

## **Annual report of progress and accomplishments -- October 1, 2011 to September 30, 2012**

Proposal Reference Number: SDS-09-021

**Proposal Title:** Extending Ozone Climate Data Records (CDRs) into the Ozone Mapping and Profiler Suite (OMPS) Era

**Institution:** NOAA/NESDIS/Center for Satellite Applications & Research

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**CDR Activities:** Total Ozone and Ozone Profile SDRs, and total column ozone and high & low vertical resolution ozone profile CDRs from OMPS SDRs

This report documents the progress and revised plans for the subject proposal as of September 2012. It is assumed that the reader has gone through the original proposal to become familiar with the scope and background information defining and motivating the work. (This report has been revised as of September 18, 2014. Notes on work completed after the end of the period covered by the report are provided in purple.)

### **Task 1 Implement a reprocessing capability for OMPS NM RDR to SDR.**

We are pursuing two approaches for hosting the IDPS OMPS SDR algorithm on Linux workstations for reprocessing use. These each leverage a set of existing work on OMPS SDR processing.

The first approach uses the JPSS implementation of IDPS algorithms under the Algorithm Development Library (ADL). The ADL is a set of programs and tools developed by Raytheon ITSS to allow the hosting of IDPS (native AIX) programs on LINUX machines. The OMPS Nadir Mapper Earth View SDR algorithms (which create the SOMTC set of products) are supported under ADL 4.1. We have installed this package on a Linux system at STAR and are investigating its use for reprocessing.

The second approach is to replicate the environment and processing system for OMPS in use at the NASA Ozone PEATE in support of the NASA OMPS NPP Science Team. We are porting an instance of the NASA-developed OMPS RDR to SDR software to NOAA STAR Linux machines both as part of our long term support for the OMPS Nadir Mapper and Nadir Profiler calibration and characterization and as part of our R2O work on implementing the OMPS Limb Profiler products on the JDE system. The native PEATE processing system has already been used to reprocess the complete OMPS Nadir Mapper chain of products (RDR through Version 8 Total Column Ozone EDR) twice in the past year.

### **Task 1 Status: Progress: YELLOW; Risk: GREEN**

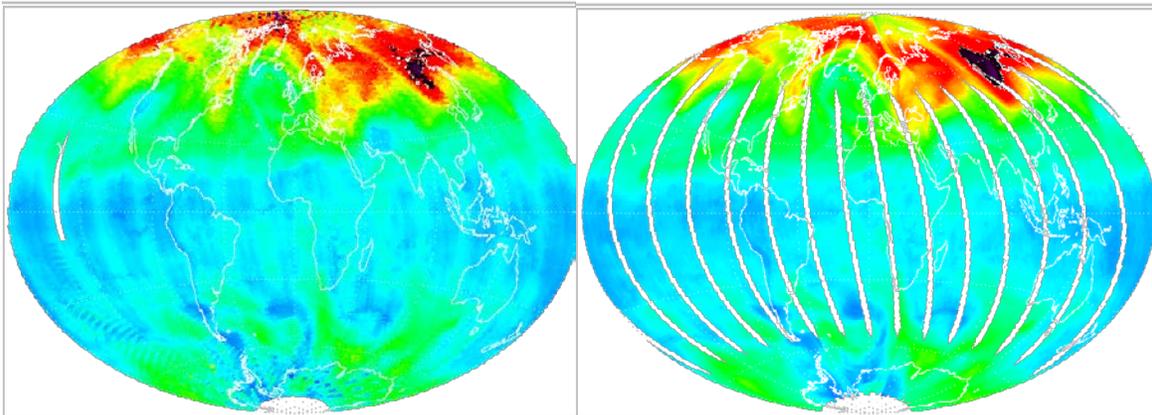
While the direct progress of this project in implementation of the OMPS NM SDR for reprocessing is not on track with the original proposal, there are several paths and efforts underway that will allow us to meet the final objectives with the shared resources. (Post period of report note: The OMPS SDR algorithms, NP and NM, as implemented in IDPS are now hosted at STAR under ADL. While this does not provide a full reprocessing capability, we have been using it for selected reprocessing and conducting studies to improve the calibration and characterization. The OMPS Calibration SDR codes in use at the NASA OMPS PEATE have also been implemented on the NOAA STAR system.)

### **Task 2 Implement a reprocessing capability for OMPS NM SDR to CDR.**

An implementation of the OMPS NM Version 8 Total Ozone code has been used to process (and reprocess) the full OMPS NM SDR record from IDPS. We have been discovering and fixing minor issues with the code and are moving to develop soft calibration adjustments to make the record consistent with other CDR components, e.g., NOAA-17, -18, and -19 SBUV/2 records.

### **Task 2 Status: Progress: GREEN; Risk: GREEN**

The basic concepts and adjustments to convert the algorithm for OMPS NM SDR reprocessing have been implemented and the successful adaptation has been demonstrated in processing the first year of OMPS NM SDR data. Appendix 1 has a color coded list of specific tasks in the conversion showing their status. There is a parallel effort by the NASA OMPS S-NPP Science Team that has processed/reprocessed and released (Beta) the first year of their OMPS Version 8 Total Ozone products at <http://ozoneaq.gsfc.nasa.gov/beta/data/omps/>. (Post period of report note: the STAR V8 system has been used to process the first two and one half years of OMPS SDR products. We lack dedicated program support to reprocess. However the V8 algorithms will be implemented in operations and the OMPS instruments have show excellent stability. These products will be archived at NCDC and will provide a good start for CDR continuation once they reach validated maturity.)



**Figure 1.** (Left) Retrieval results from STAR for the Version 8 total ozone algorithm applied to the operational OMPS NP SDRs from IDPS for March 30, 2012. (Right) NASA V8.6 Total Column Ozone from IDPS EOS Aura OMI for March 30, 2012.

**Task 3 Implement a reprocessing capability for the OMPS NP RDR to SDR**

The status of this work parallels that for the OMPS NM RDR to SDR so closely that it is not reproduced here.

**Task 3 Status: Progress: YELLOW; Risk: GREEN** – See Task 1.

**Task 4 Implement a reprocessing capability for the OMPS NP SDR to CDR**

The Version 8 Ozone Profile algorithm has been implemented with the OMPS Nadir Mapper and Nadir Profiler SDR products.

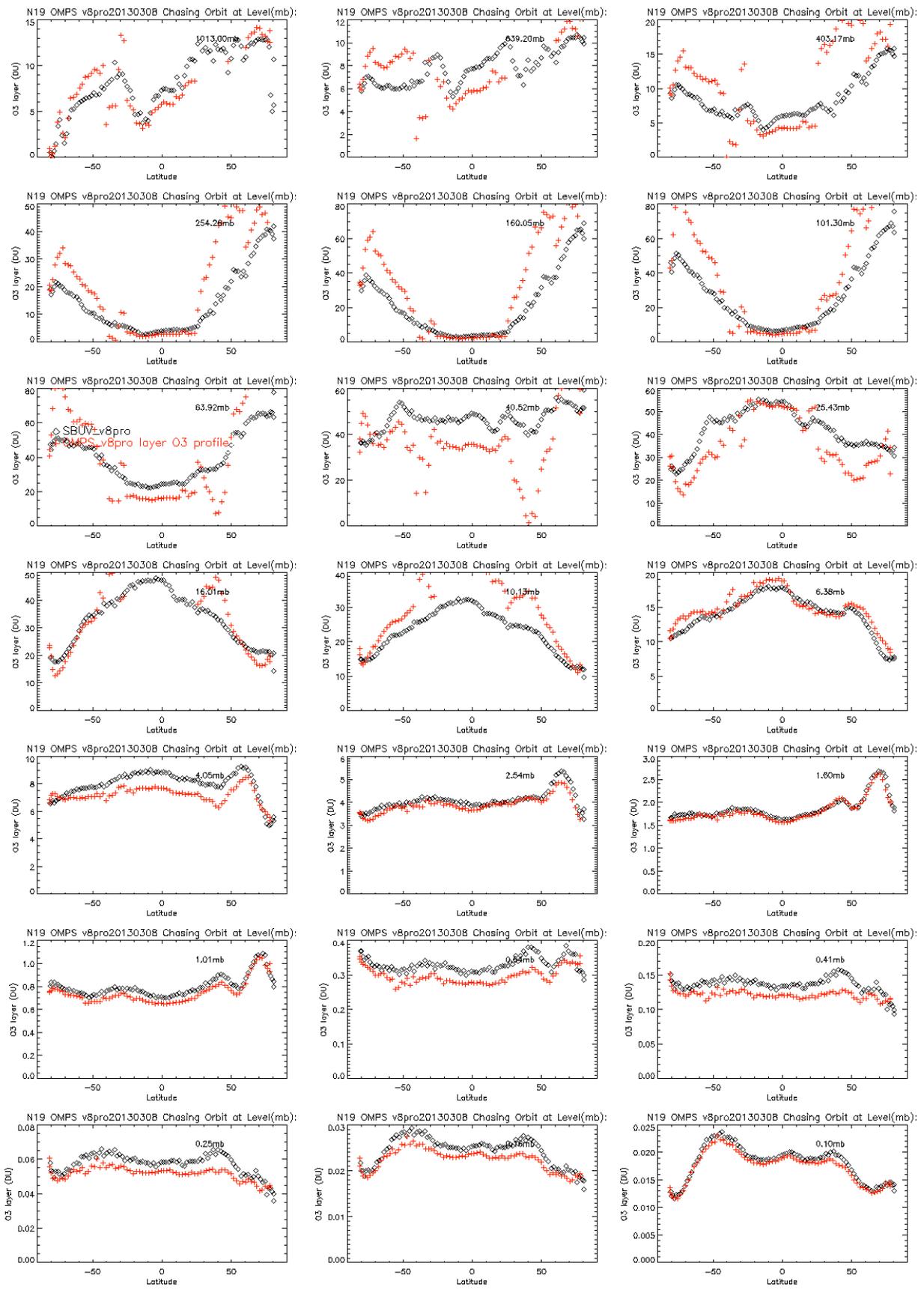
**Task 4 Status: Progress GREEN; Risk: GREEN**

The basic concepts and adjustments to convert the algorithm for OMPS NM SDR reprocessing have been implemented and the successful adaptation has been demonstrated in processing the first year of OMPS NM and NP SDR data.

**Figure 2. Chasing orbit comparisons between ozone profile retrievals from the Version 8 NOAA-19 SBUV/2 and Version 8 OMPS.** The figures on the following page show comparisons of the ozone profile retrievals estimates between S-NPP OMPS and the NOAA-19 SBUV/2 processed with the Version 8 ozone profile retrieval algorithm. The data are from a pair of orbits on March 8, 2013 where the two satellites are flying in formation (orbital tracks within 50 KM and sensing times with 10 minutes). The figures show the results of comparison for the layer amounts for 21 layers with the lower pressure boundaries for layer  $i$  at  $1013 \cdot 10^{i/5}$  hPa. The arrangement from bottommost layer (1013 hPa to 639 hPa) to topmost start in the upper left,

go across the row and then continues on the next row ending with the figure on the lower right for the highest layer (0.101 hPa to 0 hPa).

The figures show some agreement between the retrievals for the two instruments but with the OMPS NP retrieving much more variable values for the lower layers in the profiles. This is probably due to the inaccuracies in the initial calibration of the longer wavelength. Shifts in the results with Latitude for the lower levels are related to changes in the V8 channel selection with increasing SZA and current in accuracies in the OMPS calibration. Some of the biases for the upper layers could be symptomatic of stray light in the shorter wavelength channels providing information at those levels. A correction for stray light is under development. (Post period of report note: Stray light corrections have been implemented and soft calibration corrections are under development with planned completion by the end of 2014. The STAR V8 system has been used to process the first two and one half years of OMPS NP ozone profile products.)



### **Task 5 Develop monitoring tools for product calibration, validation, and evaluation**

Additional tools to assist in CDR validation and trending are under development, some with shared support from the OMPS Product Cal/Val Project. A set of monitoring figures for OMPS Version 8 total ozone and ozone profile product processing and reprocessing are available at

[http://www.star.nesdis.noaa.gov/icvs/PROD/proOMPSbeta.TOZ\\_V8.php](http://www.star.nesdis.noaa.gov/icvs/PROD/proOMPSbeta.TOZ_V8.php)

and

[http://www.star.nesdis.noaa.gov/icvs/PROD/proOMPSbeta.O3PRO\\_V8.php](http://www.star.nesdis.noaa.gov/icvs/PROD/proOMPSbeta.O3PRO_V8.php)

### **Task 5 Status: Progress GREEN; Risk: GREEN**

This work is on-track. (Post period of report note: The products continue to be monitored with regular updates to the total ozone maps, chasing orbits, initial residual time series and other new comparison now at <http://www.star.nesdis.noaa.gov/icvs/prodDemos/proOMPSbeta.php> .)

### **Task 6 Implement a reprocessing capability for OMPS LP**

The plan to implement a reprocessing capability for the OMPS LP measurements is unchanged. We are keeping up with the development of the OMPS LP RDR to SDR and SDR to EDR algorithm development by the NASA NPP Science Team. On a related note, a proposal to begin the next phase of the Research to Operations conversion for these algorithms was approved for FY-2011 funding by the SPSRB. In this phase, we have started creating the users and maintenance manuals required by the operational center, and are working with the NASA developers to ensure that the codes and input and output meet the operational processing standards. The PEATE RDR to SDR processing or OMPS LP RDRs has been transferred to STAR and initial work on the transfer to the JDE (formerly NDE) system is underway.

### **Task 6 Status: Progress GREEN; Risk: GREEN**

The development and implementation are proceeding as planned. (Post period of report note: the OMPS LP transition has been lagging the planned timeline. The NASA NPP Science Team has revised their algorithm and is now recommending that we implement Version 2.5 . We have implemented test reprocessing of Version 2.0 to STAR and had started work to implement it in an operational setting. We will now move to Version 2.5 and proceed.)

## Appendix I. Detailed Version 8 Total Ozone Implementation Tasks and Status

Key: BLACK Apply existing approach      GREEN Completed basic conversion task  
RED Remaining basic conversion task      BLUE Optional future refinement

### Documents:

ATBD given at OMI site

- eosps0.gsfc.nasa.gov/eos\_homepage/for\_scientists/atbd/docs/
- OMI/ATBD-OMI-02.pdf

Version 8 OMTO3 as applied to GOME-2

- GOME-2 Interface Control
- GOME-2 Maintenance Manual
- GOME-2 System-Description

Documents must be revised further to show OMPS modifications – FY2013 work. (Post period of report note: Both the V8 Ozone Profile and the V8 Total Ozone sets of documents were updated as part of the preliminary delivery of these algorithms for operational implementation in the JPSS IDPS system. This upgrade would not have been possible without the extensive work support by the CDR program.)

### Retrieval algorithm fundamentals

- 12 (or more) channels including 308.70; 310.80; 311.85; 312.60; 313.20; 314.40; 317.62; 322.42; 331.34; 345.40; 360.15; 372.80 nm
- New Tables with BDM cross sections
- Ring effect included via Table corrections
- Tables adapted to adjust for spectral smile and cross-track bandpass variations – pixels/rows as used
- OMPS-specific subroutine reads in the SDR and other information; The total ozone estimate sections of the code do not make any instrument-specific calculations.

Flow for OMPS NM (maintains capability to process GOME-2

Read in Tables

For Each Day

Read in day of year

Read in ancillary and auxiliary data files

Read in Solar

For Each Measurement

Read in Earth and Geo

Create and assign 12 (or more) channel N-Values

Select tables and ancillary data for Latitude, Longitude, and DOY

Adjust solar, earth, and tables for Earth wavelength scale

Call retrieval code with:

Latitude, Longitude, SZA, SAA, SVZA, SVAA

N-values and wavelength assignments

Interpolated Tables and parameters

Return retrieval results

Append results to output file

Input Files (Change to daily)

- OMPS NM SDR (Solar and Earth-view) (Awaiting final format.)
- OMPS NM GEO (DOY, Lat, Lon, SZA, SAA SVZA, SVAA) (Awaiting final format.)
- Cloud top pressure (RRS CTP)
- Snow/ice data and surface reflectivity
- Surface pressure

- Instrument tables (GOME-2 and OMPS done)
- Standard profiles
- Climatological profiles
- Solar adjustment quadratic coefficients
- N-value adjustments (Instrument specific array of daily adjustments. Currently all 0 for OMPS)
- **Need along orbit wavelength scale information.** Code is ready to make adjustments if information is provided and properly assigned. (Post period of report note: This adjustment was implemented as an SDR measurement-based correction in 2013.)

#### Parameters

- Filenames
- Wavelengths, rows, table entries
- B-pair wavelengths
- C-pair wavelengths and sensitivity test parameter
- Aerosol Index: wavelengths and **Step 3** parameters input parameter as input (currently 8 DU/N-value)
- A-pair Wavelengths and **Step 3** quadratic parameters
- SO2 wavelengths and coefficients

#### Output Files

- V8 Product Master File (PMF) Output
  - GOME-2 PMF output as basis
  - Additional work to include the following:
    - **Determine N-value adjustments** (Post period of performance note: This is ongoing and will be completed as part of JPSS cal/val activities by the end of 2014.)
    - **Layer retrieval efficiencies for B-pair and assumed profile** (code ready to compute these need to add it and output fields.) (Post period of performance note: This code has been implemented and the output now has these additional parameters.)
    - **Satellite view angles and relative azimuth angles**
    - **N-values and residuals for additional wavelengths**
    - **Multiple cloud top pressure values and choice**
- Error Message files

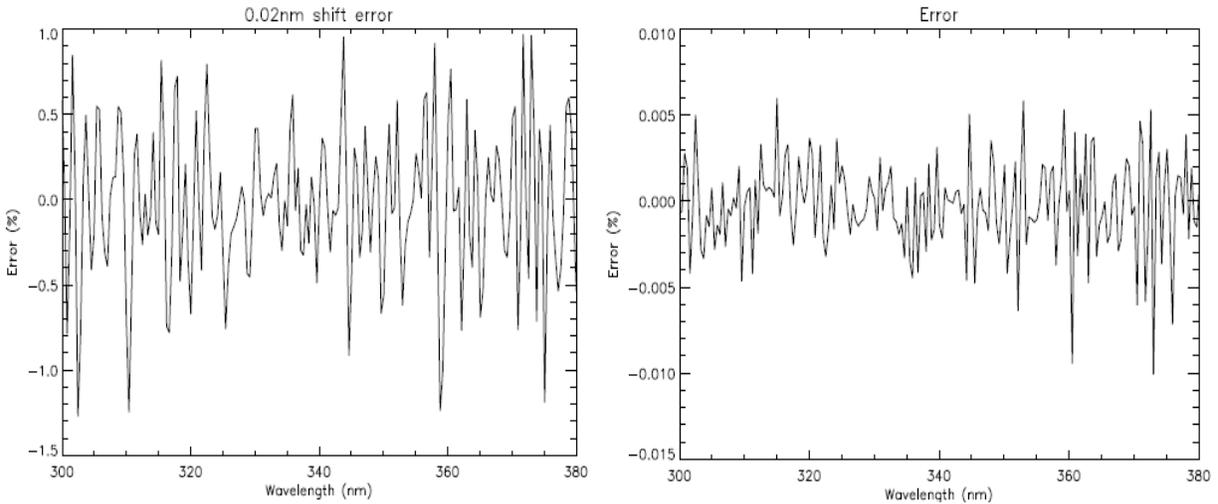
#### Specific Modifications

- **Organize daily sub-directories and data for reprocessing in ADL.** (Post period of performance note: We have not been able to devote resource to complete this work as the systems keep evolving.)
- **Read in Geolocation information (Lat, Lon, SZA, SAA, SVZA, SVAA, DOY)**
- **Handle SDR and table manipulations to make N-values before calling TOZ code.**
  - Use a linearly interpolated orbital N-value adjustment matrix (35X12X2).
  - Adjust solar to Earth-view wavelength Scale. Check and adjust Earth/Sun distance of solar SDR.
  - Allow for intra-orbit scale shifts with input-based central wavelengths.
  - Provide program wavelength sub-table selection indices for each channel.
  - Linear table interpolation in wavelength scale / bandpass.
  - Identify wavelengths for ozone, reflectivity, A-pair, and aerosol and provided parameters.
- **Make daily year of climatological files from weekly or monthly (Snow/ice, CTP, etc.)**

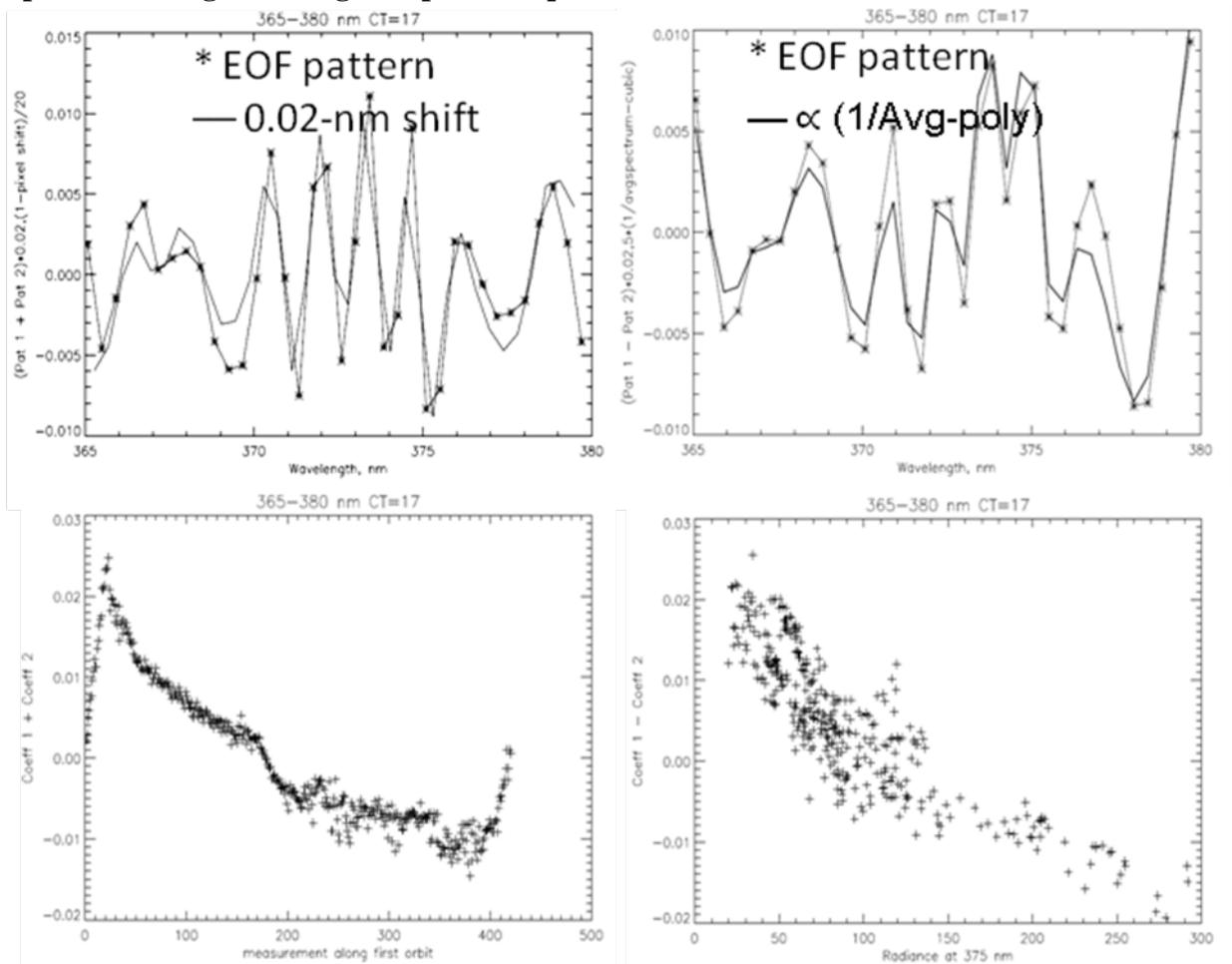
- **Output to NetCDF.** Currently in HDF with IDL code for NetCDF conversion.
  - Include the selected Standard Profile and layer retrieval efficiencies in the output.
  - Include the Effective Reflectivity in the output. (Post period of performance note: Output has been included but NetCDF format is still by post processing conversion.)
  - Include any adjustments in the output.
- Review all error codes. Check  $TOZ > 575$  DU.
- Take hard-coded options and parameters and make them run-time inputs.
- Clean up the code. (Check Layer 0/1/2 errors for cloud and surface pressures  $< 0.5$  Atm.)
- Consider using newer Snow/Ice, surface reflectivity, and CTP/CF climatologies.
- Provide tools for adjustments and validation using sensitivities and efficiencies (IDL Code exists for GOME-2 for adjustments. Code is in testing for use with OMPS.) (Post period of report note: This analysis code was used to determine soft calibration adjustments to improve the agreement of S-NPP OMPS V8 products with the EOS OMI V8 ones.)
- Check Terrain Pressure resolution relative to FOV size. Currently 1080X540. Revisit for polar regions and if FOV decreases.
- Use EOF analysis to identify SDR outliers and wavelength shifts. (Post period of performance note: Wavelength shifts have been determined and implemented in SDR processing.)
- Make variable number of total channels for main code residual calculations
- Consider incorporating subroutines
  - for better SO<sub>2</sub> estimates. (Post period of performance note: This work is proceeding well and the OMI Linear Fit SO<sub>2</sub> algorithm is in testing. We expect to complete this development work by the end of 2014.)
  - for better aerosol estimates (354 nm and 380 nm).
  - for RRS measurement-based CTPs; requires spectral interval.
  - for stray light corrections (SDR) (Post period of performance note: This correction has been implemented.)

### Specifics for New Tables

- Ring Effect
  - Redo adjustment to LUTs with latest model results
- Look Up Tables
  - Select wavelengths/bandpasses for each row that could be used for a channel; selected to cover the range of bandpasses from Nadir to extreme view with 0.07-nm spacing over interval used for each row for each side.
  - For each channel, rows are selected from the SDR to straddle the desired central wavelengths.
  - Six SVAs; ten SZAs; four with 0.25 Atm. for OMPS V8 CTPs; 12 (or more) channels; one row with adjustment for central
  - Interpolate tables to match measurement wavelengths
- Solar Adjustments
  - Weekly measurement at each cross-track position with daily Earth/Sun distance adjustment
  - Bandpass for cross-track position (High resolution)
  - Central wavelength interpolation/adjustment with quadratic wavelength scale shift sensitivity model for 196 X 35 wavelengths.



**Figure 3. Actual Difference and Final Error after Correction for 0.02-nm shifted Solar Spectrum using wavelength-dependent quadratic model.**



**Figure 4. Empirical Orthogonal Function analysis of OMPS Nadir Mapper spectra for the 365 nm to 380 nm interval.** The EOF Covariance analysis was applied to the Nadir Mapper for the central cross-track position for the 365 nm to 380 nm wavelength ranges for parts of six orbits on 1/28/2012. The first two patterns contain 90% of the variability after removing a 3<sup>rd</sup> order polynomial from Rad/AvgRad. The two patterns are combinations of Wavelength Scale Shift and Ring Effect/Stray Light variations. The figures on the Left show the sum of the first

two EOF patterns (Top) and the coefficients for the first orbit (Bottom). The Top figure also has the computed variations expected from a 0.02-nm wavelength scale shift. The two curves agree very well. The pattern of the coefficients in the Bottom may be related to wavelength scale changes produced by intra-orbital variations in the optical bench temperatures. While the shifts are small, we plan to implement a correction/adjustment to improve the ozone products. The figure on the top Right shows the differences of the first two EOF patterns. Now the additional curve is a scaled set of the variations for the reciprocal average spectra. Again, the two curves agree very well. One would expect this pattern to be produced by inelastic scattering (Ring Effect) or Out-of-Band Stray light. The figure on the Bottom Right tests this by looking at the dependence of the coefficients (y-axis) with the 375-nm radiances (x-axis). The inverse relationship between the two suggests that the major source of these variations is the Ring Effect – not Stray Light. The OMPS NPP Science Team plans to exploit this signal to create UV cloud optical centroid estimates. Given the radiance levels, a 0.01 change in the figures on the Top equates to approximately a 1% variation.

#### Nadir Mapper Refinements

- Switch to BDM ozone cross-sections
- Correct Terrain Pressure, Cloud Top Pressure layer amounts, and dN/dx layer errors
- Change from 5 DU to 1 DU for iteration convergence test
- Monitor A-Pair/B-Pair/C-Pair/D-Pair(308nm) consistency and intercalibration *a la* ICVS
- Track heritage D-Pair (306-nm channel) residuals in addition to 308 nm. (Post period of report note: the D-pair is tracked as part of the Nadir Profiler monitoring. The NM/NP performance in the overlap region from 300 nm to 310 nm has been the focus of additional studies.)

#### Progress on OMPS Product Risk/Identification/Mitigation via algorithm changes

- Solar Diffuser Characterization
  - (R) Fine Structure may limit degradation characterization
  - (I) Evaluate Solar Irradiance as incidence angles vary
- Intra-orbit spectral scale and bandpass
  - (R) Unaccounted shifts will degrade ozone products
  - (I) Use EOF analysis and spectral fits to develop functional forms for variations (Post period of report note: variations identified by EOF analysis have been used to estimate noise, stray light, and wavelength shifts.)
  - (M) Include intra-orbital shift option in look up tables
- Cloud Top Pressure
  - (R) IR estimates are inaccurate for UV measurements
  - (M) Implement UV-based Climatology or RRS algorithm (OMPS NPP Science Team)
- Stray Light
  - (R) Stray light errors will impact product accuracy
  - (I) Evaluate errors through reflectivity correlation studies
  - (M) IDPS has code in the SDR and parameters are in testing at the G-ADA.
- South Atlantic Anomaly
  - (R) Charged particles' effects will corrupt ozone profile retrievals
  - (I) Identify and flag at the SDR Level

## Appendix II. Version 8 Ozone Profile algorithm implementation status

Key: BLACK Apply existing approach      GREEN Completed basic conversion task  
RED Remaining basic conversion task      BLUE Optional future refinement

### Documents

- ATBD given at SBUV/2 site
  - [http://www.star.nesdis.noaa.gov/smcd/spb/calibration/icvs/sbuw/doc/SBUV2\\_V8\\_ATBD\\_020207.pdf](http://www.star.nesdis.noaa.gov/smcd/spb/calibration/icvs/sbuw/doc/SBUV2_V8_ATBD_020207.pdf)
- Start with Version 8 as applied to SBUV/2
  - SBUV/2 Interface Control
  - SBUV/2 Maintenance Manual
  - SBUV/2 System-Description

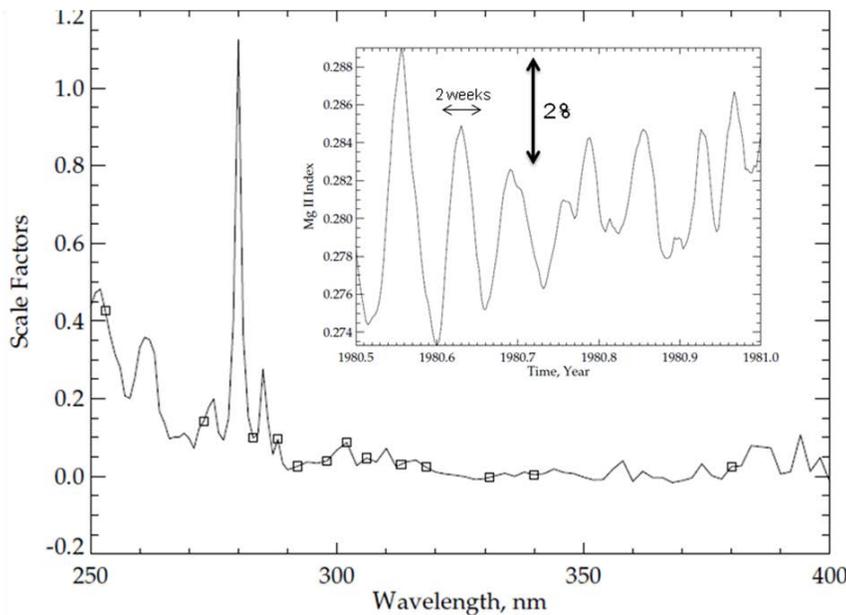
Documents must be revised further to show OMPS modifications. FY2013 work.

### Retrieval algorithm fundamentals

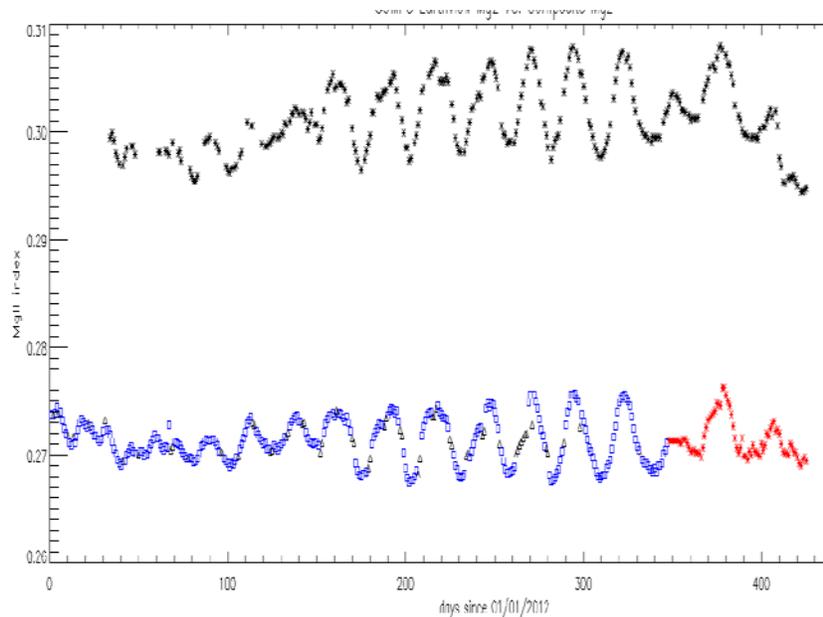
- Monthly zonal CTP from OMI RRS climatological data
- 13 (or more) channels including 253, 273, 283, 288, 292, 298, 302, 306, 313, 318, 331, 340, 380 nm (with alternate aerosol channel at 360 nm). Single 380-nm N-value repeated 12 times. (See Covariance matrix)
- New Tables with BDM cross sections (and corrected dN/dx)
- Ring effect included via Table correction.
- Tables adapted to allow for spectral scale shifts.
- Adjustments to N-value for initial calibration and daily adjustments

### Algorithm Adaptation Details

- Single scattering bandpass in code, Multiple scattering adjustments for four shortest.
- Total ozone channels averaged over 25 FOVs
- Adjustment to path length for 16° FOV (~ 1.004) (Average secants of SZA and SVA for 25 FOVs; Correct average for Solar Azimuth Angle.
- Same beginning and ending SZA and Latitude equal to average for Fractional values
- Two choices for 306-nm channel; Use OMPS NM Measurement
- Single 380 nm (no adjustment to scenes)
- Choice and parameter for Aerosol Index and adjustment
- Bracket wavelengths for wavelength scale adjustment, implement solar shift correction. (Post period of performance: An annual cycle has been observed in the wavelength scale. Given its size (+0.015 nm) it is not a high priority adjustment.
- Track initial and final residuals (in ICVS for SBUV/2)
- Use Averaging Kernels, Jacobians, and Measurement Contribution Functions to estimate and test adjustments (SBUV/2 IDL Code exists) (Post period of performance note: These approaches are in use to create soft calibration adjustments to the SDRs using calibration factor Earth tables. The OMPS NP SDR calibration will be set to match the NOAA-19 SBUV/2 calibration as of May 2014.)
- Adjust for solar activity for intra-weekly variations by using an Earth-view Mg II Index and scale factors. Earth-view Mg II Index shows good correlation with other instruments variations. Scale factor estimates have been obtained. Current solar measurements are every two weeks.
- EOF Smoothing of N-values over wavelength intervals especially for small-FOV data sets (extra work is needed in SAA with covariance adjustment). (Post period of performance note: This or a similar method will be implemented for JPPS-1 when the OMPS NP FOVs are reduced to 50 km along track.)



**Figure 5. Mg II Index scale factors (unitless %/%) for SBUV/2 with 1.1-nm FWHM bandpass. The inset plot shows the variation of the Mg II Index at solar maximum. Squares are locations of standard Version 8 channels for SBUV/2 measurements.**



**Figure 6. Comparison between an Earth-view Mg II Index from OMPS and a composite from actual solar measurements.** The OMPS EV is on the top and the index on the bottom is derived from multiple satellite observations as described at

[http://www.spacewx.com/About\\_MgII.html](http://www.spacewx.com/About_MgII.html) .

The OMPS results capture the day-to-day variations well. The drift up and the jump down at the end for the OMPS record are related to the lack of updates for dark current changes. The first update (after a year of changes) was implemented in late February 2013. Since then, weekly updates have been made. We can use the internal OMPS estimates and bi-weekly solar measurements to adjust the solar spectra for day-to-day changes if other resources are not available.

### Appendix III. Flow for OMPS NP/NM (maintains capability to process SBUV/2, add capability to process OMI and GOME-2 central FOVs)

Read in Tables (Bracketing central wavelengths)

For Each Day

Read in day of year

Read in ancillary and auxiliary data files (Bandpasses and shifts)

Read in Solar (Combine NM FOVs for OMPS)

For Each Measurement

Read in Earth and Geo (Combine NM FOVs for OMPS)

Adjust solar, earth, and tables for Earth wavelength scale

Create and assign 13 (or more) channel N-Values

Set fractional times for SZAbeg and SZAend (and Lat)

Call retrieval code with:

Latbeg/end, Longitude, SZAbeg/end, Path adj.

N-values, wavelength assignments, fractions

Interpolated Table

Return retrieval results

Append results to output file

Input Files

- SDR (Sun and Earth; Mapper average of 25 FOVs and Nadir)
- GEO (DOY, Lat, Lon, SZA, SAA SVZA, SVAA)
- Auxiliary input files
  - N-value look-up tables (data/v8shtable\_multi.nxx) (BDM + Ring)
  - N-value sensitivity look-up tables (data/v8sbdndx.nxx) (BDM + fix)
  - A priori ozone profile climatology (data/O3\_CLIM13.DAT) (.day)
  - A priori temperature profile climatology (data/TM\_CLIM13.DAT) (.day)
  - Standard profiles in fine layers (data/v8std81.dat)
  - Solar radiation reference look-up table (data/solar\_bass.dat) (BDM)
  - Terrain height pressure data (data/TERPRS.DAT)
  - Surface category code (data/SURFCAT.DAT)
  - Snow-ice cover data (data/v8snocld/v8snowice.mon) (.day)
  - Cloud pressure data (data/v8snocld/v8cldpres.mon) (.day)(RRS-based)
  - Merged a priori ozone climatology (data/mrgapprf.dat)
  - N-Value Adjustments (May be handled by changing solar or CF Earth in SDR)  
(Post period of performance note: This is handled for the off-line processing at NOAA by adjustments using initial residual comparisons between NOAA-19 SBUV/2 and OMPS NP. It will be handled operationally by changing CF Earth – in use by the end of 2014.)

Parameters

- Constants (control/CONST.nxx)
- Filenames
- Wavelengths, table entries
- B-pair wavelengths
- C-pair wavelengths and sensitivity test
- Aerosol Index: wavelength and Step 3 adjustment
- SO2 wavelengths and coefficients
- A-pair Wavelengths and Step 3 adjustment
- Measurement fractional times in scan

Output

- Weekly Solar (Daily, Earth view) Mg II Index
- V8 PMF (with averaging kernel, Jacobian, and measurement contribution functions)
  - Add N-value adjustments to output
  - Add Retrieval Covariance Matrix and Se diagonal
  - Variable number of wavelengths

#### Specific Modifications

- Read in Geolocation information (Lat, Lon, SZA, SVA, DOY)
- Handle SDR manipulations to make N-values before calling TOZ code.
  - Devise N-value adjustment matrix  $(8+25*6)*366$ . (Post period of performance note: OMPS has very good stability. Semiannual adjustments/updates to the CF Earth for the shortest three wavelengths are all that is necessary.)
  - Adjust solar to Earth-view wavelength Scale (thermal and Doppler) with quadratic. Check and adjust Earth/Sun distance of solar SDR.
  - Allow for intra-orbit scale shifts with input-based central wavelengths.
  - Provide program wavelength sub-table selection indices for each channel.
  - Linear table interpolation in wavelength scale and bandpass.
  - Identify wavelengths for ozone, reflectivity, A-pair, profile with path length, and aerosol and provided parameters.
- Make daily climatological files from weekly or monthly (Snow/ice, CTP)
- Output to NetCDF (Currently HDF with IDL conversion.)
  - Full matrix V8 Profile output
  - Include any applied N-value adjustments in the output.
- Review all error codes. Expand as needed.
- Take hard-coded options and parameters and make them run-time inputs.
- Clean up the code. (Check Layer 0/1/2 errors for pressures < 0.5 Atm.)
  - Consider using new Snow/Ice, surface reflectivity, and CTP (with cloud fraction) climatologies. Make resolutions consistent with FOV sizes.
- Consider using EOF to identify SDR outliers (including SAA) and wavelength shifts. (Post period of performance note: Flag is set for SAA as radiances are too sensitive to particle effects.)
- Make variable number of total channels for main code
- Consider incorporating results from Mapper retrievals
  - Better SO2 estimates.
  - Better aerosol estimates.
  - RRS measurement-based CTPs; requires spectral interval from SDR

#### Refinements

- Input instrument specific Single Scattering bandpasses
- Check Terrain Pressure and Cloud Top Pressure ozone layer amount adjustments
- Check Snow/ice logic
- Adjust Satellite View Path Lengths
- Include multiple scattering correction for four shortest wavelengths
- Correct dN/dx solar index table shifts
- Examine Earth-view Mg-II for intra-week solar activity adjustments
- Use Snow/Ice Forecast (not for CDR)
- Use CrIS temperatures (not for CDR)

**Appendix IV. Theory and Equations for Averaging Kernels, Measurement Contributions and Jacobians (Expanded from Year 1 Annual report with inclusion of real OMPS initial residual time series.)**

**Adjustments using A, K, and Dy**

The Averaging Kernel, A, is the product of the Jacobian of partial derivatives of the measurements with respect to the ozone profile layers, K, and the measurement retrieval contribution function, Dy:

$$A = Dy \# K$$

For a linear problem, the retrieved profile, Xr, is the sum of the A Priori Profile, Xa, plus the product of the Averaging Kernel, A, times the difference between the Truth Profile, Xt, and Xa:

$$Xr = Xa + A \# [Xt - Xa]$$

The measurement change, ΔM, is the Jacobian times a profile change, ΔX:

$$\Delta M = K \# \Delta X$$

The retrieval change, ΔXr, is the contribution function times a measurement change, ΔM:

$$\Delta Xr = Dy \# \Delta M$$

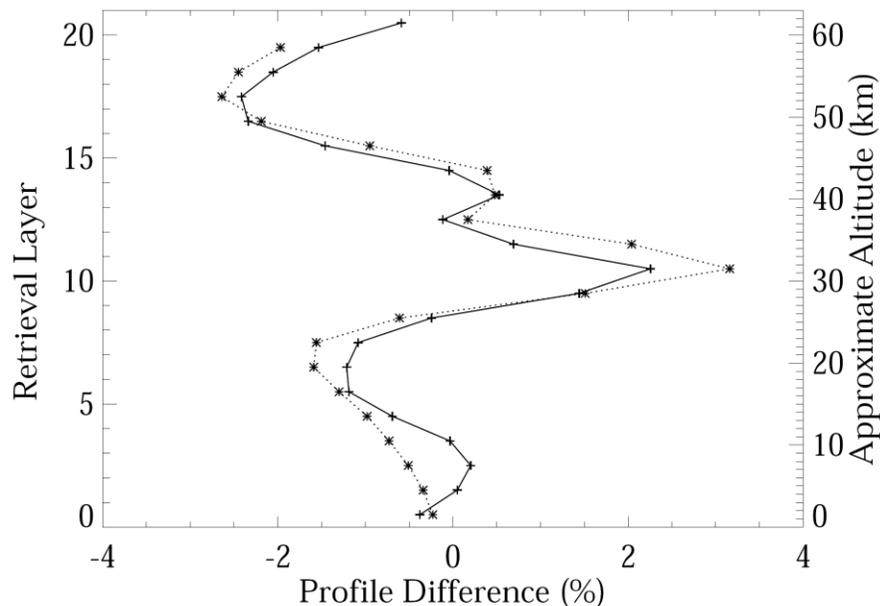
A retrieved profile from a higher resolution method, Xh, can be processed with the averaging kernel to provide a smoothed profile, Xhs, for comparison to the retrieved one

$$Xhs = Xa + A \# [Xh - Xa]$$

The innovation in a retrieved profile from can be converted to that using a forecast, Xf, as an A Priori by computing

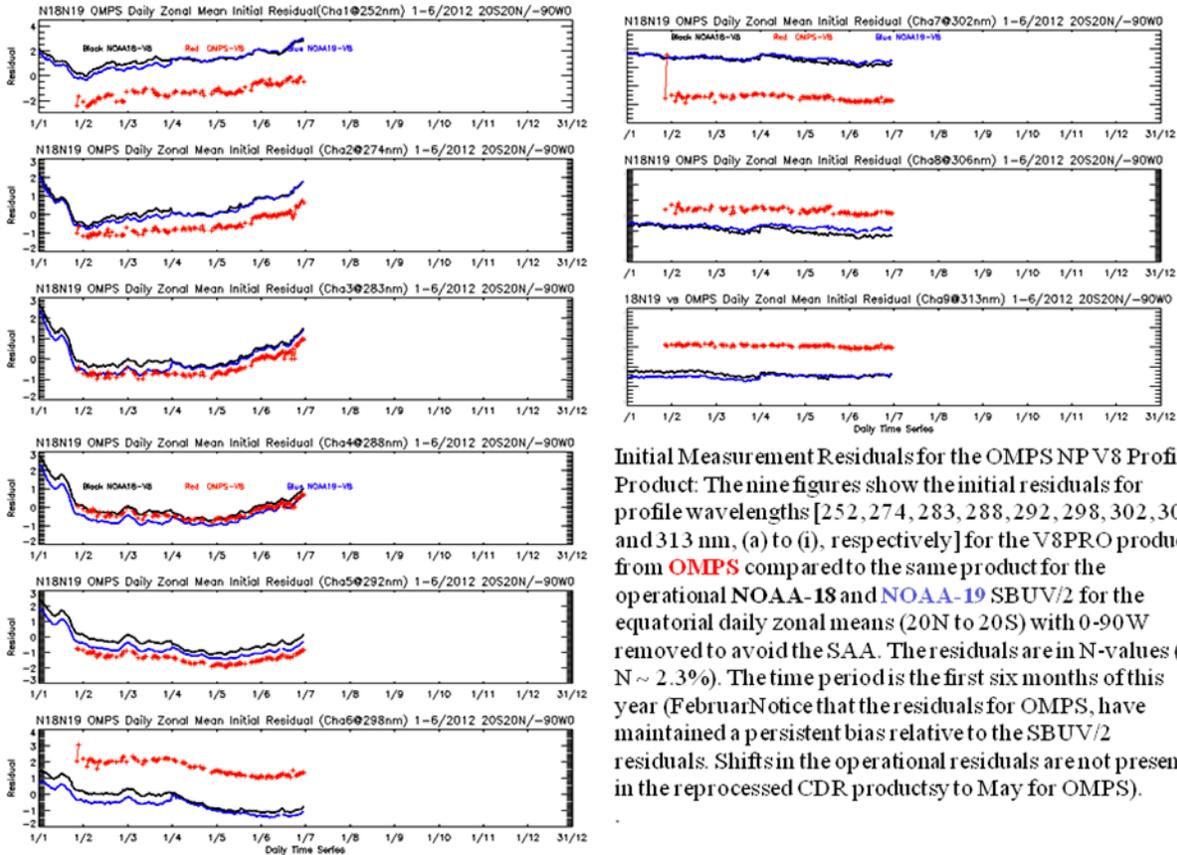
$$Xfr - Xf = Xr - Xa + A \# [Xa - Xf]$$

and then applying the retrieval and forecast covariance matrices.



**Figure 7. Comparisons of actual differences in annual tropical zonal mean profiles retrieved by NOAA-16 and NOAA-17 SBUV/2 for 2003 with those predicted by their differences in initial measurement residuals. The “+” symbols are ΔXr computed directly and the \* symbols are Dy ΔM.**

## Time series of initial V8PRO residuals for OMPS NP February through June



Initial Measurement Residuals for the OMPS NP V8 Profile Product: The nine figures show the initial residuals for profile wavelengths [252, 274, 283, 288, 292, 298, 302, 306 and 313 nm, (a) to (i), respectively] for the V8PRO product from OMPS compared to the same product for the operational NOAA-18 and NOAA-19 SBUV/2 for the equatorial daily zonal means (20N to 20S) with 0-90W removed to avoid the SAA. The residuals are in N-values (1 N ~ 2.3%). The time period is the first six months of this year (February to June). Notice that the residuals for OMPS, have maintained a persistent bias relative to the SBUV/2 residuals. Shifts in the operational residuals are not present in the reprocessed CDR products to May for OMPS).

**Figure 8. Comparisons of initial measurement residuals for NOAA-19 SBUV/2 and the OMPS NP both for Version 8 as processed at STAR.** The figures are for the nine profiling wavelengths (252, 274, 283, 288, 292, 298, 302, 306, & 313 nm) from short (top left) to long (bottom right). While the time dependencies are similar, there are obvious calibration offsets among the instruments that need to be resolved to make a consistent CDR. (Post period of performance: the initial residuals have changed from the values shown here as three improvements entered the system. 1. Weekly updates for the dark current corrections, 2. New measurement based solar spectra and wavelength scales, and 3. Implementation of a stray light correction.)