DEVELOPING AND TESTING A NEW A-PRIORI INPUT FOR NUCAPS OZONE PROFILES USING OMPS LIMB PROFILER OZONE DATA

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Abstract

Ozone is an important constituent of the Earth's atmosphere. The National Oceanic and Atmospheric Administration (NOAA) Unique Combined Atmosphere Processing System (NUCAPS) is NOAA's new generational atmosphere processing system. NUCAPS creates, among many other things, a global profile ozone product that is used in operational weather forecasting. This product is made using ozone data from the Cross Track Infrared Sounder (CrIS) for the lower atmosphere, and a tropopause-based climatology derived from ozonesondes for the upper atmosphere. It is thought that incorporating data from another satellite instrument, the Ozone Mapping and Profiler Suite Limb Profiler (OMPS-LP), as a first guess approximation for the stratosphere could improve the NUCAPS product. This project examines the process for incorporating this new data. Comparisons of OMPS-LP data with other datasets for future validation purposes of the new NUCAPS product are also examined. In particular, comparisons have been made between OMPS-LP and measurements from the Stratosphere Aerosol and Gas Experiment III onboard the International Space Station (SAGE III-ISS). These comparisons are examined in depth and show good correlation in many cases, with differences being classified further.

Introduction

Ozone

Ozone is an important part of the earth's atmosphere. Ozone in the lower troposphere, the part of the atmosphere in which we live, is dangerous to human health. In the troposphere, ozone is considered an air pollutant, and is monitored and regulated by the US Environmental Protection Agency. However, ozone farther up in the atmosphere, in the stratosphere, is vital to human survival. There, it attenuates harmful, high-energy ultraviolet sunlight, turning that energy into heat. Without this Ozone Layer in the stratosphere, the harsh ultraviolet sunlight would more easily be able to make its way down to the surface, where it has the potential to cause skin cancer and other health hazards. Therefore, monitoring ozone throughout the atmosphere is imperative; both near the surface, where it is harmful, and farther up, where it is beneficial. There are many satellite instruments and processing systems that are devoted to better understanding and characterizing atmospheric ozone distributions. This project examines the potential of combining several of these measurements together to create a more complete understanding of ozone on a global basis.

OMPS

The Ozone Mapping and Profiler Suite (OMPS) is a suite of instruments onboard the Suomi National Polar-orbiting Partnership (S-

NPP) satellite. OMPS has three instruments in total: The Nadir Mapper (NM), Nadir Profiler (NP), and Limb Profiler (LP). The LP looks behind the satellite along what is known as the limb of the earth, and measures limb scattered solar radiances in both visible and ultraviolet wavelengths. A diagram of this viewing geometry is shown in Figure 1. The scattered light from the sun measured by the instrument can be used to produce estimates of a vertical profile of ozone at each of the measurement locations.

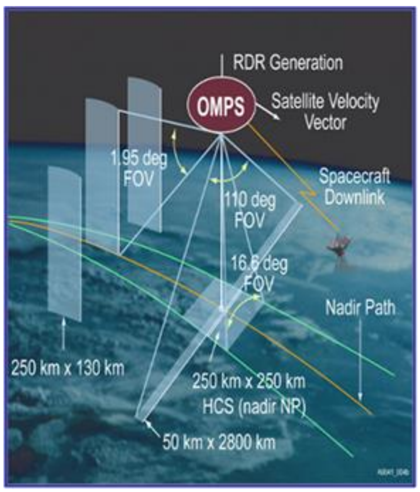

Figure 1: OMPS Viewing Geometry © NOAA

NUCAPS

The National Oceanic and Atmospheric Administration (NOAA) Unique Combined Atmosphere Processing System (NUCAPS) is NOAA's new generational atmosphere processing system. NUCAPS produces global profiles of different atmospheric constituents and parameters, including ozone. The current NUCAPS ozone profile information is obtained by combining measurements from the Cross-track Infrared Sensor (CrIS), which is also on S-NPP. To better account for the stratospheric part of the profile, a tropopause-based climatology derived from ozonesonde measurements is used as an a-priori first guess profile. Being an infrared sensor, CrIS views radiation emitted from the earth, as opposed to the scattered solar radiation that OMPS observes. This means that CrIS and OMPS measurements are sensitive to ozone variations in different parts of the atmosphere.

SAGE III-ISS

The Stratospheric Aerosol and Gas Experiment III (SAGE III) is an occultation instrument on the International Space Station (ISS) that measures aerosols and trace gases, such as ozone and water vapor, in the atmosphere. Occultation is a similar measurement technique to the limb scattering that was discussed in the previous OMPS section. The difference with occultation is that it makes measurements using transmitted solar (or lunar) radiation as opposed to scattered solar radiation. SAGE takes measurements during sunrise and sunset events, following the sun (or moon) as it rises or sets through the atmosphere, which enables it to retrieve high resolution vertical profiles of the atmosphere. Occultation measurements have high vertical resolution but come at the cost of only being able to take measurements during sunrise and sunset events.

Development of a New NUCAPS A-Priori

TOAST

Like NUCAPS, Total Ozone from Assimilation of Stratosphere and Troposphere (TOAST) is another processing scheme made by NOAA to produce a global map of ozone concentration at several different pressure levels. TOAST has evolved over the years, combining satellite data from High Resolution Infrared Sounder (HIRS), Solar Backscatter Ultraviolet Instrument (SBUV/2), CrIS, and now OMPS measurements. Each of the versions of TOAST since its inception have been created by using a combination of both infrared and UV/Visible measurements. The first version of TOAST was made by combining SBUV/2 and HIRS measurements, while its most recent iteration combines CrIS and OMPS data in different ways to create three different versions of TOAST. Two of these variations use a 12-layer analysis, while the third uses a 100-layer analysis. The two 12-layer analyses, TOAST v05 and v05.2, are made at 12 umkehr layers. The difference between the two is that v05 is made using NOAA's granule OMPS data, while v05.2 is made using the NASA PEATE daily OMPS data files. The 100-layer analysis, TOAST v05.100, is what will be used to create the new NUCAPS a-priori, as NUCAPS is also a 100-layer product.

The first step in this process is to generate the TOAST ozone fields. This involves developing the stratospheric TOAST ozone fields using OMPS-LP data, though data from the OMPS Nadir Profiler or SAGE III-ISS could also be used. This task began with the tools developed for the TOAST product, received from Dr. Jianguo Niu at the NOAA Center for Weather and Climate Prediction in College Park, MD. TOAST profiles are produced using Fortran code which is run using a KornShell script. An Interactive Data Language (IDL) script was made for this project in order to automate the process of creating the TOAST profiles. The IDL code was made to iterate through each day of data, running the KornShell script and producing TOAST profiles for each day. An example of a v05 TOAST analysis can be seen in Figure 2 (which can be found at the end of this document in the Appendix), which shows the 12-layer analysis from July 25, 2018. Of note, these plots were made using just OMPS-LP data and have not incorporated CrIS data yet. In the 12 plots shown, the top left, layer 1, is the highest in the atmosphere at 0.25mb while layer 12 in the bottom right is the lowest at 1013mb. Once CrIS data is incorporated into the analyses, it will replace the bottom 4 layers (layers 9, 10, 11, and 12), while OMPS will still be used for the upper 8 layers.

<u>NUCAPS A-Priori</u>

In creating the ozone fields, there are several aspects to keep in mind. When considering the inputs for the fields for use as an a-priori, both the vertical resolution of the data and the covariance of the inputs must be considered. There will also inevitably be some filtering or quality control that needs to be performed on the inputs to ensure a high-quality end product. As the study progresses, it would be possible to compare the fields produced by different inputs (OMPS-LP, OMPS-NP, SAGE III) as a way of comparing the inputs themselves. This would be a proper method to see how changing the input data from, for example, OMPS-LP to SAGE III affects the resulting product.

After the TOAST fields have been created, they will be converted to match the NUCAPS layers. TOAST and NUCAPS have different vertical resolutions, so in order to combine the two, the TOAST fields will need to be converted to the resolution of NUCAPS. NUCAPS produces higher resolution layers than TOAST, so an interpolation or spline will be used to change the TOAST levels to match those for NUCAPS. This means that there will be a conversion from the initial high resolution of OMPS, down to the medium resolution of TOAST, and then back up to the high resolution of NUCAPS. This will be the basis for the new NUCAPS a-priori.

Once the TOAST fields are produced at the NUCAPS resolution, an a-priori covariance matrix will be created. This will start as a simple diagonal or banded covariance matrix designed to allow greatly increased variability for layers below the tropopause. This part of the project will prove to be very experimental, as the effects of varying the magnitude of the values along with their dependence on latitude and height will be explored and analyzed.

New Product Validation

After establishing both the TOAST a-priori and the a-priori covariance matrix, NUCAPS retrievals can be produced. The process will be run with both new a-priori to create two new NUCAPS products: One with an OMPS-LP/TOAST-based a-priori, and one with an a-priori covariance. These retrievals will then be compared to the baseline NUCAPS case and to the input a-priori. Comparisons will be made between the different products, classifying what changes happened, where the changes occurred, and the magnitude of the changes. Comparisons will also be made with the original NUCAPS ozone profiles, the original TOAST profiles, and daily total ozone measurements from satellite instruments such as OMPS Nadir Mapper, the Ozone Monitoring Instrument (OMI), Microwave Limb Sounder (MLS), and SAGE III ISS to see how they compare. There is also potential to make comparisons with ozone profile retrievals from a new Differential Absorption Lidar (DIAL) instrument that has been installed at Hampton University. In addition, an ozonesonde system has been installed at HU for ozone measurements up to approximately 35 km altitude. The Department of Atmospheric and Planetary Sciences at Hampton University also operates a Direct Broadcast receiving system, which downloads data from satellite overpasses of the area, and has capability to produce NUCAPS profiles. In the future, the DIAL and ozonesonde systems can be used in conjunction with satellite overpasses to do near-real-time validation with NUCAPS profiles. There is potential to make the new a-priori operational, depending on its success and how it compares to the other ozone products.

SAGE III ISS Comparisons

In preparation for the future validation efforts of the new NUCAPS product, comparisons have been made between OMPS-LP and SAGE III ISS ozone measurements. SAGE III was launched in February 2017 began taking measurements in June 2017. At the time of writing this, data from June 2017 through February 2019 has been released. Extensive comparisons have been made between OMPS-LP and SAGE III data up through November 2018, with the remaining SAGE data to be compared in the near future.

In order to perform the comparisons, the closest OMPS profile by distance was found for each SAGE III profile for each day. With data being grouped by days, differences in time between profiles was not considered a limiting factor for finding profiles to compare. This was done assuming that ozone in the stratosphere in a given location would not change significantly within a day.

As noted earlier, SAGE III has a higher vertical resolution than OMPS. SAGE reports its ozone measurements at half kilometer intervals starting at 500 meters, while OMPS-LP reports its measurements at 1-kilometer intervals starting at 500 meters, with both instruments reporting measurements in terms of number density. This allows for 1-to-1 comparisons to be made easily by directly comparing every other data point of SAGE to every data point of OMPS. This method was chosen over taking an interpolation or spline of the data, as only measured data was used in this case. With over 10,000 profile comparisons, profiles were grouped into seasons to be able to examine the data more easily. An example of a season from OMPS-LP can be seen in Figure 3, while the corresponding season from SAGE III can be seen in Figure 4. These two plots show every profile taken by SAGE III (and the corresponding OMPS-LP profiles) during June, July, and August of 2018 (JJA 2018). Absolute differences between the seasonal plots were also calculated, and the resulting difference plot for JJA 2018 can be seen in Figure 5. The difference plots show higher values of SAGE III in red and higher values of OMPS in blue, with values near 0 difference represented by white.

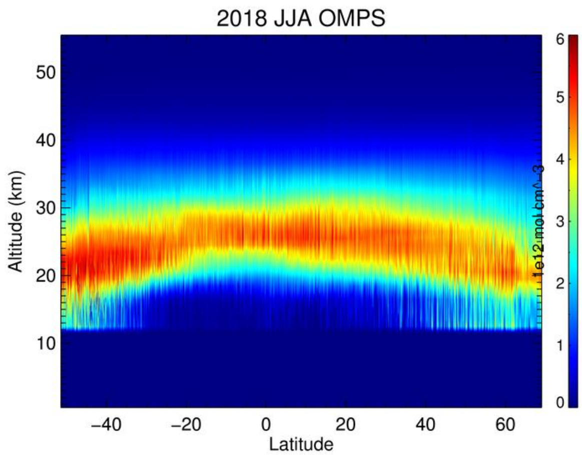

Figure 3: OMPS-LP Seasonal Plot for June-July-August 2018, showing every profile corresponding to a SAGE measurement

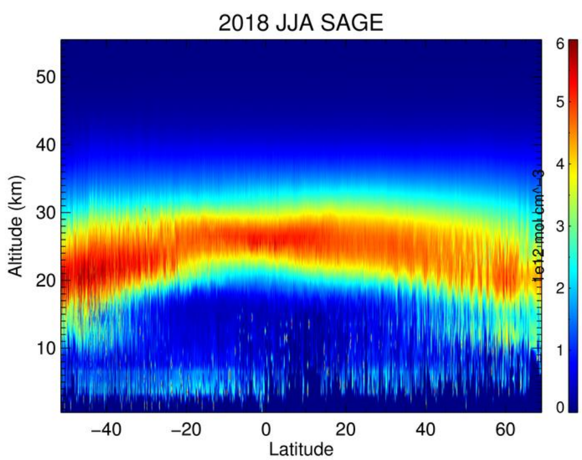

Figure 4: SAGE III Seasonal Plot for June-July-August 2018, showing every SAGE III measurement in that time

An example of a SAGE/OMPS individual profile comparison can be seen in Figure 6, along with the associated percent difference plot in Figure 7. In Figure 6, the SAGE profile is shown in black while the OMPS profile is shown in blue. The error associated with each are shown as the gray and cyan error bars, respectively. In the percent difference plot, the black line represents the percent difference between the two profiles, and only shows where both instruments had measurements, while the area shaded in gray denotes ±10%. This profile was selected because it represents the “best” profile from JJA 2018. In order to find the “best” comparison, the average of the absolute value of the percent difference for each profile was determined, and this quantity was minimized. This helped to determine which profile had, on average, the smallest deviations from 0% difference in the profiles. Correlation values and Chi Squared values were also calculated for each set of profiles, so those statistics could also have been used to find the best comparing profiles.

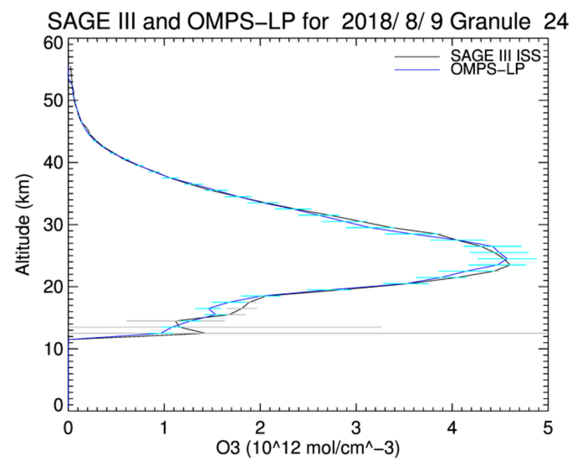

Figure 5: Statistical “Best” comparison profile between SAGE III and OMPS from JJA 2018, taken on August 9, 2018

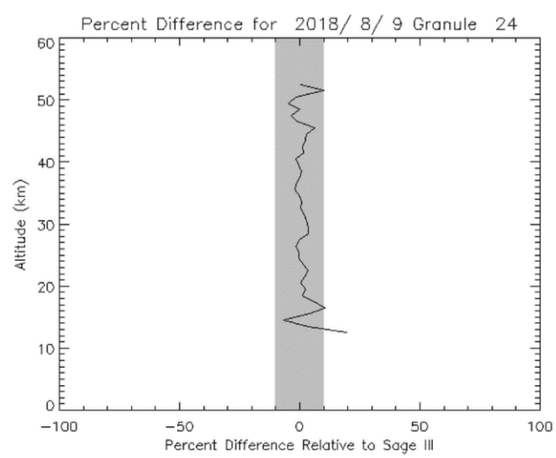

Figure 6: Percent Difference values for the profiles shown in Figure 5

Discussion

SAGE III and OMPS Statistics

Examining the correlation and chi-squared statistics for the SAGE and OMPS comparisons allows for an in-depth look at how well the 2 instruments are comparing over longer timescales. Correlation values were determined two different ways: by correlating individual profiles together within a season and correlating the seasonal plots themselves. These two methods for correlating resulted in similar, yet slightly different, values. Correlating the seasonal plots themselves resulted in correlation values between about 93% and 95% for each season. When correlating each individual profile and grouping those by season, the mean correlation values rise slightly to between about 94% and 96%, with median values ranging from 96% to 98%. Specifically, for JJA 2018, the mean correlation for the individual profile comparisons was 94.67%. Seeing correlation values this high, regardless of method, shows that the instruments do compare well overall.

During this study, both OMPS-LP and SAGE III received data version updates. OMPS updated from version 2.4 to version 2.5 in June of 2017. SAGE III updated from its preliminary release version, version 5.00, to version 5.10. In both cases, data fields that were previously being used had been changed or eliminated completely, which presented challenges. For OMPS, a weighted average had to be applied to two different ozone measurements (an ultraviolet product and a visible product) to create a profile spanning the entire vertical range. Version 5.10 of the SAGE III data improved the comparisons made with OMPS. All comparisons that have been shown here have used the version 5.10 data. The version 5.00 data had more inconsistencies in select profiles, including one profile with an altitude registration issue. Average correlation for profiles and seasons showed similar values between both versions of the data, but less low outliers were present in the v5.10 data.

In order to examine some of the lower correlation values seen in the comparisons, correlation for each profile was examined as a function of distance and time separation between compared profiles. The resulting plot of this can be seen in Figure 8. Figure 8 shows each correlation value for all measured profiles plotted as a function of distance between profiles. The points are colored to represent time separation. In doing this, it was expected that the lower correlation profiles would be separated by large amounts of time or space compared to most profiles. This, however, proved to be untrue. The profiles with the lowest correlation values tended to be relatively close in both space and time, while the profiles with the largest separation in space all tended to have very high correlation. These outliers will have to be examined and classified further.

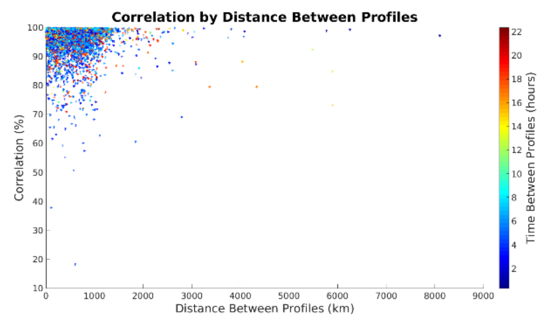

Figure 8: Correlation Values between all SAGE and OMPS comparisons plotted as a function of distance between profiles and colored by time separation

TOAST and NUCAPS

With OMPS-LP TOAST profiles created, the next step in the development of the new NUCAPS a-priori should be incorporating CrIS measurements and creating the TOAST v05.100 profiles. Part of this process will require determining at which pressure level the OMPS and CrIS data sets should be merged. The v05.100 product is relatively untested at this point but will be an important step in developing the a-priori. CrIS and OMPS pressure levels have been examined briefly at this point, specifically looking at the region of the OMPS profile where the retrieval switches from visible measurements to UV measurements. This transition occurs around 30 km in altitude, with the visible product being used for lower altitudes and the UV product for higher altitudes. CrIS, like NUACPS, has 100 vertical pressure levels, while OMPS has approximately 60. The pressure levels of the two instruments do not seem to share many values from these preliminary examinations, but more time will need to be spent examining them more in depth to see if a common scale exists, or if there is a particular level where the two could be combined easily.

Coverage differences between OMPS, CrIS and NUCAPS have also been examined using data from the Direct Broadcast System at Hampton University. In a given swath, CrIS has an approximately 15km resolution at nadir, while NUCAPS is approximately 50km at nadir, which makes CrIS higher horizontal resolution. OMPS, instead of being an image like the other two measurements, has a single pass of measurements that run through the middle of the other two. This will result in one OMPS measurement being used for many different NUCAPS measurements.

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Appendix

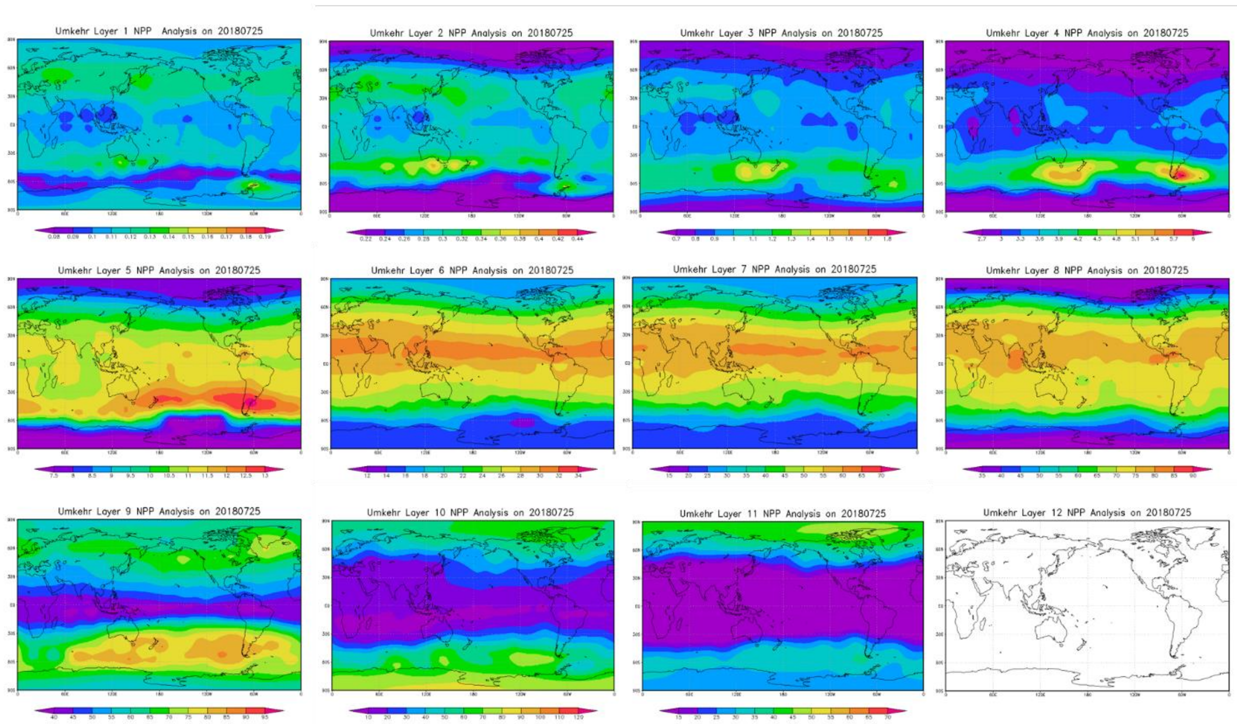

Figure 2: An example of TOAST v05 12-layer analysis for July 25, 2018 made using OMPS-LP data. The bottom right panel is the lowest in the atmosphere, while the top left panel is the highest. The lowest four layers will be made using CrIS data in the future.