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# Strategies for Stratosphere-Troposphere Separation of Nitrogen Dioxide Columns from the TEMPO Geostationary Instrument

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## The Problem

Observations of $NO_2$ from satellite-based instruments have provided unprecedented global insight into tropospheric $NO_2$ concentrations. Stratosphere-troposphere separation (STS) is a crucial step in the application of these observations. The tropospheric vertical column density ($VCD_{trop}$) is calculated by:

$$VCD_{trop} = \frac{SCD - (VCD_{strat} \cdot AMF_{strat})}{AMF_{trop}}$$

where *SCD* is the slant column density (obtained by spectral fitting of solar backscattered radiation), $VCD_{strat}$ is an estimate of the stratospheric vertical column density, and $AMF_{strat}$, $AMF_{trop}$ are the stratospheric and tropospheric air mass factors. Observations from low-earth orbit (LEO) provide a daily global view, with coverage over pristine areas where the $NO_2$ column is dominated by the stratosphere. This can be used to interpolate the stratospheric column elsewhere.

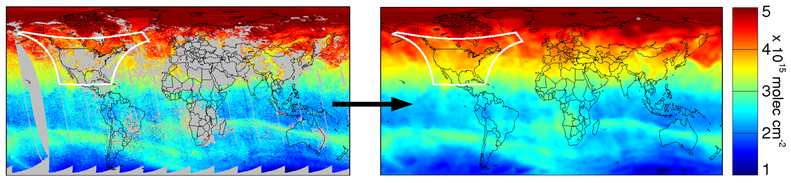


Figure 1: Estimating global stratospheric $NO_2$ based on interpolation between pristine areas (July 15, 2007). The white polygon shows the anticipated TEMPO field of regard

**Instruments in geostationary orbit (GEO) will not have this global context, and will require hourly estimates of the stratospheric $NO_2$ column.** The TEMPO instrument [1], to be centered over North America and expected to launch between 2018-2021, will be part of a constellation of geostationary instruments dedicated to monitoring tropospheric pollution around the world.

## Spatial Filtering Approach

We use OMI observations clipped to the anticipated TEMPO field of regard to test strategies for STS. We start with a spatial filtering approach based on the current operational algorithm [2]. After removing a prior estimate of the troposphere (from an observation climatology), we mask regions that are likely to have strong signal coming from the troposphere. The threshold allows for polluted pixels to remain if the lower tropospheric signal is suppressed by clouds (and conversely exclude pixels that are not necessarily polluted but have high surface reflectivity):

$$\frac{VCD_{trop,\,prior} \cdot AMF_{trop}}{AMF_{strat}} > 0.3 \times 10^{15}\ cm^{-2}$$

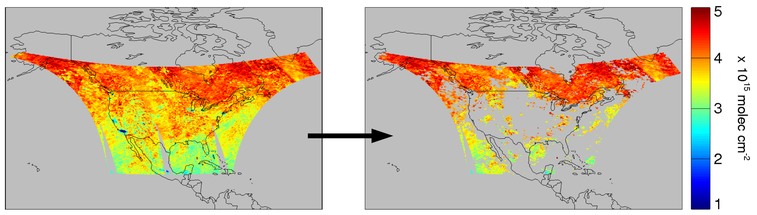


Figure 2: On average, 60% of data in the TEMPO field is removed as a result of this threshold. Masked areas can be filled in using a smoothing and interpolation algorithm.

## Context from Low-Earth Orbit

Where the averaging windows overlap with the field edges, the observations may be disproportionately influenced by continental signal instead of the pristine ocean regions outside of the boundaries. Suppose we have LEO observations from a different time of day, and that we understand the relative diurnal pattern in stratospheric $NO_2$. We propose to use these observations as context near the TEMPO edges during the smoothing step.

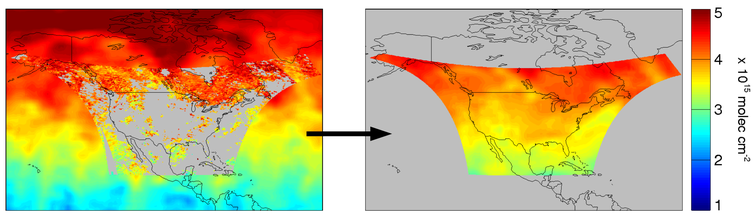


Figure 3: Context outside the TEMPO field derived from GOME-2 observations on the same observation day, corrected for OMI overpass time based on their monthly mean ratio (left). Final stratospheric estimate based on smoothing and interpolation (right).

## Performance

Here we compare our TEMPO algorithm with the global algorithm.

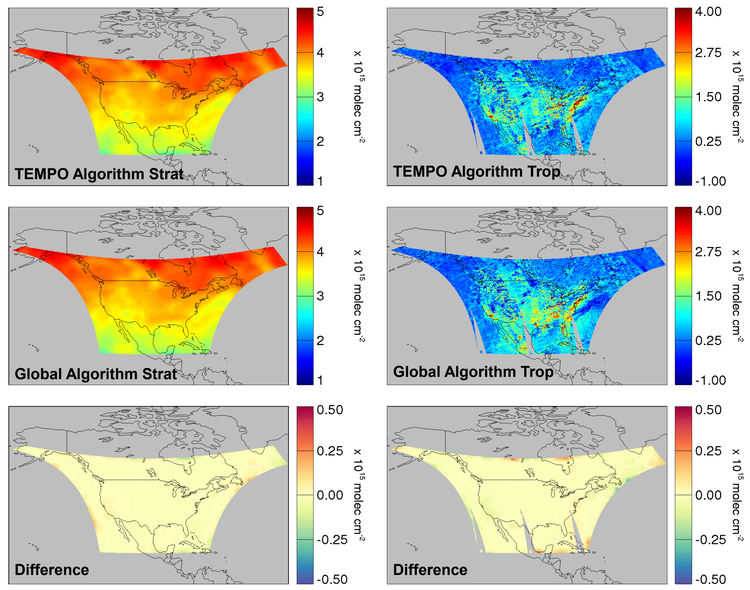


Figure 4: Comparing the TEMPO and Global algorithms for July 15, 2007. Much of the continent is unaffected compared to our global algorithm due to the size of the averaging windows. Small differences are seen near the TEMPO boundaries.

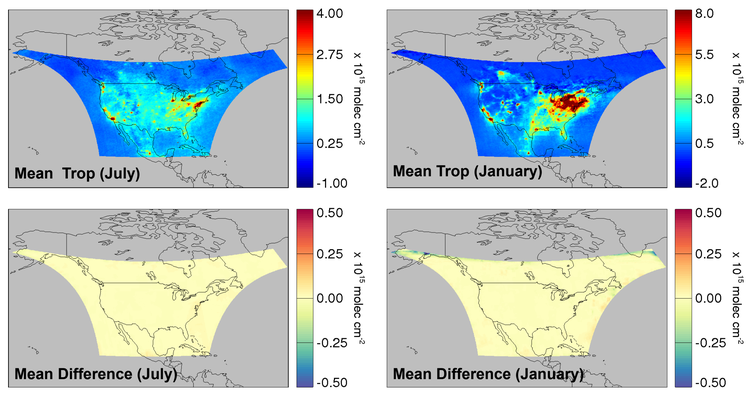


Figure 5: Mean tropospheric $NO_2$ from the TEMPO algorithm for July and January, and the difference between our TEMPO algorithm and our global algorithm. Errors on individual days are randomly distributed, and negligible in the monthly mean.

We find the spatial filtering approach generally performs very well over the TEMPO field of regard. Carrying out the same algorithm without incorporating the low-earth orbit observations shows how this supporting information can be important, especially near the southeast corner of the field of regard. We note that even small differences in the stratospheric $NO_2$ column estimate can result in an order of magnitude discrepancy (or more) in the tropospheric column, as a function of the $AMF_{strat}/AMF_{trop}$ ratio:

$$VCD_{trop,2} - VCD_{trop,1} = \frac{AMF_{strat}}{AMF_{trop}} \left( VCD_{strat,2} - VCD_{strat,1} \right)$$

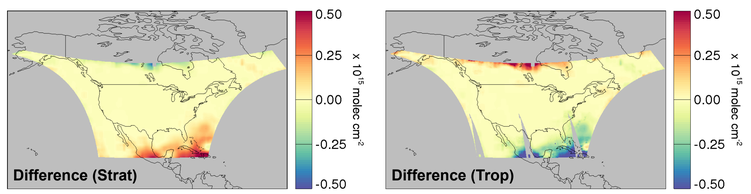


Figure 6: Difference between the TEMPO algorithm and global algorithm (July 15, 2007), excluding the low-earth orbit observations for context in the TEMPO algorithm.

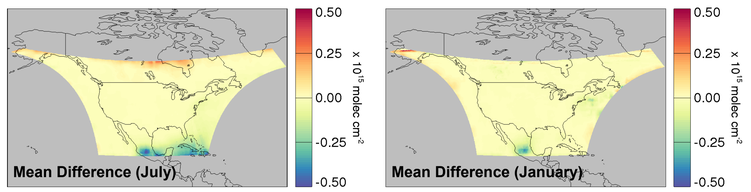


Figure 7: Difference in mean tropospheric $NO_2$ for July and January between our TEMPO algorithm and our global algorithm, excluding the complementary low-earth orbit observations for context in the TEMPO algorithm. Errors on individual days are systematic, persisting in the monthly mean.

## Cloudy Pixels

Cloudy scenes (CF>0.9) where lower tropospheric signal is suppressed may be useful for STS. Mid-level clouds (600-400 hPa) will be least likely to contain NOx mixed in from the surface, or lightning NOx associated with higher clouds. We find that around 60% of pixels that meet these criteria are already retained by our original masking algorithm (due to the threshold's dependence on radiative transfer). Incorporating the other cloudy pixels in the masked data increases data coverage only by about 4% in July (and even less in January). The value of cloudy pixels will be explored further in future work.

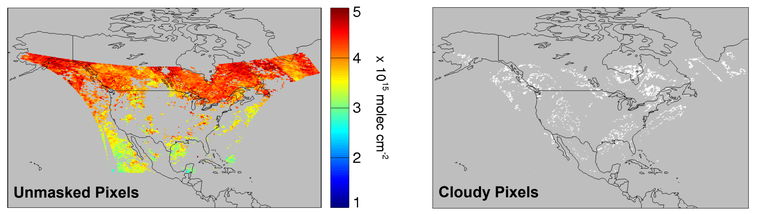


Figure 8: Comparing unmasked pixels (July 15, 2007) with cloudy pixels (CF > 0.9) that match our pressure criteria on the same day.

## Near-Real-Time Retrieval Considerations

Incorporating independent observations from a low-earth orbit instrument may not always be feasible for near-real-time data products (i.e. within an hour of the observation). Moreover, observations from the west coast will not be available in the early morning over eastern North America (and vice versa in the late afternoon over western North America). An alternative for real-time retrieval may be the "reference sector" approach. A first-order stratospheric estimate could be derived as a function of latitude from all the available unfiltered observations in the current hour.

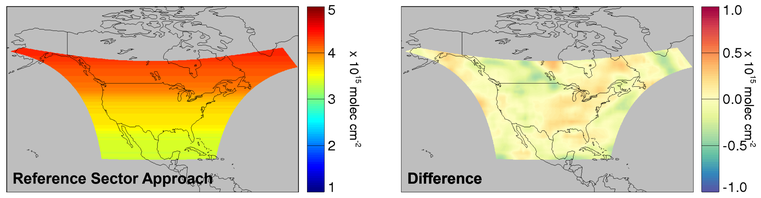


Figure 9: A reference sector estimate of stratospheric $NO_2$ from July 15, 2007 (right), and the difference between this estimate and our TEMPO algorithm for the same day (right).

Another alternative would be to use a "recent" climatology based on observations at the same time of day from the previous several days. This would account for some persistent longitudinal variability that can be important in the midlatitudes. Either approach (or a combination of both) could be useful for near-real-time retrieval products.

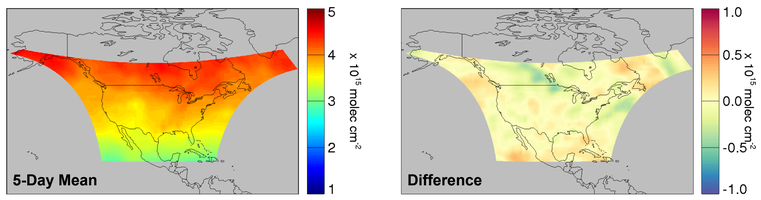


Figure 10: Mean stratospheric $NO_2$ estimate from July 10-14, 2007 (right), and the difference between this and our TEMPO algorithm for July 15. 2007 (right).

## Summary & Recommendations

- A spatial filtering approach to STS works well for geostationary observations of $NO_2$ over North America from the TEMPO instrument field of regard
- Incorporating independent observations from low-earth orbit helps remove STS bias in the TEMPO domain near field-of-regard boundaries
- At high $AMF_{strat}/AMF_{trop}$ ratios, uncertainty in stratospheric column can be magnified by more than an order of magnitude in the troposphere, suggesting screening based on AMFs should be good practice
- Cloudy pixels may offer supporting information, but mid-level clouds don't add substantial coverage to our current spatial filtering algorithm
- Estimated stratospheric columns from a reference sector or from previous days at the same hour could be used for initial near-real-time data products

[1] Zoogman et al. (2016) *J. Quant. Spectrosc. Radiat. Transfer*, 186, 17-39.
[2] Bucsela et al. (2013) *Atmos. Meas. Tech.*, 6, 2607-2626.