An Innovative Satellite SO_2 and HCHO Retrieval Algorithm based on Principal Component Analysis: Contribution to the Sentinel-5P Mission

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ATOMOS 2015 Conference

Air quality session

University of Crete, Heraklion, Greece, 8-12 June 2015

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Outline

- Introduction to the NASA GSFC PCA algorithm
- Application to OMI SO_2 retrievals
- New Development
- Application to HCHO retrievals
- Contribution to the Sentinel-5P Mission

Methodology (Framework): PCA

Instead of explicit modeling of ozone, RRS, and other instrumental features, we use a **data-driven approach** based on principal component analysis (PCA) with spectral fitting

Measured N-value spectrum

SO_2 column amount

$$N(\omega, \Omega_{SO_2}) = \sum_{i=1}^{n_v} \omega_i v_i + \Omega_{SO_2} \frac{\partial N}{\partial \Omega_{SO_2}}$$

PCs from SO_2-free regions, (O_3 absorption, surface reflectance, RRS, measurement artifacts etc.) **other than SO_2 absorption**

Pre-calculated SO_2 Jacobians (assuming O_3 profiles, albedo, etc.)

Fitting of the right hand side to the spectrum on the left hand side -> SO_2 column amount and coefficients of PCs

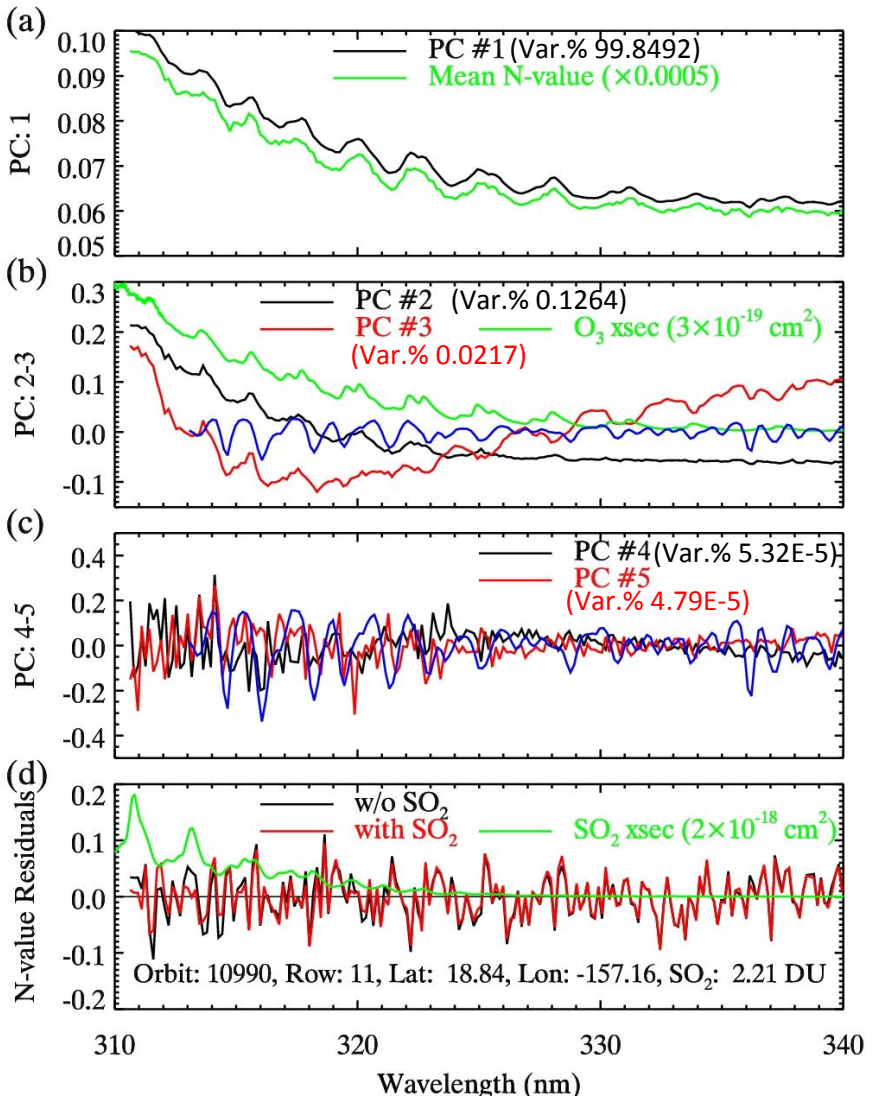
(See Guanter et al., 2012; Joiner et al., 2013; Li et al., 2013)

Principle Components and Residuals

Example PCs from **entire row** # 11, Orbit 10990

(a-c) First few PCs
Blue line: scaled reference Ring spectrum

(d) Least squares fitting residuals for a pixel near Hawaii



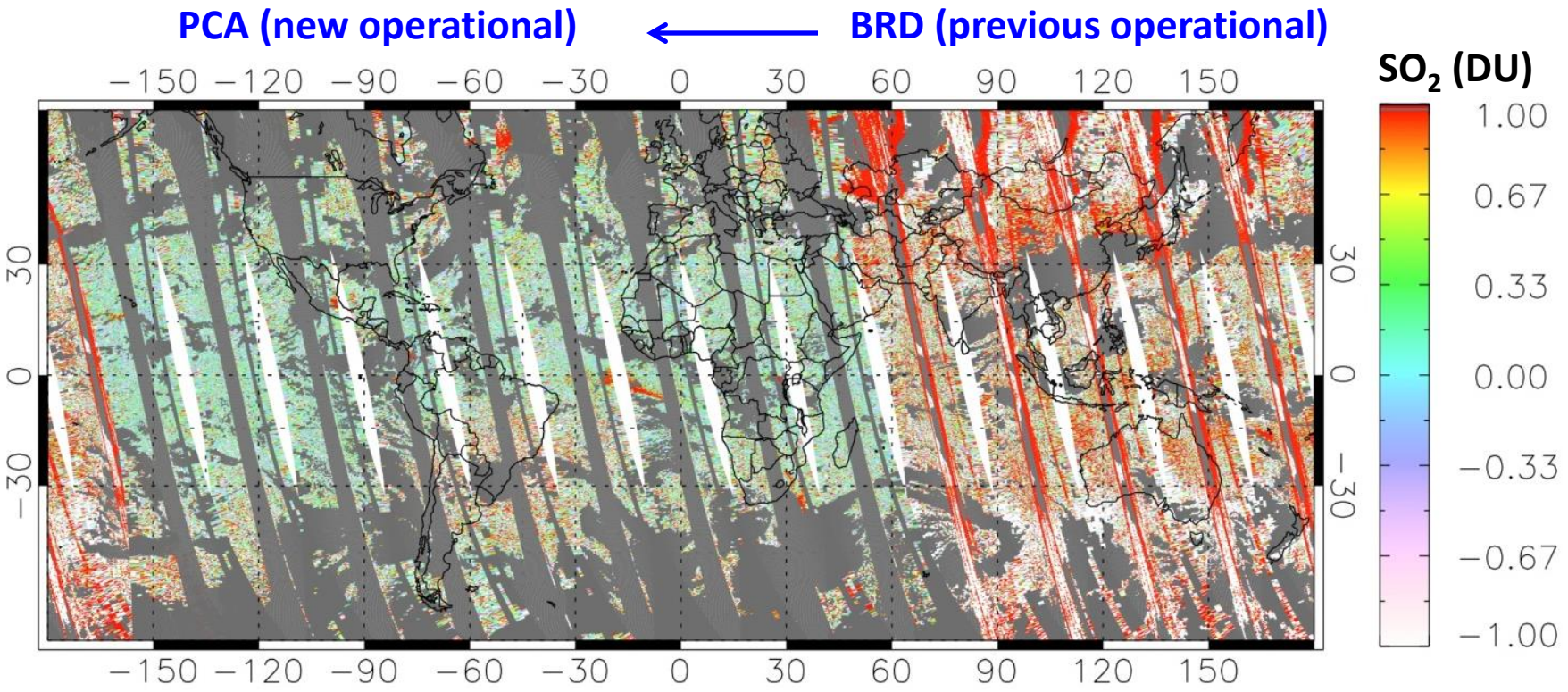
PC #1: Mean spectrum

PC #2: O_3 absorption
PC #3: Surface reflectance (also Ring signature)

PCs #4 and #5: likely measurement artifacts, noise (>99.99% variance explained)

Smaller residuals with SO_2 Jacobians fitted

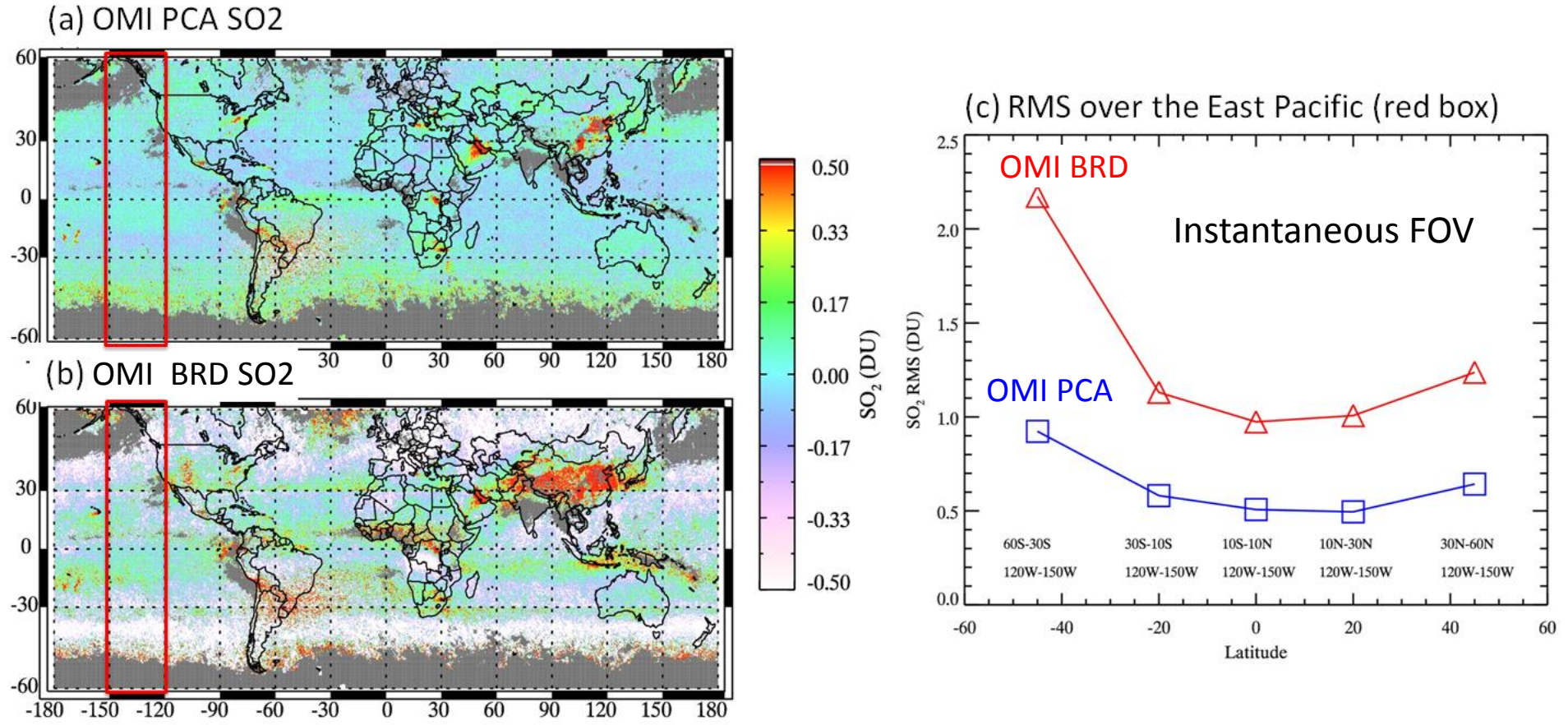
The OMI PCA SO_2 Algorithm Became Operational on 09/18/2014, Data Released in October



Both Retrievals assume the same simplified, fixed conditions in retrievals (SZA = 30°, VZA=0°, mid-latitude O_3 profile with O_3 = 325 DU, cloud-free, R = 0.05, SO_2 mostly in the lowest 1 km of the atmosphere)

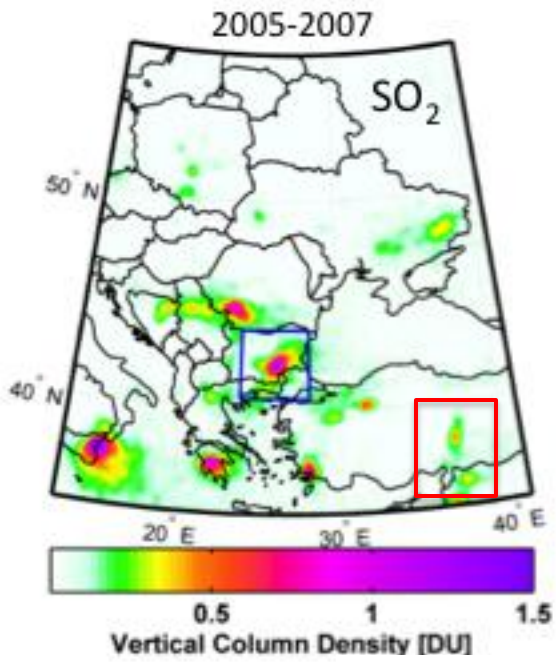
Results: noise and artifact reduction

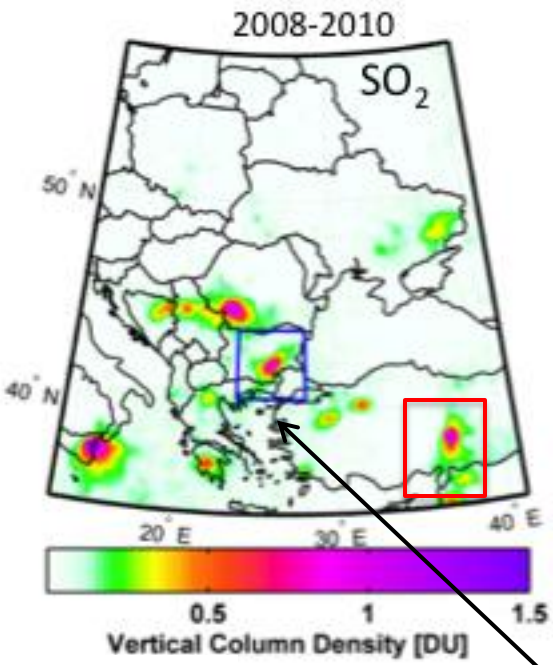
August, 2006

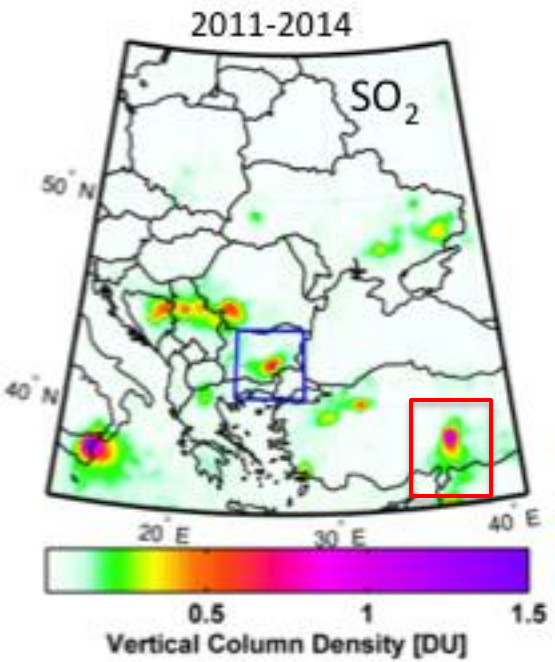


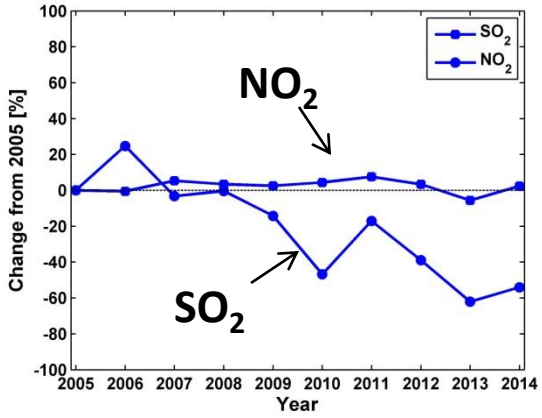
- PCA algorithm reduces retrieval noise by a factor of two as compared with the BRD algorithm
- SO_2 Jacobians for PCA algorithm calculated with the same assumptions as in the BRD algorithm

OMI PCA Retrievals show Changes in SO_2 in Eastern Europe and Turkey





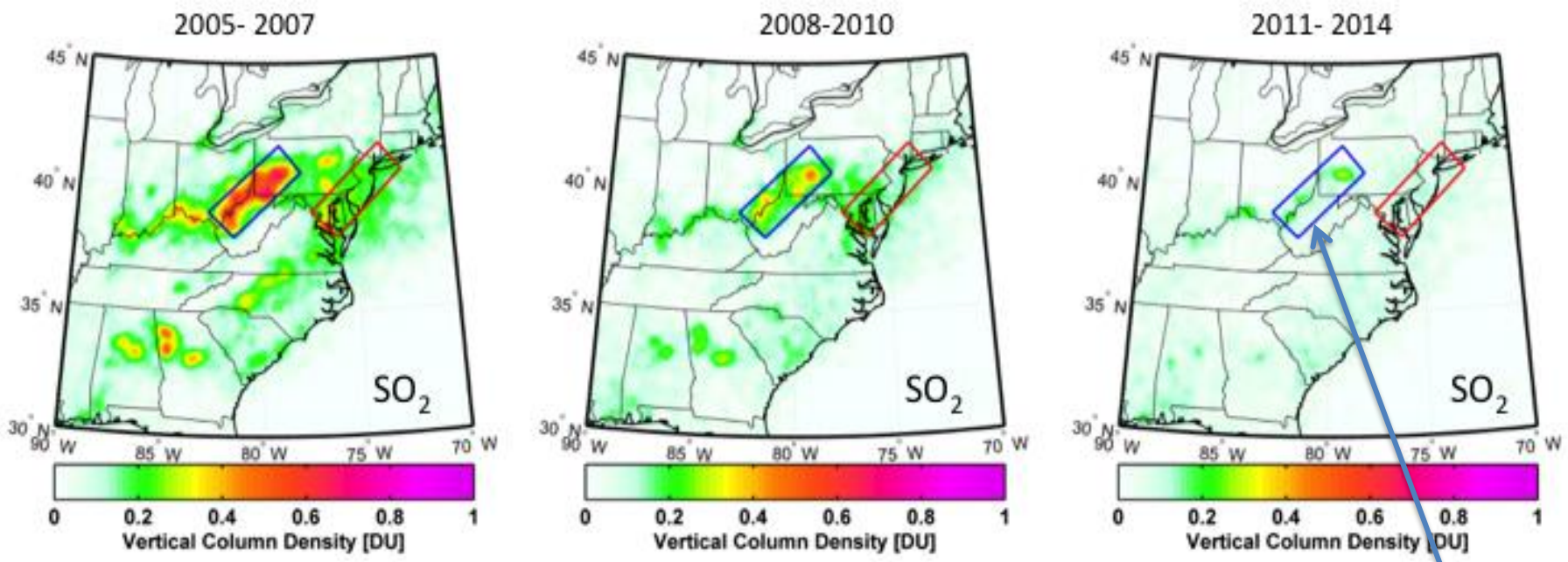


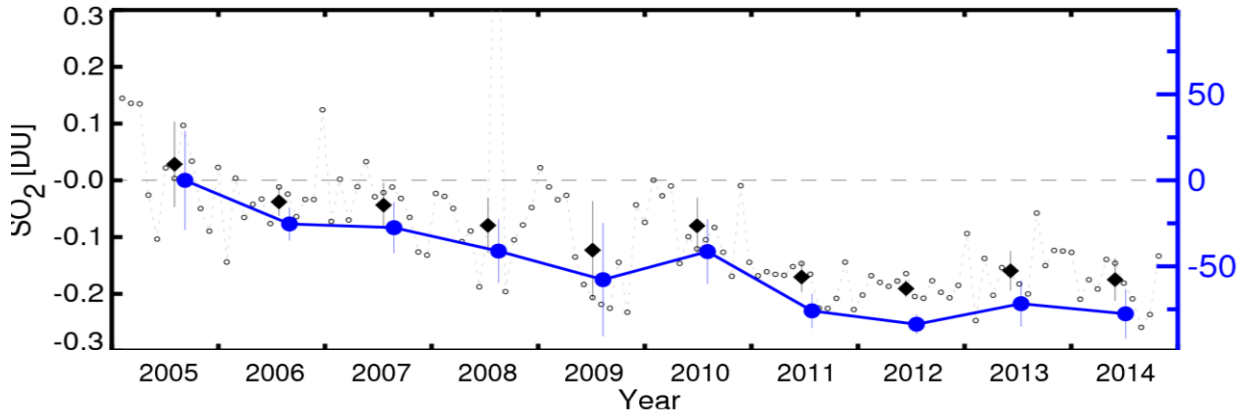


Maritsa Power Station

(Krotkov et al., ACP OMI special issue, in prep)

OMI PCA Retrievals show dramatic decrease in SO_2 point sources in Eastern US

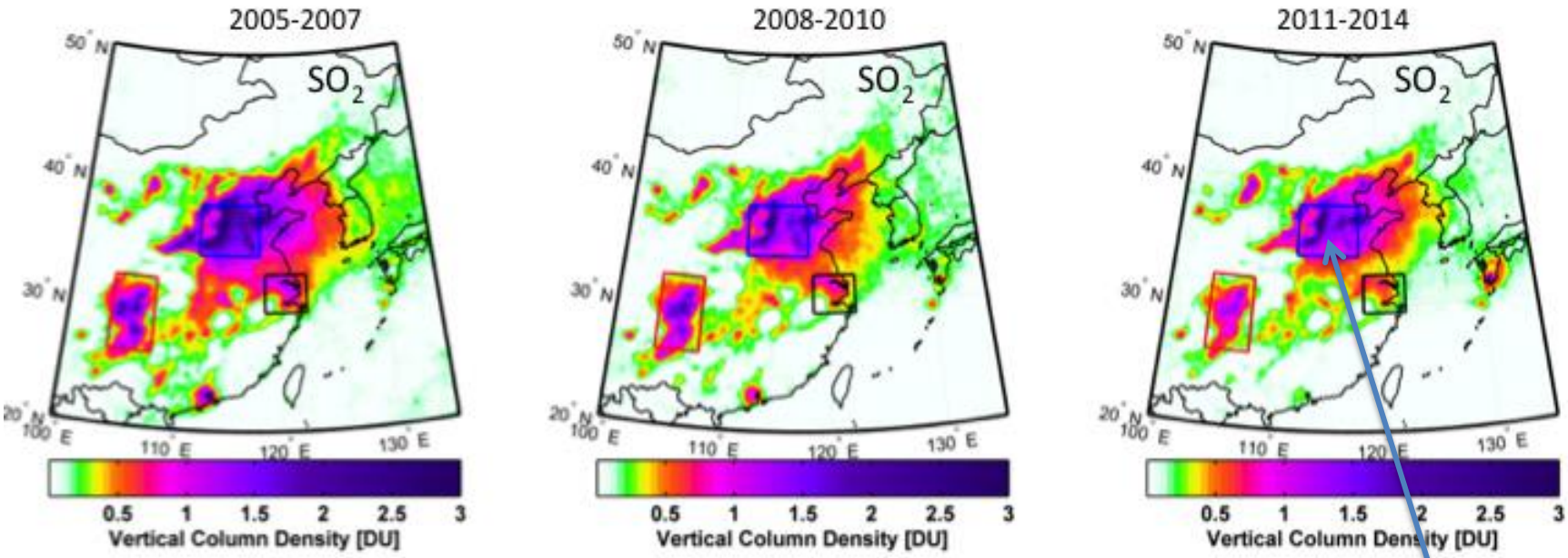


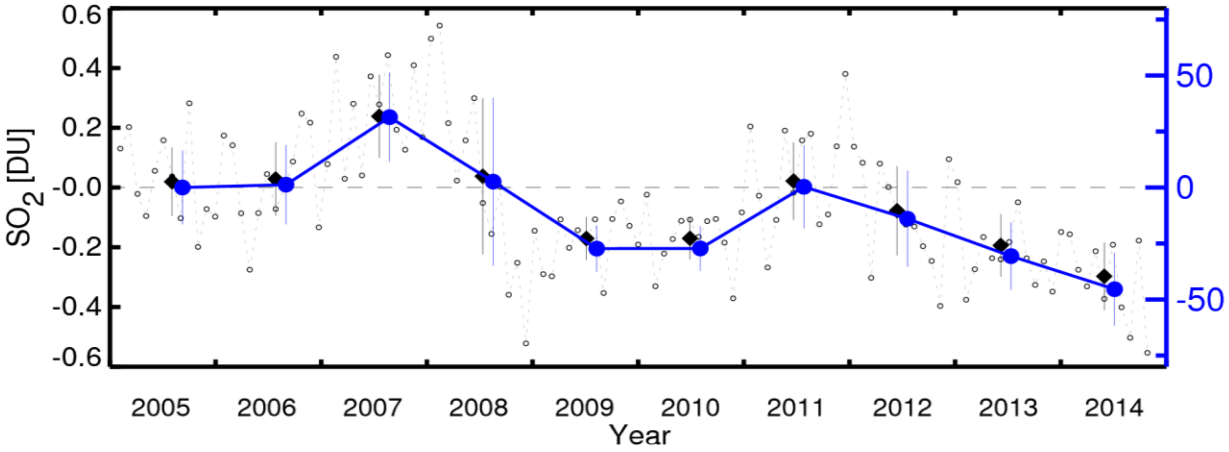


Ohio valley Power Plants: -80%

(Krotkov et al., ACP OMI special issue, in prep)

OMI PCA Retrievals show decrease in SO_2 pollution in Eastern China

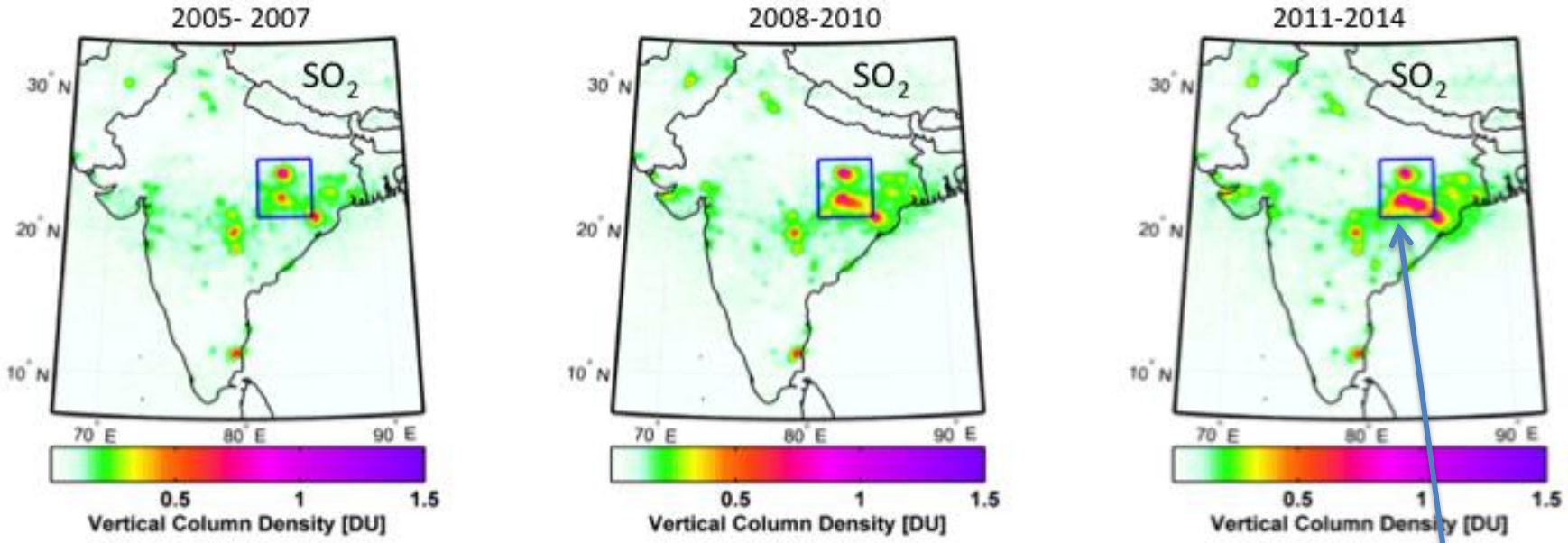


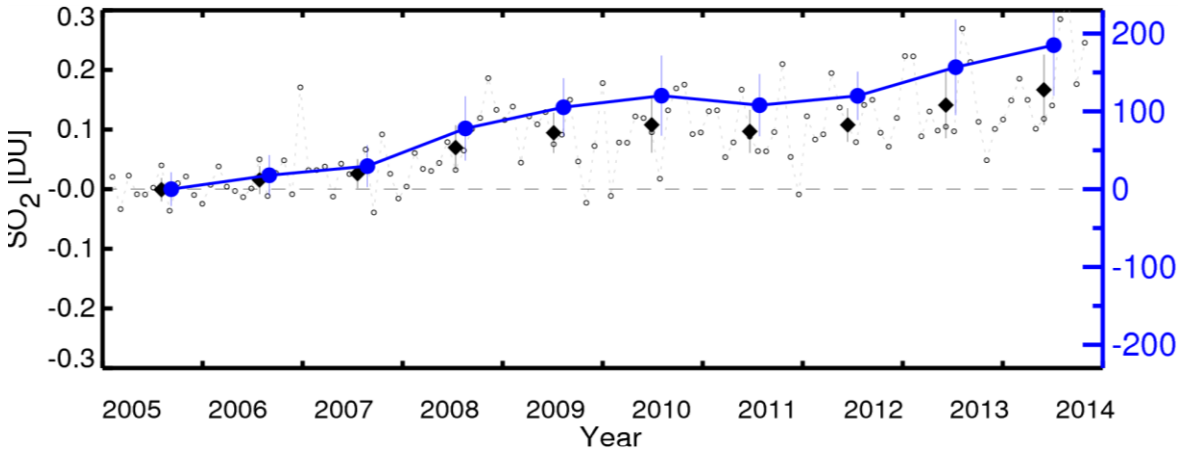


Eastern North China: -50%

(Krotkov et al., ACP OMI special issue, in prep)

OMI PCA Retrievals show dramatic increase in SO_2 pollution in North Eastern India



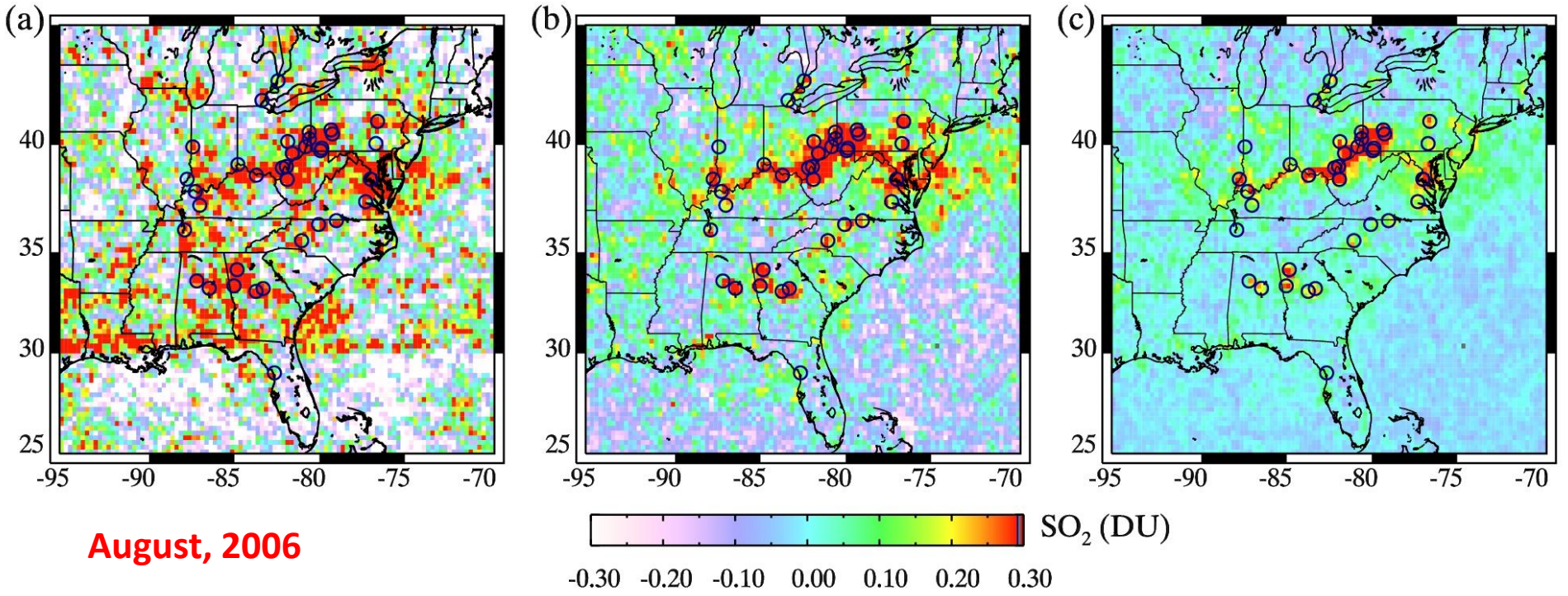


Eastern North India: +200%

(Krotkov et al., ACP OMI special issue, in prep)

Development: Table Lookup Approach for More Accurate Jacobians

Past (BRD) | Present (PCA , simple LUT) | Future (PCA , Updated LUT)



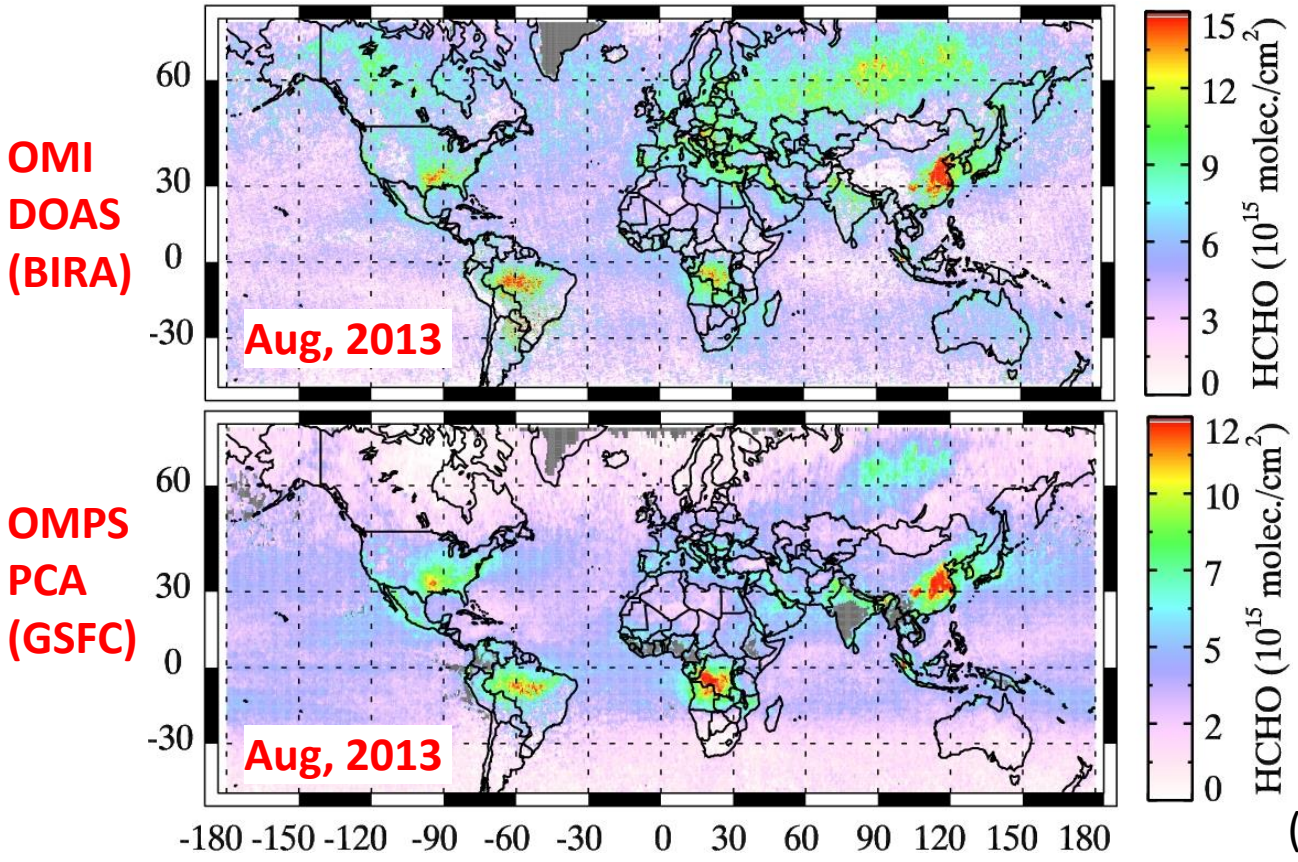
August, 2006

Use of lookup table to account for effects of viewing geometry, O_3, reflectivity, clouds, and vertical distribution on SO_2 Jacobians

Application to S-NPP OMPS HCHO Retrievals

Ozone Mapping and Profiler Suite (OMPS):

- Flying on NASA/NOAA Suomi National Polar-orbiting Partnership spacecraft
- Nadir mapper similar to OMI, but lower spectral (~1 nm) and spatial resolution (50 × 50 km^2 at nadir)
- HCHO NOT a required/anticipated product from OMPS



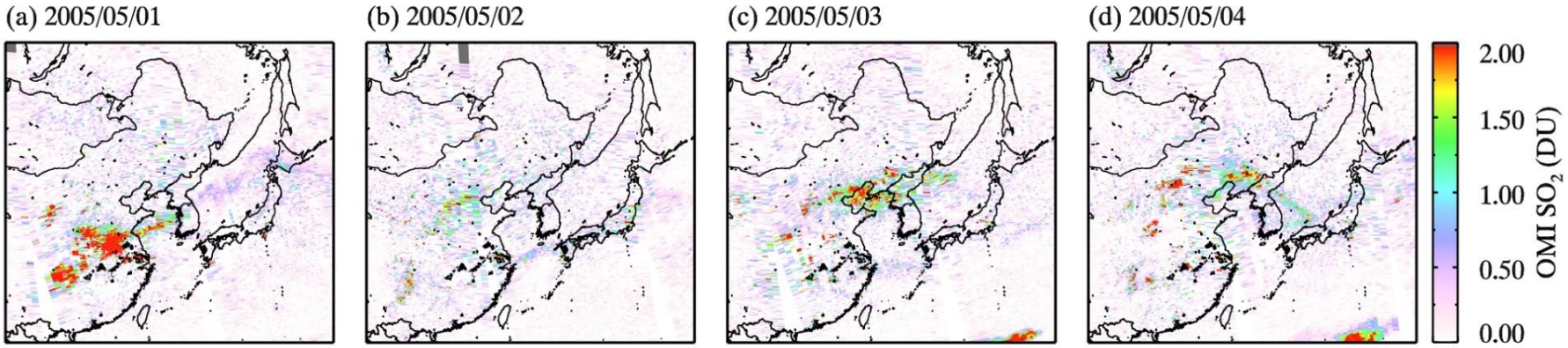
Two independent retrievals show fairly consistent spatial patterns in HCHO.

OMPS HCHO ~15-20% smaller than OMI, probably due to several instrumental and algorithmic factors (e.g., *a priori* profiles etc.).

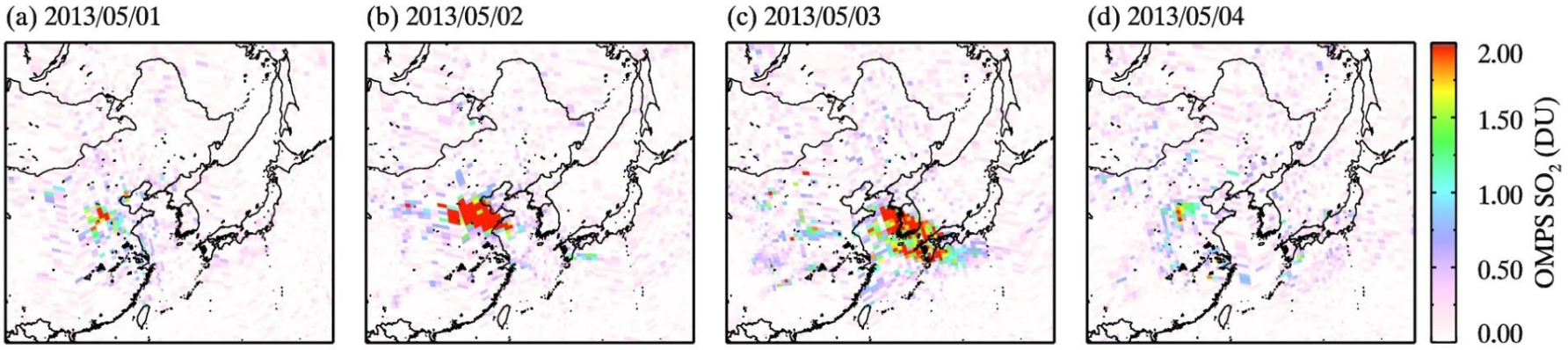
(Li et al., GRL, 2015)

OMI and OMPS PCA SO_2 Retrievals – Daily Regional Air Quality and Transport Episodes

OMI SO_2 Retrievals, May 01-04, 2005



SNPP/OMPS SO_2 Retrievals, May 01-04, 2013



Proposed contribution to the Sentinel-5P Mission

- During the pre-launch phase (2015- early 2016): continue the comparisons of our SO_2 and HCHO PCA retrievals with BIRA's retrievals using official TROPOMI algorithms as applied to OMI;

- During the commissioning phase (2016): apply PCA algorithms to selected subset of TROPOMI L1B spectra and compare with the ESA's provisional SO_2 and HCHO products;

- During the operational phase (2017-2021): apply PCA algorithm and oversampling techniques to selected subsets of TROPOMI L1B data (point/area sources) to produce SO_2 and HCHO time series that will overlap with OMI records to facilitate study of long-term emission trends and pollutant lifetime;