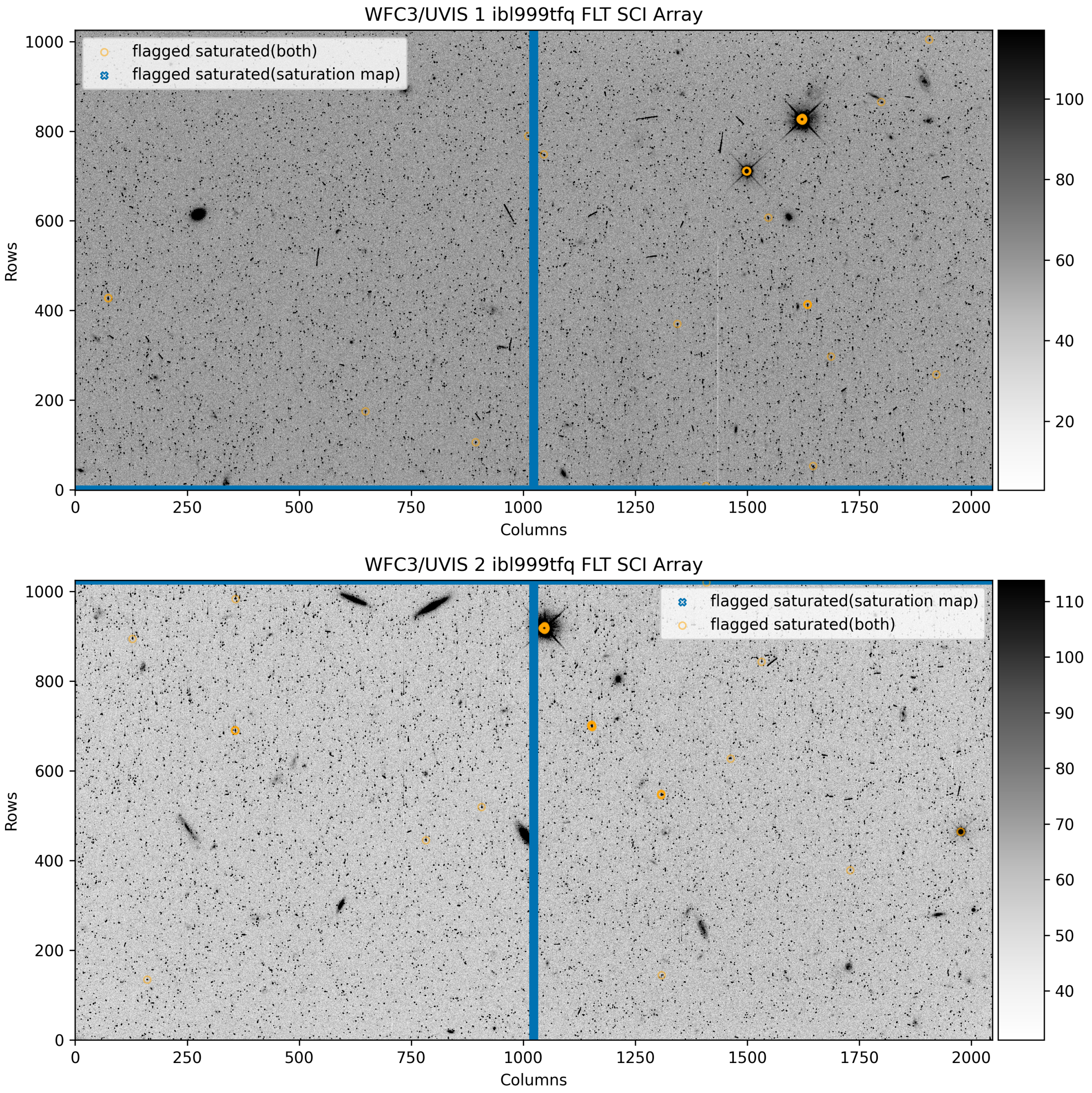


Figure 10. Saturated pixels (orange apertures) identified by both the CCDTAB and saturation maps in the 2x2 binned science arrays of dataset ibl999tfq. Pixels flagged by only the saturation maps are located in the overscan and in mixed rows and columns (as the saturation threshold of those regions is $0\,e^-$); their locations are marked by blue apertures that appear as borders due to the density.

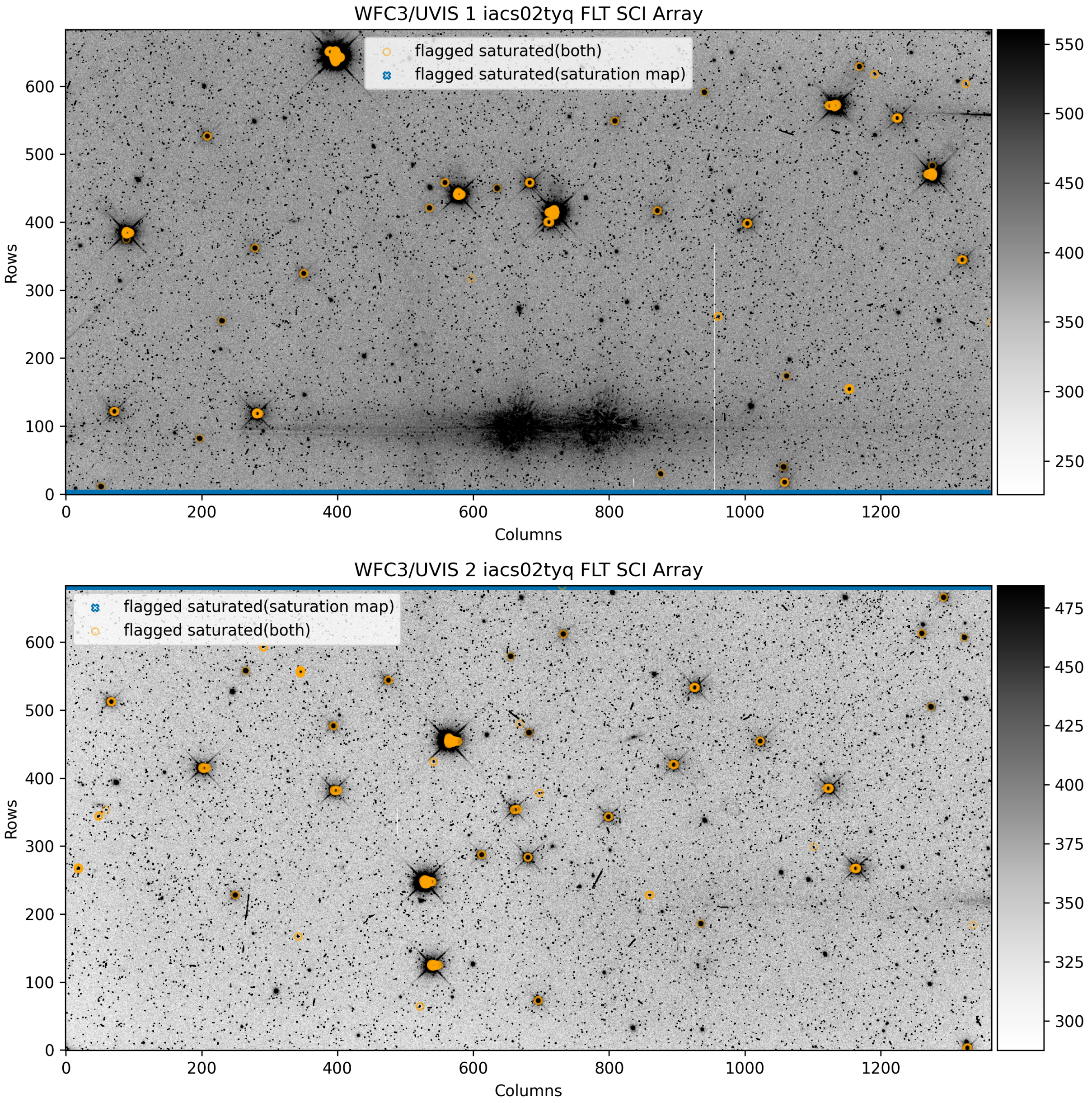


Figure 11. Saturated pixels (orange apertures) identified by both the CCDTAB and saturation maps in the 3x3 binned science arrays of dataset iacs02tyq. The pixels flagged by only the saturation maps (blue apertures) are located in the mixed rows near the chip gap. There are no pixels flagged only by the CCDTAB.

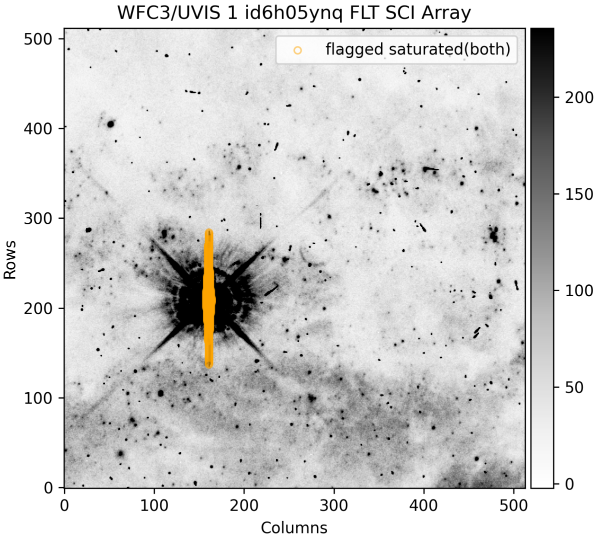


Figure 12. Saturated pixels (orange apertures) identified by both the CCDTAB and saturation maps in the unbinned subarray dataset id6h05ynq. As there are no overscan regions or mixed rows/columns in a subarray image, there are no pixels that are only flagged by one method.

5. Conclusions

Prior to the release of `calwf3` v3.7.1, saturated pixels were flagged in UVIS images using a single-scalar threshold given in the CCDTAB. The new saturation map reference files were delivered to CRDS: for both full-frame and subarray images, 2x2 binned, and 3x3 binned images. As of December 7, 2023, the pipeline applies the appropriate saturation reference file as specified by the SATUFILE keyword in the primary header of the raw file to flag full-well saturated pixels.

At present, the only material difference between the updated and previous methods of saturation flagging is that the mixed rows and columns of binned images will be flagged as saturated. This first delivery of the saturation map reference files effectively performs the same flagging as the single scalar value from the CCDTAB. To do so, the saturation maps are offset by the UVIS amplifier commanded bias levels, since the saturation maps are applied after the overscan subtraction in the `calwf3` pipeline. This can cause negligible disagreement in the number of pixels flagged by the saturation maps versus the single scalar value when the measured overscan levels in an image differs slightly from the commanded bias levels.

However, the updates to `calwf3` and the introduction of a new reference file type make possible the future implementation of saturation maps that account for the spatially-variable nature of pixel full-well saturation depth, thereby improving the accuracy of saturation flagging.

6. Recommendations

Data retrieved through MAST from December 7, 2023 use `calwf3` v3.7.1 (`CAL_VER` keyword), and saturation maps: no action required. In this section we examine two scenarios that may face users with data retrieved prior to December 2023. **Note: Since these were primarily infrastructure changes, users do not need to re-retrieve or reprocess their data.** However, should users choose to reprocess: **1)** data retrieved through MAST before August 14, 2023 (`calwf3` versions 3.6.2 or earlier, no SATUFILE keyword) **2)** data retrieved through MAST between August 14, 2023 and November 2, 2023 (calwf3 v3.6.2, keyword present, but not populated) **3)** data retrieved through MAST in November 2023 (`calwf3` v3.6.2, keyword present, and populated), please refer to the following steps for reprocessing using `calwf3` v3.7.1. Figure 13 summarizes these scenarios and suggestions in the form of a decision tree. The Appendix contains a brief tutorial for editing FITS file headers using the `Python` library `Astropy`.

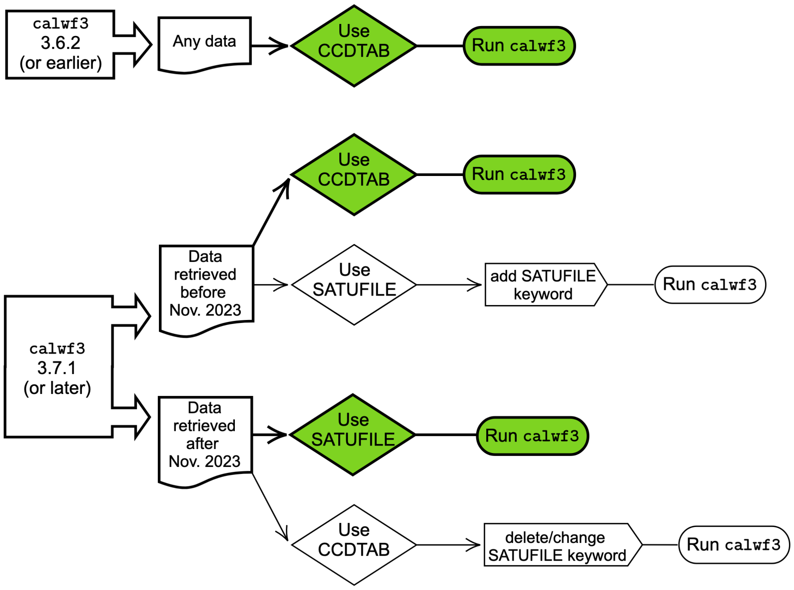


Figure 13. Decision tree for how to reprocess UVIS data (retrieved before or after November, 2023) using the updated `calwf3` version 3.7.1 or using 3.6.2 (and prior). The green boxes are the default behavior.

- **Scenario 1**: To reprocess data downloaded from MAST **prior to** November 2, 2023, saturation flagging will only be done using the CCDTAB unless SATUFILE keyword is added and/or populated with the appropriate reference file in the raw primary header. To do so, the user should do the following:
    1. Add the SATUFILE keyword to the primary header of the raw FITS file (if not present).
    2. Set the SATUFILE value to the appropriate reference file (see Appendix A).
- **Scenario 2**: To reprocess data downloaded from MAST **between** November 2, 2023, and December 7, 2023, SATUFILE keyword is present and populated, and can be run with `calwf3` v.3.7.1 to apply the saturation maps.
- **Backwards-compatibility using calwf3 version 3.7.1**: Users can still perform saturation flagging using the CCDTAB values by doing one of the following to bypass the saturation map flagging step:
    1. Delete the SATUFILE keyword (see Appendix A).
    2. Set the SATUFILE keyword to a non-valid value, i.e. 'N/A' (see Appendix A).

Importantly, when processing data with `calwf3` v3.7.1, if the SATUFILE keyword cannot be read from the file's primary header, the software will simply revert to using the CCDTAB to flag saturated pixels.

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HRFI Document: https://newcdbs.stsci.edu/doc/Section11.html

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Appendix: Modifying FITS files with Python

As of `calwf3` v3.7.1, there now exist two ways to flag WFC3/UVIS saturated pixels; the original method uses the CCDTAB and the updated method (**Recommended**) applies a new reference file defined by the SATUFILE keyword. This keyword must be present and set to the appropriate reference file in the image header before reprocessing to utilize the maps. *Because `calwf3` v3.7.1 is backwards-compatible, using the CCDTAB values is still possible as long as the SATUFILE keyword is void, or does not exist.*

Various use cases are outlined in Section 6 and are summarized in a flowchart (Figure 13). While there are many ways to modify FITS file headers, this Appendix demonstrates how to do so using the Python package `Astropy`[3]. First, we import the `fits`[4] package from `Astropy`, and we define the path to an example raw file.

```
from astropy.io import fits
filepath = 'directory/to/files/if4001yeq_raw.fits'
```

Only the primary header (the zeroth FITS extension) will need to be edited. We can easily open the FITS file, add the keyword and value pair, write out the modified header data unit (HDU) to a new file, and close the original file without modifying it.

```
hdu = fits.open(filepath)
hdu[0].header.set('SATUFILE', 'satmap.fits')
hdu.writeto('NEW_if4001yeq_raw.fits')
hdu.close()
```

Adding the keyword and overwriting the original file is also simple. Here we open the file in "update mode" so we can call the `flush()` method to write all changes back to the original file.

```
with fits.open(filepath, mode='update') as hdu:
   hdu[0].header.set('SATUFILE', 'satmap.fits')
   hdu.flush()
```

Finally, either approach can be used to remove the keyword or set it to a null value.

```
hdu = fits.open(filepath)
hdu[0].header.remove('SATUFILE')
hdu.writeto('NEW_if4001yeq_raw.fits')
hdu.close()

with fits.open(filepath, mode='update') as hdu:
   hdu[0].header.set('SATUFILE', 'N/A')
   hdu.flush()
```

---

[3] Astropy Collaboration (Robitaille et al., 2013, Price-Whelan et al., 2018)

[4] For more in-depth documentation, see https://docs.astropy.org/en/stable/io/fits/index.html