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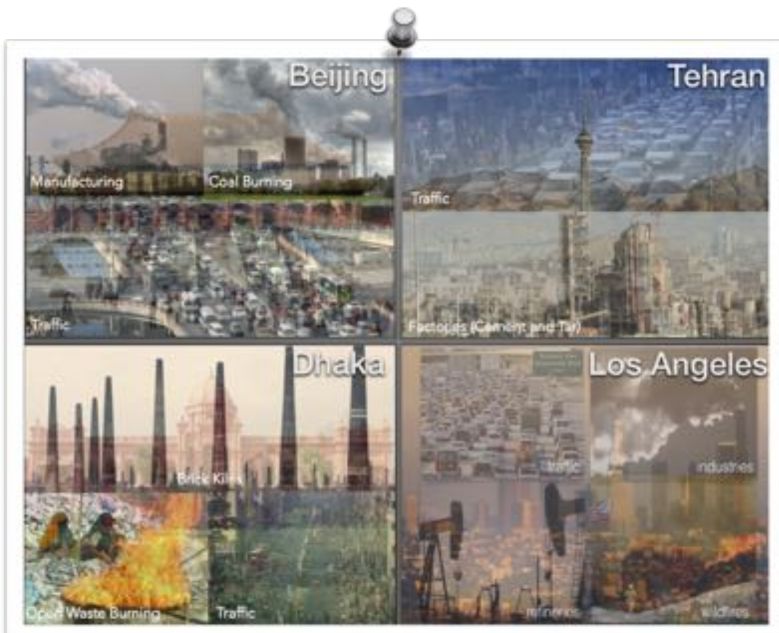
Improvement of Quality Flags on IASI Products for an Optimized Data Assimilation in CAMS:

A Specific Application to
Multi-Species Analysis of Anthropogenic Pollution Trends
Using IASI and AC SAF Retrieval Products



Executive Summary

A four-month program of research was conducted in LATMOS to better understand how best to utilize AC SAF products, particularly with the IASI retrievals of O_3 and CO, in optimizing observational constraints for prediction systems of atmospheric composition like CAMS. Such systems are becoming a useful tool to monitor, assess, and predict the states of our atmosphere, in response to the growing demand for high-level information to support decision and policy making. Yet, these systems (while evolving) still lacks the fidelity needed for an accurate and consistent prediction. The AC SAF suite of products offer an opportunity to provide important multi-instrument and multi-variate/species constraints to these systems. In this program, we first assess the quality flags for IASI O_3 and CO, leveraging from previous and on-going work by the IASI team on improving the general data quality of its products. We focus on assessing the sensitivity of our inference on species abundance and their associated spatiotemporal patterns to the choice of quality flags. Second, we estimate the trends of the enhancement ratios derived from IASI O_3 and CO over major combustion regions (i.e., megacities) to provide a baseline diagnostic for prediction systems to capture. This is an important step towards a more robust way to confront models of atmospheric composition, not only using single species evaluation but including an evaluation of how well these models show consistency across species. This is especially true for reanalysis activities where the relatively long term multiple products of IASI (O_3 and CO in particular) can provide observational constraints.

Our initial results show that changes in quality flags did not alter the main results of the trend analysis. However, depending on the scientific application, the choice between nighttime and daytime data warrants further investigation. In addition, the trends in the degrees of freedom for signal (DOFS) and relative retrieval error for CO (but not for O_3) show a slight increasing (and decreasing) trend which indicate sensitivity of retrievals to more improved level 2 (L2) inputs from EUMETSAT. DOFS and relative error for O_3 are stable across the 9-year IASI record. Enhancement ratios of IASI O_3 to CO show intriguing differences across megacities in China. In particular, Beijing and Shenzhen shows a positive linear trend (0.58±2.15 and 0.38±0.42 %/yr respectively) while Shanghai shows a negative trend (-062±0.67%/yr). This may be attributed to differences in VOC-NOx-O_3 regime between these cities, which the models should be able to capture. On the other hand, enhancements of O_3 derived from these ratios show a pattern of decreasing to increasing trend across Beijing, Shanghai, and Shenzhen which may indicate differences in combustion-related activity between these cities consistent with the developing economic status of these cities. More scientific evidences corroborating these results are needed in the future. Evaluation against other datasets (ground-based, airborne, or other retrievals – e.g., MOPITT CO and GOME-2 NO_2 and O_3) is recommended to enhance the rigor of these findings.

This study offers an impetus towards characterizing other species relationships (e.g., IASI NH_3, CH_4) not only as basis for monitoring consistency in atmospheric composition but also as a way to fully utilize the information content of these retrieval products in the context of data assimilation and reanalysis.

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Introduction

Anthropogenic Pollution. Increasing population and rapid growth and development of urban areas around the world present a compelling and urgent need to understand, assess, and predict the accelerating stresses on our changing environment. Urban agglomeration, particularly megacities (i.e., cities with >10 million inhabitants) are expected to continue growing (in size and number) over the coming decades (United Nations, 2015). This is especially problematic since it is in these megacities where human (anthropogenic) activities are most intense, accompanied by immense energy consumption mainly in the form of fossil-fuel combustion (Kennedy et al., 2015). These directly lead to enhanced emissions of air pollutants, greenhouse gases, and waste energy, largely impacting air quality, climate, and ecosystems (e.g., Baklanov et al., 2016; Lelieveld et al., 2015; Zhu et al., 2012). At present, estimates of emissions from fossil-fuel combustion remain uncertain, especially in rapidly developing regions where combustion is poorly characterized due to lack of detailed information on energy-use, combustion practices, and pollution control strategies (e.g., Creutzig et al., 2015). Our understanding of how combustion and other anthropogenic-related pollution (e.g., deforestation, agriculture) evolve in space and time is still rather limited. This alone precludes us to accurately assess the changes in atmospheric composition due to anthropogenic activities at scales that is relevant to air quality, energy, and environmental policy. In this broad context, it is imperative that we provide more accurate and consistent analysis of anthropogenic pollution emissions.

Pollution Signatures Seen from Space. Our capability to observe atmospheric composition has been unprecedented in recent decades. In particular, the NASA's EOS satellite platforms (Terra, Aqua, and especially Aura), as well as ESA's Envisat and Eumetsat's MetOp satellites have provided remarkable opportunities to study tropospheric constituents and monitor the abundance of combustion-related chemical species such as CO (MOPITT, AIRS, TES, Sciamachy, IASI), NO_2 (GOME-2, Sciamachy, OMI), O_3 (TES, OMI, Sciamachy, IASI), CO_2 (AIRS, TES, Sciamachy, OCO-2, IASI), CH_4 (AIRS, TES, Sciamachy, IASI), SO_2 (OMI, Sciamachy, GOME-2, IASI), HCHO (Sciamachy, GOME-2, OMI) and NH_3 (IASI, TES, AIRS) among others; as well as aerosols through data on optical depths and backscatter (AOD or AI from MODIS, MISR, OMI, CALIPSO, Sciamachy, GOME-2, and IASI). In twenty years or so, we made progress in identifying and quantifying regional and sectoral sources of these pollutants using these satellite products (i.e., top-down), in conjunction with ground-based networks and aircraft campaigns. With these products and with advances in modeling and chemical data assimilation systems (CDAs), we have also improved our predictive capability and understanding of the spatiotemporal patterns of these pollutants through chemical weather forecasting and reanalysis (e.g., Copernicus/CAMS, Inness et al., 2015). IASI retrievals has played a major role not only on our scientific progress but more importantly in providing critical data for public information services (e.g., Clerbaux et al., 2015 and references therein). However, despite this progress, gaps still exist in our understanding of the major drivers of the changes in emission patterns/trends that we observed, including inconsistencies in emission estimates between inversion methods, retrievals, and more importantly between species (e.g., Frost et al. 2013 and references therein; Stavrakou et al., 2015). In fact, we have yet to directly connect and reconcile top-down estimates with bottom-up emission inventories through improvements in characterizing combustion activity levels/fuel consumption and/or combustion efficiency and emission factors (Streets et al., 2013).

The IASI Remote Sensor. The Infrared Atmospheric Sounding Interferometer (IASI) mission is a versatile mission that was designed to fulfill the needs of three communities: numerical weather prediction, climate research and atmospheric composition monitoring. Ten years of data are now readily available, and the series will be continued by a 3rd instrument to be launched in the fall of 2018 on EUMETSAT MetOp-C. The recorded radiance spectra exhibit signatures associated with spectroscopic absorption/emission lines of molecules present along the optical path between the Earth's surface and the satellite detectors, and from these, geophysical data such as temperature profiles and atmospheric concentrations can be derived in selected spectral windows (Clerbaux et al., 2009). The instrument has unprecedented horizontal coverage, providing more than 1.2 million (15 GB) radiance spectra per day with a footprint on the ground of 12 km diameter pixel (at nadir). As demonstrated by the LATMOS group, IASI is also a ground-breaking remote sensor for atmospheric composition sounding, allowing near-real-time mapping of chemical species and aerosols, contributing to air traffic safety, and to our understanding of atmospheric transport processes. An example of this is shown in Figure 1 where large enhancements of CO were observed from IASI during a recent pollution episode in China. Its radiometric performance is so good that it has unexpectedly allowed the distribution mapping of short-lived pollutants, permitting, for example, derivation of emission sources for ammonia and formic acid.

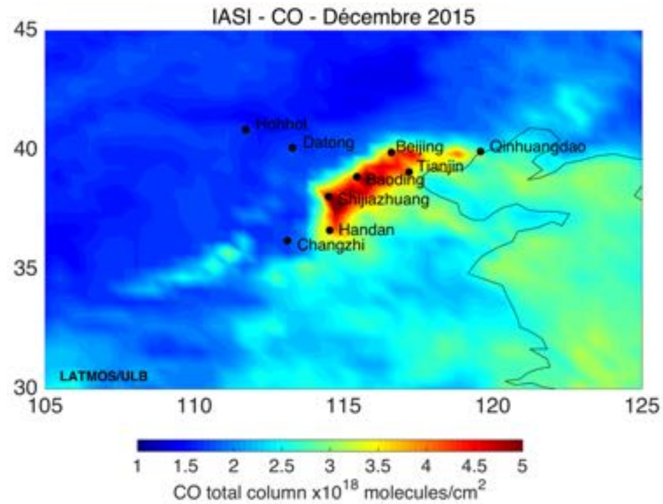

Figure 1. Total column abundance of CO retrieved from IASI during a winter pollution event in China (Source: Cathy Clerbaux).

Power of Chemistry. The relative abundance of atmospheric constituents, as observed from space, should provide a means to understand from an emission process level the integrated properties of anthropogenic pollution. When combined, these retrieval products altogether provide a unique opportunity to investigate human fingerprints in the atmosphere. Each of these constituents exhibits distinct atmospheric signatures that depend on fuel type, combustion technology, process, practices and regulatory policies. Distinguishable patterns and relationships between the increases in concentrations (or enhancements) across a region due to emissions of these constituents enable us to: a) identify trends in pollution 'activity' and 'efficiency', and b) reconcile discrepancies between state- to country-based emission inventories and modeled concentrations of these constituents. While important work has been carried out in recent years toward understanding anthropogenic pollution emissions (incl. fires) through analysis of enhancements of chemical species (including isotopes) based on ground, aircraft, and satellite observations, most of these analyses (including those from this investigator) are focused on specific regions or chemical ratios (Parrish et al. 2009; Fortems-Cheiney et al., 2012; Lopez et al., 2013; Silva et al., 2013; Reuter et al., 2014; Konovalov et al., 2014 and 2016; Hassler et al. 2016; Hakkarainen et al. 2016; Silva and Arellano, 2017; Tang and Arellano, 2017). Limited studies have focused on analyzing multiple datasets for estimating emissions. To a large extent, the synergies between these retrieval products (and between ground, aircraft, and satellite data streams) have yet to be fully explored especially with regards to providing accurate and consistent emission estimates. While it is well recognized that there are spatiotemporal sampling issues and limitations in information content of many of these observations, the integration of these datasets should provide insights towards full characterization of anthropogenic pollution; in light of the current gaps in estimating emission especially in poorly observed yet rapidly growing megacities. The key to addressing these gaps and limitations is to exploit the information from multiple observations together with different models of atmospheric chemistry and physics. This is especially true with simultaneous measurements (and near-global twice-daily coverage) of atmospheric pollutants from IASI (e.g., Boynard et al., 2014; Thonat et al. 2015; Barré et al., 2015) which eliminate collocation issues. In addition, chemical data assimilation systems (CDAs), which effectively integrate and synthesize heterogeneous information, offer a coherent picture that goes well beyond the snapshots that can be derived from measurements or models alone. However, while such information systems have been developed and matured in recent years, individual system still lacks the capability to properly characterize errors and quantify uncertainties. Issues with regards to representativeness (especially with mismatch in scale), model errors, and fully extracting information content are often dealt with in an ad-hoc manner without regard to consistency to other quantities in the coupled physical system. This results to inaccuracies and inconsistencies in the top-down estimates of the abundance, emissions, and impacts of radiatively- and chemically-active trace gases and aerosols produced from anthropogenic activities on our local to regional environment.

Research Opportunity. There is a growing need to improve the accuracy and consistency in our estimates of dynamic chemical states of the atmosphere to better monitor, assess, and report changes in air quality and climate. This is especially true as regional to global prediction systems for atmospheric composition like CAMS are being further developed for high-resolution multi-species forecasting and reanalysis including monitoring carbon human emissions which are mostly generated from megacities of the world. As a direct consequence, the quality and consistency of observational constraints (including their associated trends) on these atmospheric states becomes critical in minimizing misattribution of the drivers on the changes inferred by these systems. The trends in IASI-derived dO_3/dCO (in conjunction with dO_3/dNO_2 from GOME) offers a unique opportunity to establish a baseline on the changes in O_3 enhancements over megacities. This is particularly useful as a diagnostic when confronting AC prediction systems. The relationships of tropospheric O_3 to its precursors are presently under-explored and poorly evaluated precluding more accurate and consistent forecast and reanalysis. In this regard, this work will benefit AC SAF users (such as CAMS) as point of comparison on the drivers of O_3 trends. This also highly complements and adds value to current decadal trend investigations of IASI (and GOME-2) O_3 products (e.g., Wespes et al., 2017; Boynard et al., 2017 to be submitted).

Objectives

This study explores the value of simultaneous retrievals of multiple species of atmospheric composition from IASI instrument in providing a basis of evaluating the consistency in model predictions of anthropogenic pollution. We carry out a 4-month data analysis activity on IASI O_3 and CO in LATMOS Paris for this purpose. Here, we first assess the quality flags for IASI O_3 and CO, leveraging from previous and on-going work by the IASI team on improving the general data quality of its products. We focus on assessing the sensitivity of our inference on O_3 and CO abundance and their associated spatiotemporal patterns to the choice of quality flags. Second, we estimate the trends of the enhancement ratios derived from IASI O_3 and CO over major combustion regions (i.e., megacities) to provide a baseline diagnostic for prediction systems to capture. This is an important step towards a more robust way to confront models of atmospheric composition, not only using single species evaluation but including an evaluation of how well these models show consistency across species. This is especially true for reanalysis activities where the relatively long term multiple products of IASI (O_3 and CO in particular) can provide observational constraints. This work is also a direct extension of IASI studies on O_3 and CO trends, but with a particular focus on the time series of this enhancement ratio over megacities.

In close collaboration with Cathy Clerbaux and the IASI team, we conduct our investigation under the purview of the following questions:

1. How can we better use satellite retrievals as observational constraints on anthropogenic combustion monitoring, assessment, and prediction?
2. How can we better attribute changes in O_3 enhancements resulting from combustion-related activities?
3. How sensitive are the trends derived from IASI to the choice of quality flags?
4. How can we 'best integrate' multiple observational constraints of anthropogenic pollution emissions?

Methodology

We focus our analysis on large sources of combustion, where anthropogenic pollution is most intense. Here, we investigate the trends in combustion products (i.e., CO, in conjunction with NO_2) over major cities in China (red marks in Figure). For each city, we extract data from IASI CO and O_3 across a 2 deg radius, grid them into 0.1 deg, and calculate the average for a given month. We then conduct a geometric mean regression analysis (or reduce major axis regression) between pairs of O_3 and CO data across each sampled space to estimate the linear slope (enhancement ratio) and intercept (background). Long-term trends are derived using the widely-used Seasonal Trend decomposition using LOESS (locally weighted scatterplot smoothing) or STL. A linear trend is then estimated from STL output of long-term trend.

Different sets of IASI CO and O_3 data are tested for consistency with other retrievals like MOPITT and sensitivity of ensuing trends to the choice of quality flags. For CO, we use data from AERIS (http://cds-espri.ipsl.upmc.fr) varying them based on quality flag filters (superflag 0 to 2). We also use CO and O_3 data from a newer FORLI version (v20151001) with IASI-team supplied recipe for data quality filtering. The quality flags, which have been recently established for O_3 and CO, are leveraged in this work (please see Appendix A for description of quality flags).

The specifics of our final version of trend analysis are outlined below:

1. Extract daytime retrievals at 2-deg radius around city center (see Figure 1 for an example)
2. Do the same for 2-deg grids surrounding the city grid
3. Grid data at 0.1-deg for each 2-deg box and average across each month
4. Conduct linear regression analysis (slope and intercept) between species and across 2-deg (20x20 points). Consider +ive significant slopes only
5. Do the same for the surrounding grids
6. Calculate statistics across time and grids

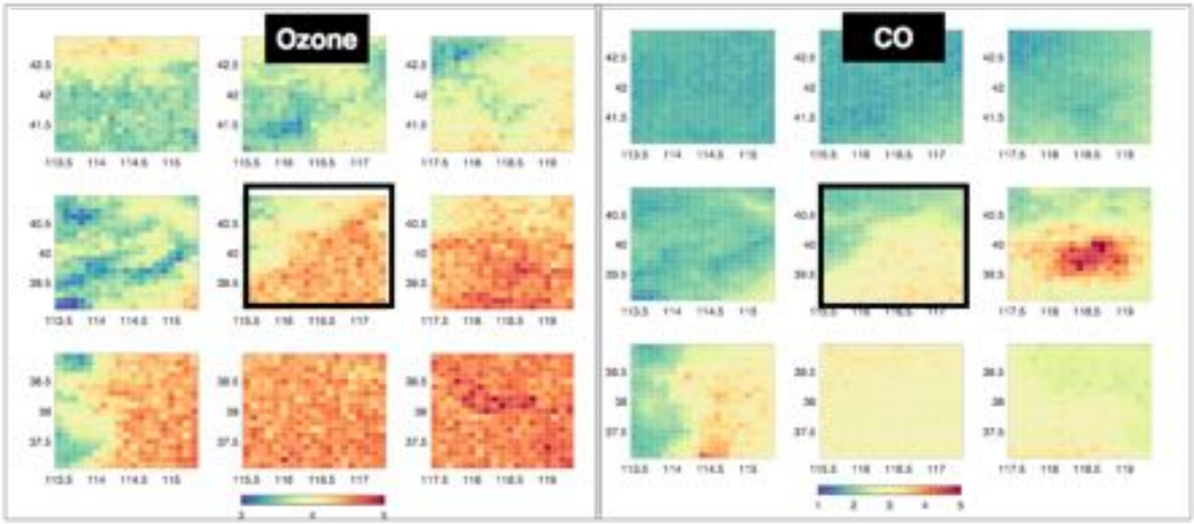

Figure 1. Monthly-mean O_3 and CO in Beijing and surrounding regions

Results and Discussion

Assessment of IASI CO and O_3

We show in Figure 2 our results on trend analysis for IASI CO and comparison with previous studies with MOPITT CO and OMI NO_2. While the relative magnitudes are slightly different (i.e, IASI tends to be consistently below which may be due to a shorter period of trend analysis), the progression from decreasing to increasing dCO/dNO_2 across less developed to more developed cities appears to be robust. This is driven not only by increasing to decreasing dNO_2 (Shenyang to Shenzhen) but also by decreasing to leveling off of dCO. We associate this progression with changes in activity and efficiency (incl. control technology and policy), and shift in fuel mixtures as the city socioeconomically evolves. Enhancements of CO from IASI show lower slopes than dCO derived from MOPITT.

Our tests on different combinations of quality flags for IASI CO total columns in AERIS show that the derived trends are not sensitive to the choice of superflag settings (from recommended superflag==0 to superflag<=2) (at least from the perspective of abundance, [CO]). Using the newer version of FORLICO (v2015+) results to slightly higher slopes that are closer to MOPITT (except in Shenzhen). We also find that there is no 'significant' difference in the trends of [CO] when selecting daytime or nighttime data. However, differences can be seen in the trends of relative error with nighttime data to be decreasing at a steeper rate in Beijing and Los Angeles suggesting larger variability of CO retrievals over these cities, which is not apparent in the [CO] trends. This has important implications to using the data in assimilation/reanalysis (e.g., CAMS/ECMWF) and/or decadal inverse modeling studies. Lastly, we also find that there appears to be a slight increasing trend in the degree-of-freedom-to-signal (DOFS) (& decreasing error) which may affect [CO] trend analysis. Its impact, however, can be minimized using enhancements (dCO). Unlike CO, IASI O_3 DOFS and error appear to be stable (Figure 3). Future work will include extending to 2017 and potentially exploring GOME-2 O_3, and NO_2 depending on the relative ease in analyzing these products and more importantly its interpretation in the context of IASI-derived trends.

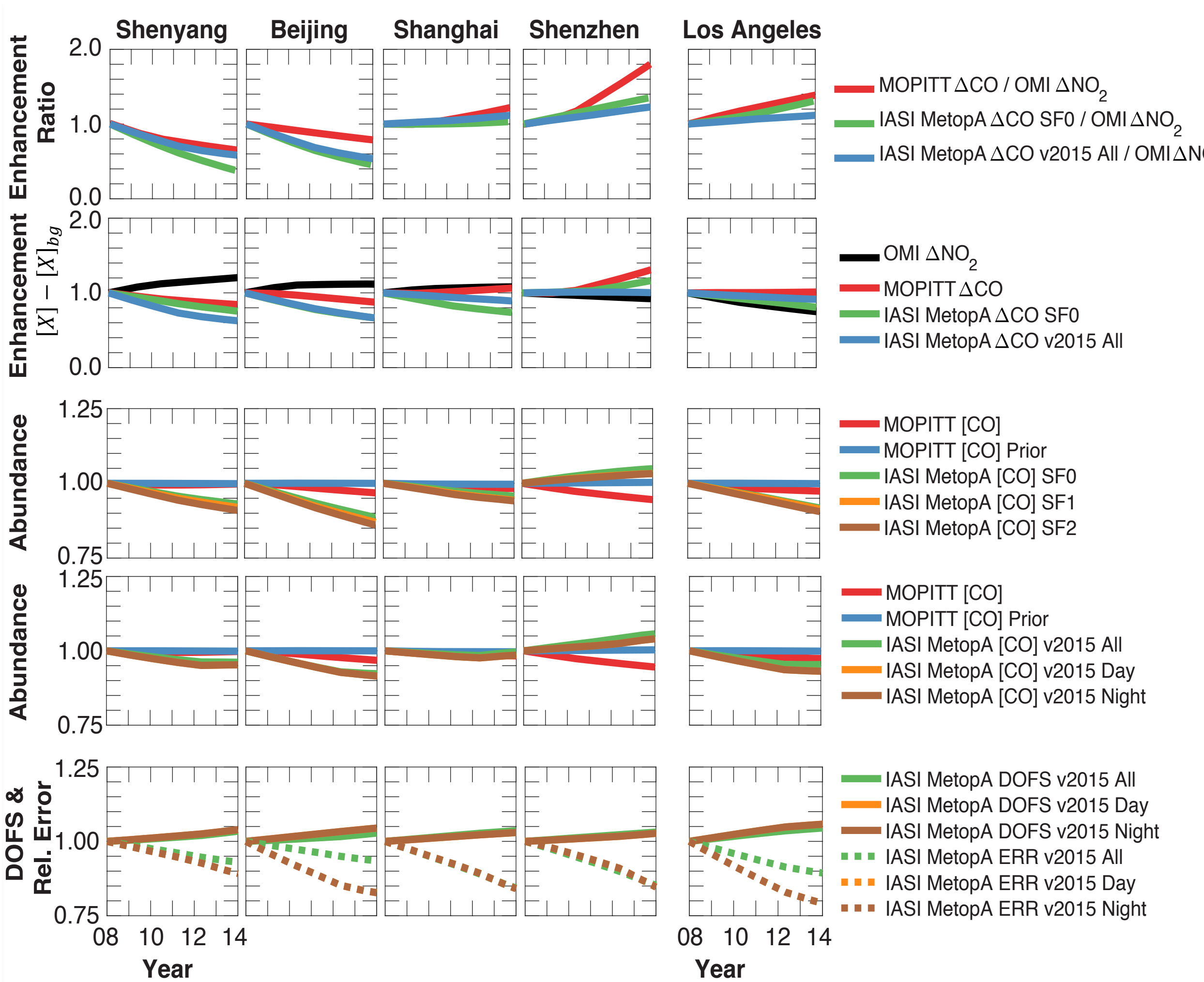

Figure 2. Trends of IASI CO, MOPITT CO and OMI NO2.

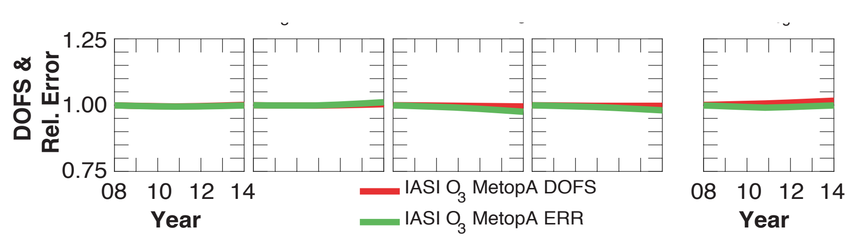

Figure 3. Trends in DOFS and Relative Error for IASI O_3

Emergent Relationships in IASI O_3 and CO Retrievals

We show in Figure 4 our results for trend analysis over major cities in China. In particular, we show the fitted data from STL analysis for O_3, CO and dO_3/dCO for the period of the study (starting from 2008). Superimposed on these plots is the long-term trend in black solid thick line and an estimate of linear trend (from the long-term trend derived from STL) in black solid line. We have also included the associated standard deviations (in red) and enhancements (in blue). Note that the standard deviation corresponds to spatial variability across the 2-degree grid of this study and not time variability. These enhancements are derived from the analysis based $\Delta O_3 = (\Delta O_3/\Delta CO)\ (CO\text{-}CO_{bg})$ where CO_{bg} was derived from the intercept in IASI CO and OMI NO_2 regression. We will explore in the future the use of GOME-2 NO_2 (within the purview of QA4ECV activity).

The mean O_3 concentrations in Beijing, Shanghai, and Shenzhen appear to be decreasing with time (-1.35±0.99, -0.56±0.06, -0.27±0.10 % year) which is consistent with Wespes et al. ACPD, (2017) findings of significant decreasing O_3 trend in the Northern Hemisphere mid-high latitudes during summer. We also see decreasing trend in Los Angeles (-1.37±0.38 %/yr). Note that Wespes et al. (2017) used a more sophisticated trend analysis algorithm than what is used here (i.e., STL). For CO, we find statistically significant decreasing trend in Beijing (-1.01±0.88 %/yr) while CO over Shenzhen appears to be increasing (0.75±0.22 %/yr). This indicate differences combustion activity and/or efficiency in Beijing versus a more developed city like Shenzhen. Similar decreasing trend in O_3 standard deviation can be also be seen. However, there appears to be decreasing CO standard deviation across all cities including Los Angeles. This is consistent with decreasing anthropogenic emissions (precursors of O_3) in these cities in the recent years.

Enhancement ratios of O_3 to CO show differences between cities (see Table 1 below for trend estimates). Beijing and Shenzhen show increasing trend (although not statistically significant for Beijing within 95% confidence interval) similar to Los Angeles while Shanghai shows a decreasing trend. This suggests that the sensitivity of O_3 production due to combustion is potentially difference between these cities (e.g., even though CO in Shenzhen show opposite sign of trend with Beijing). The rate at which CO and O_3 is decreasing is an important aspect to investigate, in particular to test consistency in modeled O_3 and CO. Verification with MOPITT CO will be conducted to test the robustness of these findings. With regards to O_3 enhancements, we find a progression of decreasing to increasing trend in Beijing, Shanghai and Shenzhen which appears to be consistent with our previous analysis of CO and NO_2 trends over these cities. Enhancements of CO follows the same pattern as its standard deviation (decreasing trend which is more prominent in Beijing). This is an interesting finding which shows the utility of satellite retrievals (in this case AC SAF IASI) to monitor emerging patterns across cities.

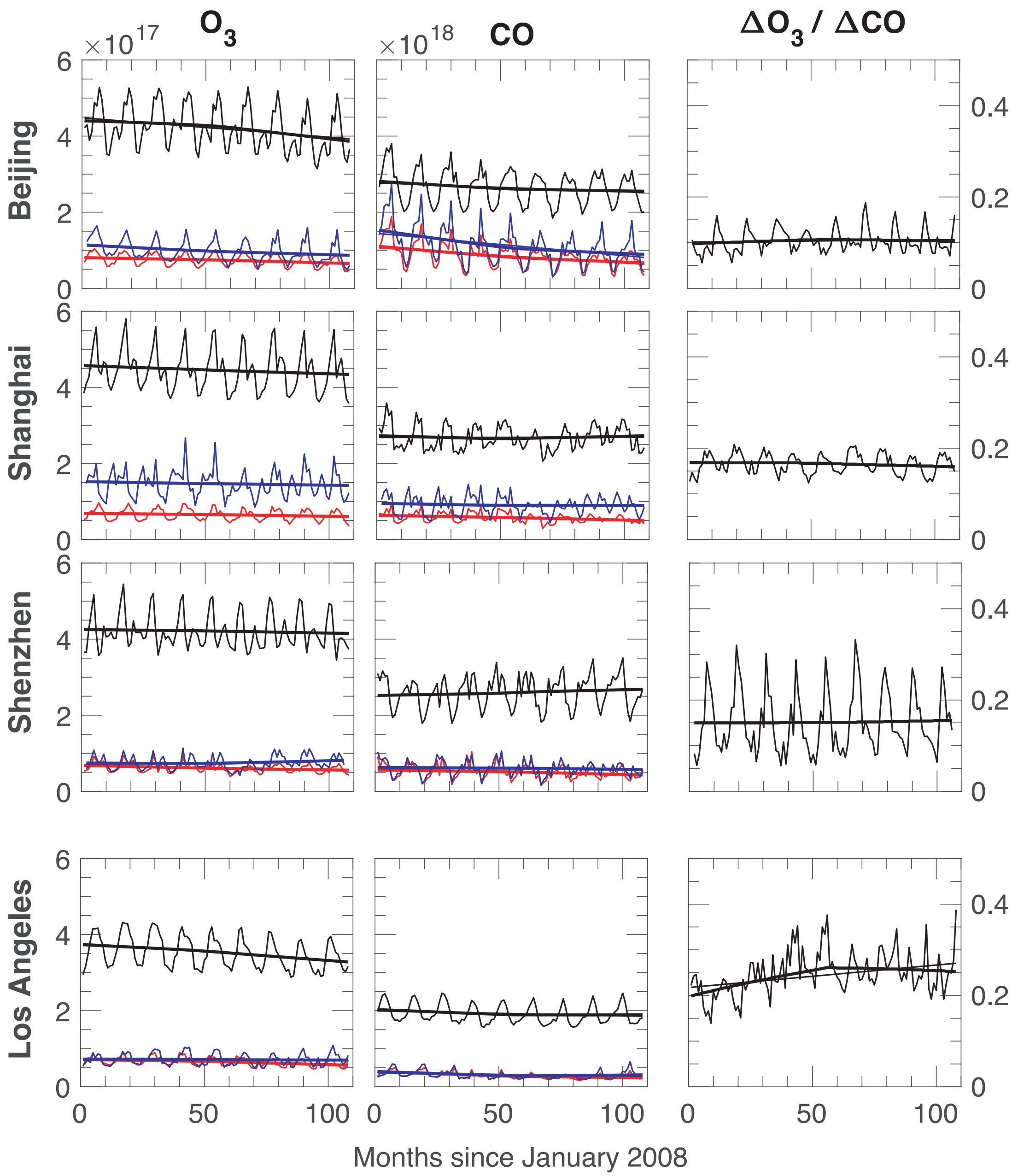

Figure 4. Estimates of O_3, CO and dO_3/dCO patterns. Black lines in column 1 and 2 panels correspond to mean O_3 or CO while red and blue lines correspond to the associated standard deviation and enhancements for the species, respectively.

9-year Linear Trend (% per year)

	Beijing	Shanghai	Shenzhen	Los Angeles
ΔO_3	-2.63±1.18	-0.72±0.17	1.14±1.89	-0.47±0.17
ΔCO	-4.85±4.45	-0.60±0.90	-0.98±0.58	-2.68±6.27
$\Delta O_3/\Delta CO$	0.58±2.15	-0.62±0.67	0.38±0.42	2.69±4.46

Evolution of O_3 Production in Chinese Cities

We show in Figure 5 the relative changes in enhancement ratios of O_3 to CO and O_3 to NO_2 to place our analysis in the broad context of O_3 production due to combustion in these megacities. Briefly, there is an important difference between Beijing and more developed cities like Shenzhen and Shanghai. The sensitivity of O_3 to CO is increasing while O_3 to NO_2 is decreasing in Beijing. In contrast, the sensitivity of O_3 to CO in Shanghai and Shenzhen show a decreasing to stable pattern while sensitivity of O_3 to NO_2 is increasing. Differences in combustion mixture across these cities and/or combustion efficiencies may account for these differences (although meteorology cannot be discounted at this point). Again, our findings point to the utility of using these satellite retrievals to monitor trends of atmospheric composition. This is especially true for poorly observed regions of the world (yet are key drivers of pollution). This also shows the utility of these retrievals as observational constraints on prediction systems like CAMS.

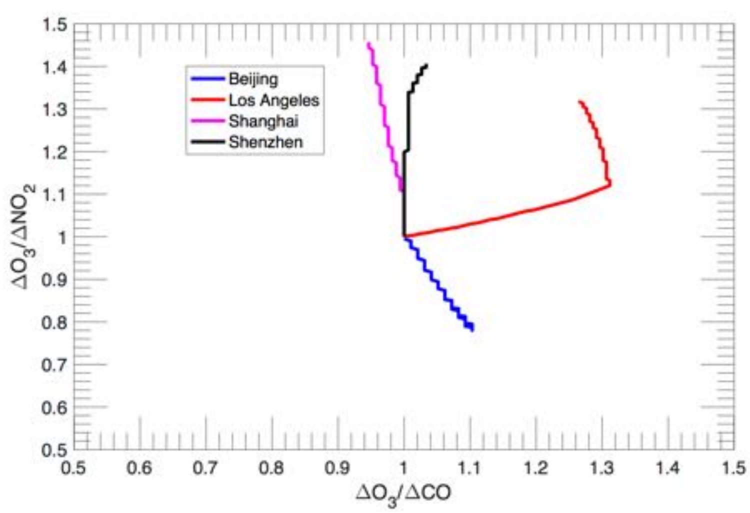

Figure 5. Evolution of dO_3/dCO and dO_3/dNO_2 relative to January 2008.

Summary and Future Directions

In light of rapid urbanization and its impacts on our changing environment, it is imperative that we provide more accurate and consistent analysis of anthropogenic pollution emissions to advance our monitoring, assessment, and predictive capabilities. Here, we explore the use of multiple AC SAF satellite retrieval products, particularly from the IASI instrument on EUMETSAT MetOp satellite, in conjunction with retrievals from other instruments like MOPITT and OMI, towards characterizing and quantifying emissions from anthropogenic combustion. Thus far, the IASI instrument has provided long-term hyperspectral Earth observational records critical to advancing our current capabilities in Numerical Weather Prediction (NWP), atmospheric composition monitoring, and climate studies. A suite of multiple regression analysis of available collocated IASI retrievals (e.g., O_3, CO) is conducted to derive long-term patterns of abundance and chemical ratios over major pollution regions of the world. This analysis is based on an approach originally applied to ambient CO and NOx concentration to infer vehicular emission ratios. Data quality and data filters are systematically assessed to attain a more robust analysis on the patterns of these ratios and emergent relationships between species as well as across pollution regions. Retrieval characteristics (e.g., averaging kernels, error covariances, systematic biases, pixel resolution) are taken into consideration in assessing the information content (and synergies) of these retrievals.

Our initial results show that changes in quality flags did not alter the main results of the trend analysis. However, depending on the scientific application, the choice between nighttime and daytime data warrants further investigation. In addition, the trends in the degrees of freedom for signal (DOFS) and relative retrieval error for CO (but not for O_3) show a slight increasing (and decreasing) trend which indicate sensitivity of retrievals to more improved level 2 (L2) inputs from EUMETSAT. DOFS and relative error for O_3 are stable across the 9-year IASI record. Enhancement ratios of IASI O_3 to CO show intriguing differences across megacities in China. In particular, Beijing and Shenzhen shows a positive linear trend (0.58±2.15 and 0.38±0.42 %/yr respectively) while Shanghai shows a negative trend (-062±0.67%/yr). This may be attributed to differences in VOC-NOx-O_3 regime between these cities, which the models should be able to capture. On the other hand, enhancements of O_3 derived from these ratios show a pattern of decreasing to increasing trend across Beijing, Shanghai, and Shenzhen which may indicate differences in combustion-related activity between these cities consistent with the developing economic status of these cities. More scientific evidences corroborating these results are needed in the future. Evaluation against other datasets (ground-based, airborne, or other retrievals – e.g., MOPITT CO and GOME-2 NO_2) is recommended to enhance the rigor of these findings.

This study offers an impetus towards characterizing other species relationships (e.g., IASI NH_3, CH_4) not only as basis for monitoring consistency in atmospheric composition but also as a way to fully utilize the information content of these retrieval products in the context of data assimilation and reanalysis. There is utility in multi-species analysis of satellite retrievals on atmospheric composition, especially from combustion-related constituents over megacities. Confronting model simulations, forecast, and analysis with multi-species constraints may be the way to go in ensuring consistency in our estimates. Lastly, this has implications to future missions (i.e., collocated measurements of species within the nexus of AC constellation).

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I would like to thank EUMETSAT AC SAF for IASI data and for financial support of my sabbatical in LATMOS France. I especially thank Seppo Hassinen of EUMETSAT for his guidance. I am also very grateful to the members of LATMOS IASI team: Cathy Clerbaux, Juliette Hadji-Lazaro, Anne Boynard, Maya George, Camille Viatte, and Sarah Safieddine as well as ULB IASI Team especially Catherine Wespes for help and significant guidance on IASI data. I acknowledge the members of CAMS global prediction team for helpful discussions on data assimilation activities in CAMS.

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Appendix A

The table below is a summary of the quality flags discussed and tested.

IASI Flag Definitions

(from AERIS: http://cds-espri.ipsl.upmc.fr/etherTypo/index.php?id=1707&L=1)

Flag Number*	Simple Description	Technical Description (from Juliet's Notes)	Corresponding Variable Name(s)	Additional Notes from Juliet
1 (desc)	If surface altitude in our model is negative	If Z0 < 0	AMP_NEGZ0	we treat the obs and warn the user with this flag (+AMP_ANC = if Z0<0.25, AMP_ERROR)
2 (desc)	If Tskin is missing in IASI level 2 data AND is replaced by the brightness temperature at 2143.25 cm^{-1} in our model	If Tskin from EUMETSAT = NaN AND is replaced by Ts @ 2143.25/cm	AMP_TSKIN	and warns the user with this flag (+AMP_L2 = flags related to L2 EUMETSAT Met variables)
3 (desc)	If the difference in absolute value between Tskin of IASI level 2 data and the brightness temperature at 2143.25 cm^{-1} is higher than 5K	If |Tskin - Ts @ 2143.25/cm | >5K	AMP_TDIFF	+AMP_L2
4 (desc)	If a desert is detected at the Earth's surface	If Desert >=5 where Desert=(2*BT(844)-BT(1097.5)-BT(1128.5)) / 2	AMP_DESERT	+AMP_L2

5 (fit)	If the maximum number of iterations is reached without convergence	If dfit < (L_nParames*Tolerance) and ((old_cost-cost)<1 and |bias|<0.5xRMS) Tolerance=0.1	AMP_ITERATIONS	bAlt +AMP_ERROR +AMP_FIT (may need to check units)
6 (fit)	If the fit residual bias is sloped	If |slope| > RMS	AMP_SLOPE	+AMP_FIT
7 (fit)	If the contrast of CO lines is weak	If |radiance(2157.25)-radiance(2156.5) |x 2e-2 < NOISE	AMP_CONTRAST	+AMP_L1 = flags related to L1 EUMETSAT Met variables)
8 (fit)	If the averaging kernel vector includes strange values (generally too high)	If A(j) > 2 and (A(j+2)-A(j)) > 1 and (A(j+1)-A(j))>0.5	AMP_AVK	break? +AMP_FIT
		Additional "Flags"		
	one to indicate that the fit residual root mean square is too high	RMS>2.0*NOISE	AMP_RMS	+AMP_FIT
	one to indicate that the fit residual bias is too high	|Bias|>0.15*NOISE OR |Bias|>0.2*RMS	AMP_BIAS	+AMP_FIT
			AMP_FIT	from FORLI
			AMP_ERROR	from FORLI

Additional flags used in newer version of FORLICO (20151001)

Flag Number*	Simple Description	Technical Description (from Juliet's Notes)	Corresponding Variable Name(s)	Additional Notes from Juliet
		CO>= 20e18 molec/cm2		
		If 1 or 2 levels in the H_2O profile from EUMETSAT have NaN values	AMP_INCOMPLETE	Or if Pskin=NaN +AMP_ERROR +AMP_L2 the obs is treated H2O_lev2(i)=H2O_lec2(i+1) and the user is notified with this flag (only warning) from 3 levels of H_2O = NaN AMP_ERROR(alone)
		If one partial column of CO, H_2O, CO_2, N_2, or N_2O is negative	AMP_NEGPC	break? +AMP_ERROR +AMP_FIT

Additional flags used O_3

Flag Number*	Simple Description	Technical Description (from Juliet's Notes)	Corresponding Variable Name(s)	Additional Notes from Juliet
		If determinant of Shat<e-68	AMP_CONDITION	balt Must be positive definite

From AERIS website, the superflag is equal to:

0	a) all desc and fit flags are zero (null) OR b) the cloud cover is less than 12 % (but higher than 0) and only flag 2 is equal to 1 ;
1	a) all the fit flags are zero (null) with at least one desc flag equal to 1 OR b) all the fit flags are null with only flag 2 equal to 1 and the cloud cover equal to 0 OR c) all the fit flags are null with only flag 2 equal to 1 and the cloud cover higher or equal to 12 %
2	at least one fit flag is equal to 1.

FLAG=
AMP_NEGZ0+
AMP_TSKIN+
AMP_TDIFF+ (for CO)
AMP_DESERT+
AMP_ITERATIONS+
AMP_DIVERGED+ (for CO and O3)
AMP_SLOPE+
AMP_CONTRAST+
AMP_AVK+ (for CO and O3)
AMP_RMS+
AMP_BIAS+
AMP_FIT+
AMP_ERROR+ (for CO and O3)
AMP_ANC+
AMP_L2+
AML_L1+
AMP_EMPTY + (for CO and O3)
AMP_INCOMPLETE + (for CO and O3)
AMP_CONDITION +
AMP_NEGPC (for CO and O3 – note species dependent treatment of NEGPC)
CO >= 20e18 (for CO)
O3(0-6km)/O3(total) < 0.085 (for O3)
For CO (FORLI 20151001)
RMS<=2.7e-9, -0.15e-9<ABIAS<0.25e-9

For O3:
RMS<3.5e-8, 0.75e-9<ABIAS<1.25e-9

Note: For CAMS/ECMWF, superflag=0 is used. EUMETSAT data uses superflag=2 for AERIS superflag=0.