The capability of the OMPS Linear Fit SO_2 (LFSO2) algorithm for implementation at NDE

Jianguo Niu
System Research Group Inc.at NOAA/STAR

C. Trevor Beck, Lawrence E. Flynn
NOAA/NESDIS/STAR

Kai Yang
University of Maryland

Goal for LFSO2 implementation at NOAA

1. Provide near real time ***alerts*** of volcanic SO_2 clouds.

2. Provide O_3 ***corrections*** when large amounts of SO_2 are present.

3. Provide ***accurate SO_2 total column amounts*** to address the shortfall of the existing products in the Version-8 ozone algorithm.

Residuals and Linearization

The algorithm starts from N-values: $$N_m(\Omega, \Xi, R, \lambda_i) = N(\Omega, \Xi, R, \lambda_i) + \varepsilon_r \qquad (1)$$

We linearize the problem with differentials at $\Omega = \Omega_0$, $\Xi = \Xi_0$, $R = R_0$:

$$N_m(\lambda_2) - N_0(\lambda_2) = \Delta\Omega \left.\frac{dN(\lambda_2)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_2)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_2 - \lambda_0)^j\right) \left.\frac{dN(\lambda_2)}{dR}\right|_{R=R_0} + \varepsilon_r$$

$$N_m(\lambda_3) - N_0(\lambda_3) = \Delta\Omega \left.\frac{dN(\lambda_3)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_3)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_3 - \lambda_0)^j\right) \left.\frac{dN(\lambda_3)}{dR}\right|_{R=R_0} + \varepsilon_r$$

$$N_m(\lambda_4) - N_0(\lambda_4) = \Delta\Omega \left.\frac{dN(\lambda_4)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_4)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_4 - \lambda_0)^j\right) \left.\frac{dN(\lambda_4)}{dR}\right|_{R=R_0} + \varepsilon_r \qquad (2)$$

$\ldots$

$\ldots$

$$N_m(\lambda_i) - N_0(\lambda_i) = \Delta\Omega \left.\frac{dN(\lambda_i)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_i)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_i - \lambda_0)^j\right) \left.\frac{dN(\lambda_i)}{dR}\right|_{R=R_0} + \varepsilon_r$$

$N_0(\lambda)$: radiative transfer model computed at $N_0(\Omega_0, \Xi_0, R_0, \lambda)$.

$N_m(\lambda)$: measured N-value.

$N_m(\lambda) - N_0(\lambda)$: V8TOZ Algorithm output residuals.

15-Granule Bias Estimates

The ozone retrieval provided residual includes biases along-orbit. To eliminate these residual biases, A 15-granule implementation technique is designed. Residual averages <ψ(λ)> over three five-granule intervals (corresponding to ~10° latitude) are calculated at the 12 wavelength bands and 35 cross tracks. Each individual average residual within these three averaged intervals are calculated by interpolation. The corrected residual,

$\psi(\lambda) = N_m(\lambda) - N_0(\lambda) - \langle\psi(\lambda)\rangle$ is called the "adjust residual", then:

$$
\begin{aligned}
\psi(\lambda_2) &= \Delta\Omega \left.\frac{dN(\lambda_2)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_2)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_2 - \lambda_0)^j \right) \left.\frac{dN(\lambda_2)}{dR}\right|_{R=R_0} + \varepsilon_r \\
\psi(\lambda_3) &= \Delta\Omega \left.\frac{dN(\lambda_3)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_3)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_3 - \lambda_0)^j \right) \left.\frac{dN(\lambda_3)}{dR}\right|_{R=R_0} + \varepsilon_r \\
\psi(\lambda_4) &= \Delta\Omega \left.\frac{dN(\lambda_4)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_4)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_4 - \lambda_0)^j \right) \left.\frac{dN(\lambda_4)}{dR}\right|_{R=R_0} + \varepsilon_r \\
&\cdots \\
&\cdots \\
\psi(\lambda_i) &= \Delta\Omega \left.\frac{dN(\lambda_i)}{d\Omega}\right|_{\Omega=\Omega_0} + \Delta\Xi \left.\frac{dN(\lambda_i)}{d\Xi}\right|_{\Xi=\Xi_0} + \left(\Delta R(\lambda_0) + \sum_{j=1}^{2} c_j (\lambda_i - \lambda_0)^j \right) \left.\frac{dN(\lambda_i)}{dR}\right|_{R=R_0} + \varepsilon_r
\end{aligned}
\tag{3}
$$

These linear equations can be converted into a matrix expression.

Matrix Formulation

$$\begin{pmatrix} \psi(\lambda_2) \\ \psi(\lambda_3) \\ . \\ \psi(\lambda_i) \\ . \\ \psi(\lambda_{11}) \end{pmatrix} = \begin{pmatrix} \frac{dN(\lambda_2)}{d\Omega} & \frac{dN(\lambda_2)}{d\Xi} & \frac{dN(\lambda_2)}{dR} & (\lambda_2-\lambda_0)\frac{dN(\lambda_2)}{dR} & (\lambda_2-\lambda_0)^2\frac{dN(\lambda_2)}{dR} \\ \frac{dN(\lambda_3)}{d\Omega} & \frac{dN(\lambda_3)}{d\Xi} & \frac{dN(\lambda_3)}{dR} & (\lambda_3-\lambda_0)\frac{dN(\lambda_3)}{dR} & (\lambda_3-\lambda_0)^2\frac{dN(\lambda_3)}{dR} \\ .... & & & & \\ \frac{dN(\lambda_i)}{d\Omega} & \frac{dN(\lambda_i)}{d\Xi} & \frac{dN(\lambda_i)}{dR} & (\lambda_i-\lambda_0)\frac{dN(\lambda_i)}{dR} & (\lambda_i-\lambda_0)^2\frac{dN(\lambda_i)}{dR} \\ ..... & & & & \\ \frac{dN(\lambda_{11})}{d\Omega} & \frac{dN(\lambda_{11})}{d\Xi} & \frac{dN(\lambda_{11})}{dR} & (\lambda_{11}-\lambda_0)\frac{dN(\lambda_{11})}{dR} & (\lambda_{11}-\lambda_0)^2\frac{dN(\lambda_{11})}{dR} \end{pmatrix} \begin{pmatrix} \Delta\Omega \\ \Delta\Xi \\ \Delta R \\ c_1 \\ c_2 \end{pmatrix} + \begin{pmatrix} \varepsilon(\lambda_2) \\ \varepsilon(\lambda_3) \\ . \\ \varepsilon(\lambda_i) \\ . \\ \varepsilon(\lambda_{11}) \end{pmatrix}$$

The sensitivities differ depending upon the assumed height of the SO_2 layer. Estimates of the total column SO_2 using this Matrix formula is obtained for three different heights: Lower Troposphere (TRL), Middle Troposphere (TRM) and Lower Stratosphere (STL). Other technique is used to estimate Planetary Boundary Layer (PBL) SO_2.

Retrieval Parameters

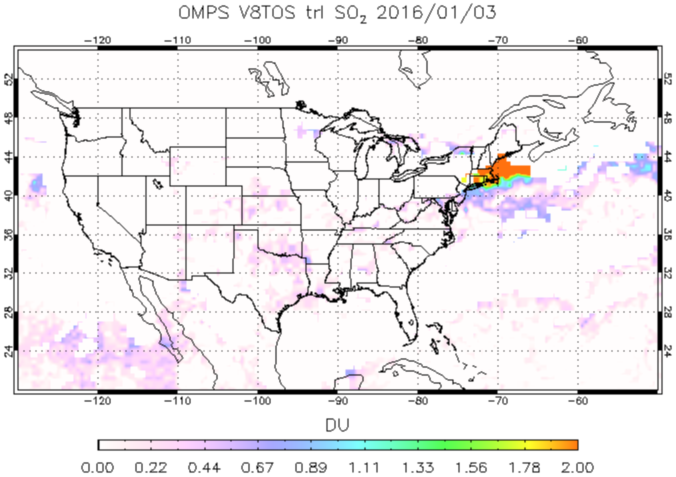
Name	Type	Description	Dimension	Units	Range
s_AlgorithmFlag_PBL	32 bit integer	PBL algorithm flag	105 x 15	Unitless	0, 1, 11
s_AlgorithmFlag_STL	32 bit integer	STL algorithm flag	105 x 15	Unitless	0, 1, 2, 11, 12
s_AlgorithmFlag_TRL	32 bit integer	TRL algorithm flag	105 x 15	Unitless	0, 1, 2, 11, 12
s_AlgorithmFlag_TRM	32 bit integer	TRM algorithm flag	105 x 15	Unitless	0, 1, 2, 11, 12
s_QualityFlags_PBL	32 bit integer	PBL quality flag	105 x 15	Unitless	0 ~ 65535
s_QualityFlags_STL	32 bit integer	STL quality flag	105 x 15	Unitless	0 ~ 65535
s_QualityFlags_TRL	32 bit integer	TRL quality flag	105 x 15	Unitless	0 ~ 65535
s_QualityFlags_TRM	32 bit integer	TRM quality flag	105 x 15	Unitless	0 ~ 65535
s_STLO3	32 bit float	STL corrected total column of O3	105 x 15	Dobson	0 ~ 1000
s_TRLO3	32 bit float	TRL corrected total column of O3	105 x 15	Dobson	0 ~ 1000
s_TRMO3	32 bit float	TRM corrected total column of O3	105 x 15	Dobson	0 ~ 1000
s_ColumnamountSO2_STL	32 bit float	STL total column of SO2	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_TRL	32 bit float	TRL total column of SO2	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_TRM	32 bit float	TRM total column of SO2	105 x 15	Dobson	-10 ~ 2000
s_deltaRefl331	32 bit float	Delta Reflectivity at 331 nm	105 x 15	Percent	-100 ~ 100

Retrieval Parameters

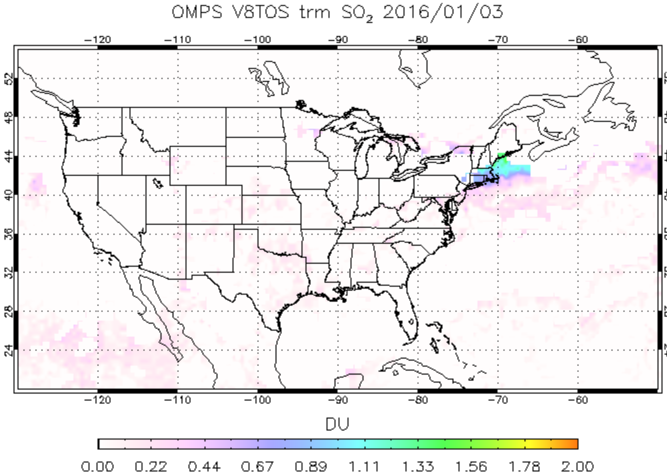
Name	Type	Description	Dimension	Units	Range
s_ChiSquareLfit	32 bit float	Chi-square of linear fit	105 x 15	Uniteless	> 0
s_dN_dSO2_STL	32 bit float	dN/dSO2(STL)	12 x 105 x 15	Per Dobson	-1 ~ 100
s_dN_dSO2_TRL	32 bit float	dN/dSO2(TRL)	12 x 105 x 15	Per Dobson	-1 ~ 1000
s_dN_dSO2_TRM	32 bit float	dN/dSO2(TRM)	12 x 105 x 15	Per Dobson	-1 ~ 100
s_Slope	32 bit float	C_1 in linear equ.	105 x 15	Uniteless	-1 ~ 1
s_Qterm	32 bit float	C_2 in linear equ.	105 x 15	Uniteless	-1 ~ 1
s_ResidualAdjustment	32 bit float	Averaged residual of nvalue	12 x 105 x 15	Uniteless	-10 ~ 10
s_ColumnamountSO2_PBL	32 bit float	Planetary Boundary Layer (PBL) SO2	105 x 15	Dobson	-300 ~ 1000
s_ColumnamountSO2_PBLbrd	32 bit float	PBL SO2 by BRD method	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_STLbrd	32 bit float	STL SO2 by BRD method	105 x 15	Dobson	-10 ~ 2000
s_ColumnamountSO2_TRMbrd	32 bit float	TRM SO2 by BRD method	105 x 15	Dobson	-10 ~ 2000
s_SO2indexP1	32 bit float	Partial adjust residual for 310 and 311	105 x 15	Uniteless	-100 ~ 100
s_SO2indexP2	32 bit float	Partial adjust residual for 311 and 313	105 x 15	Uniteless	-100 ~ 100
s_SO2indexP3	32 bit float	Partial adjust residual for 313 and 314	105 x 15	Uniteless	-100 ~ 100

Products from the LFSO2 algorithm

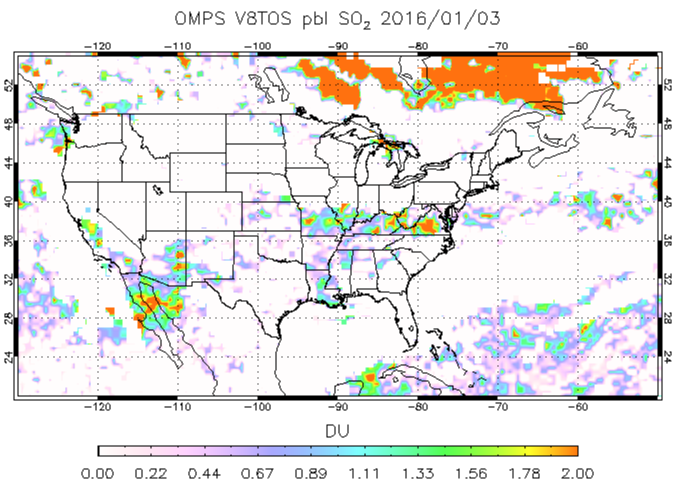
Umkhr-0: 0~5.5km



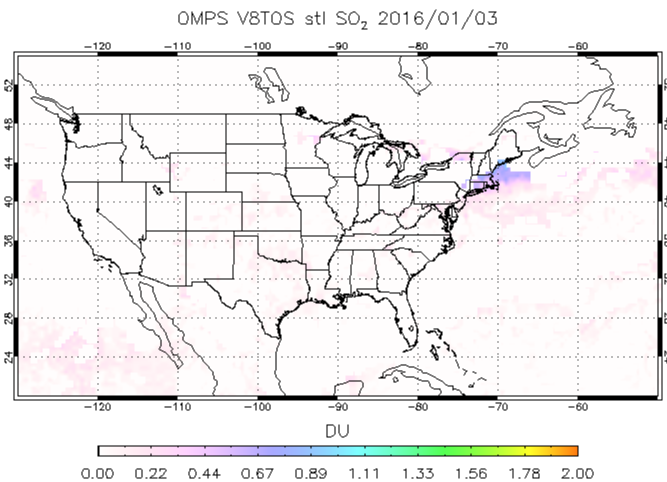
Umkhr-1: 5.5~10.3 km



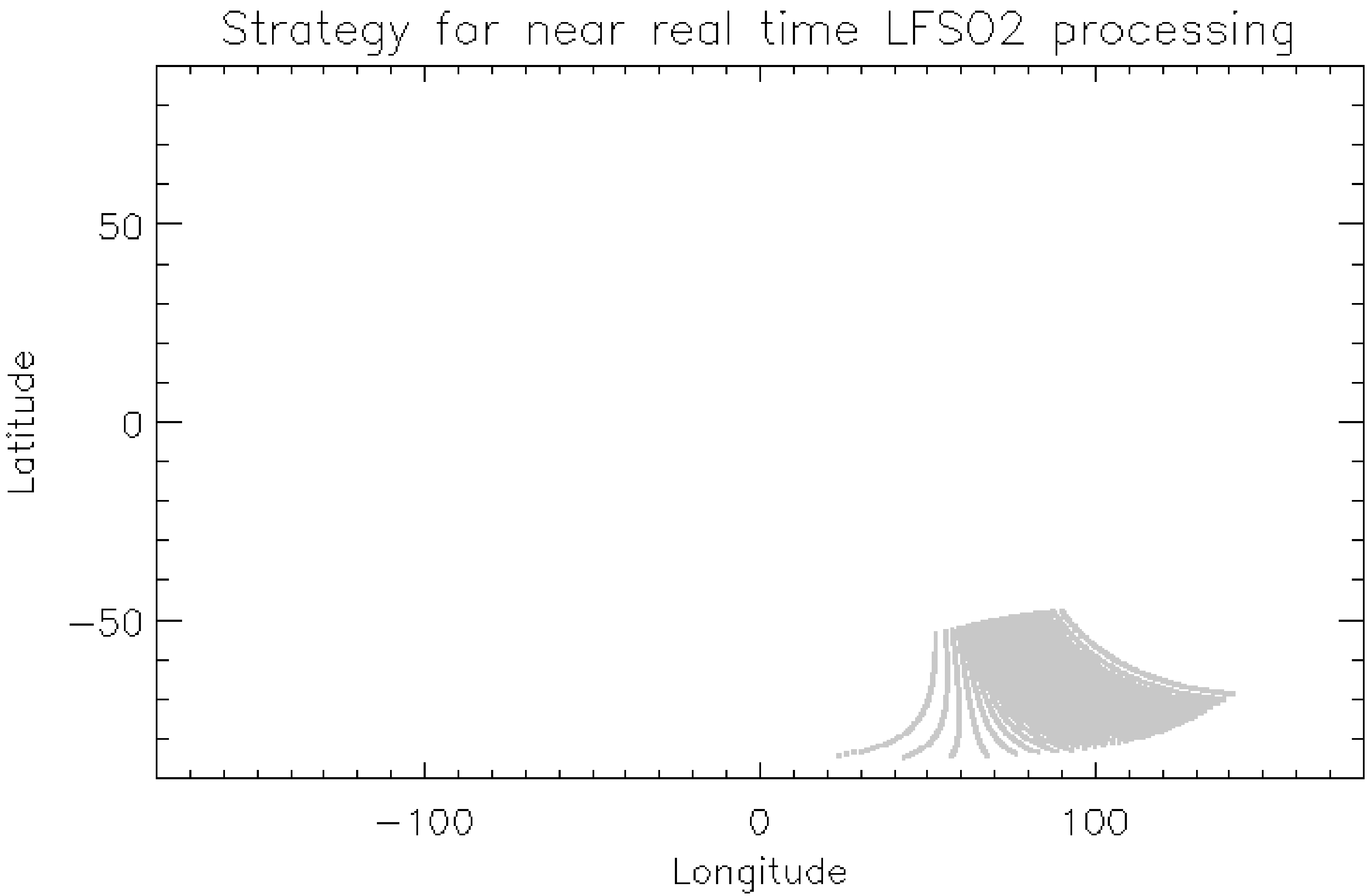
PBL: 0~2km



Umkhr-3: 14.7~19.1km

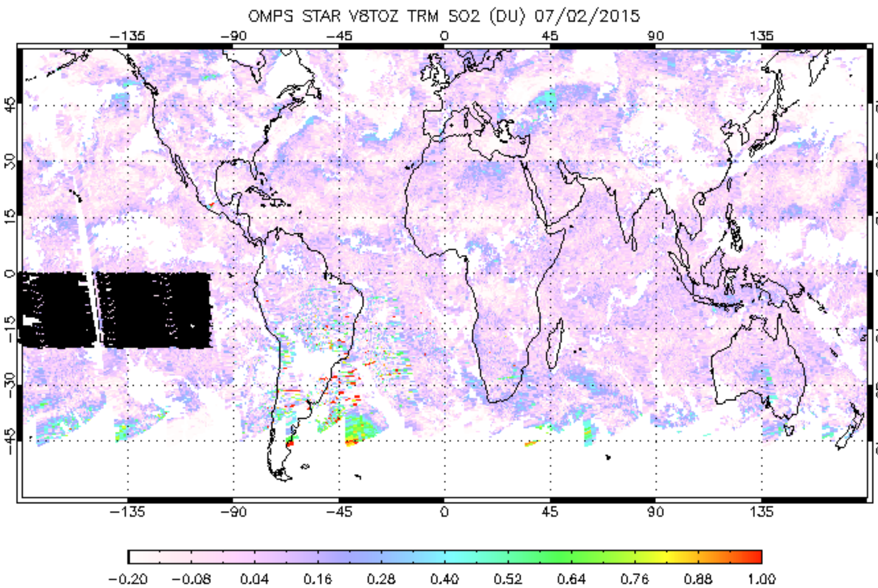


Strategy for running LFSO2



Estimates ***minimum detectable SO_2*** *for single IFOV*

	# IFOV	Average (DU)	STD (DU)
STL	5480	0.0037	0.069
TRM	5480	0.0057	0.09
TRL	5480	0.0125	0.18
PBL	5480	0.0624	0.6



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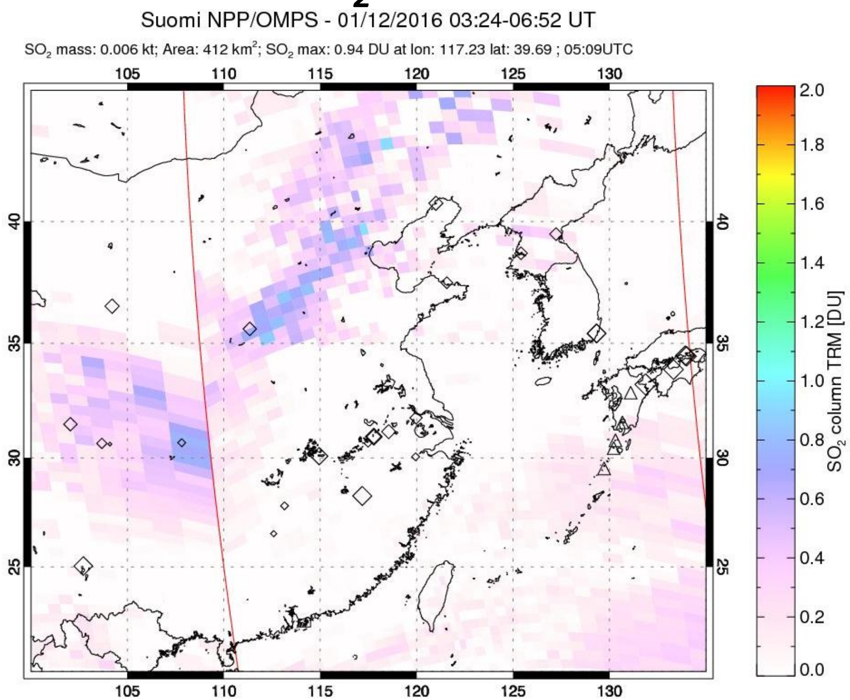
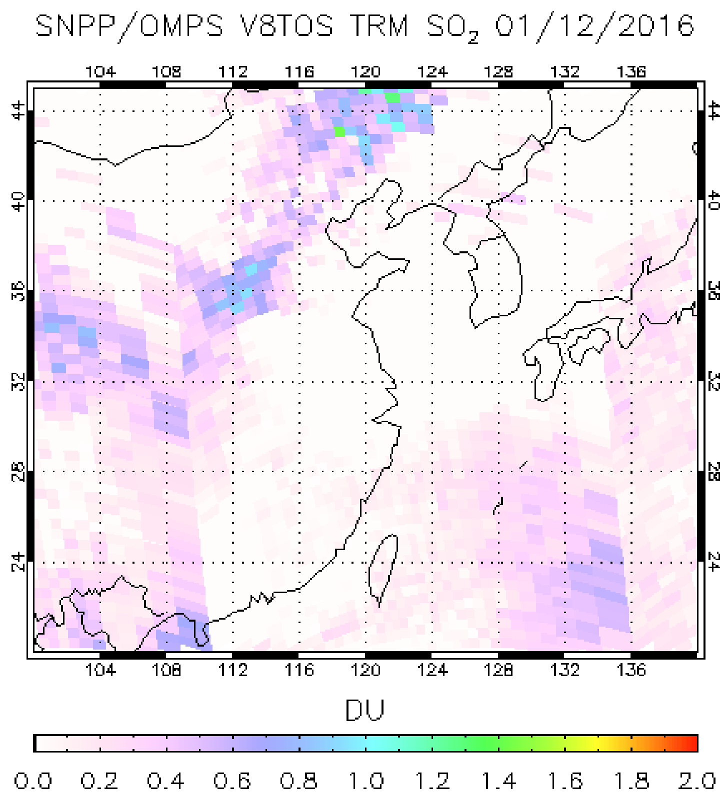
SO_2 in 5~10km (TRM) over East China

From PEATE SO_2 website

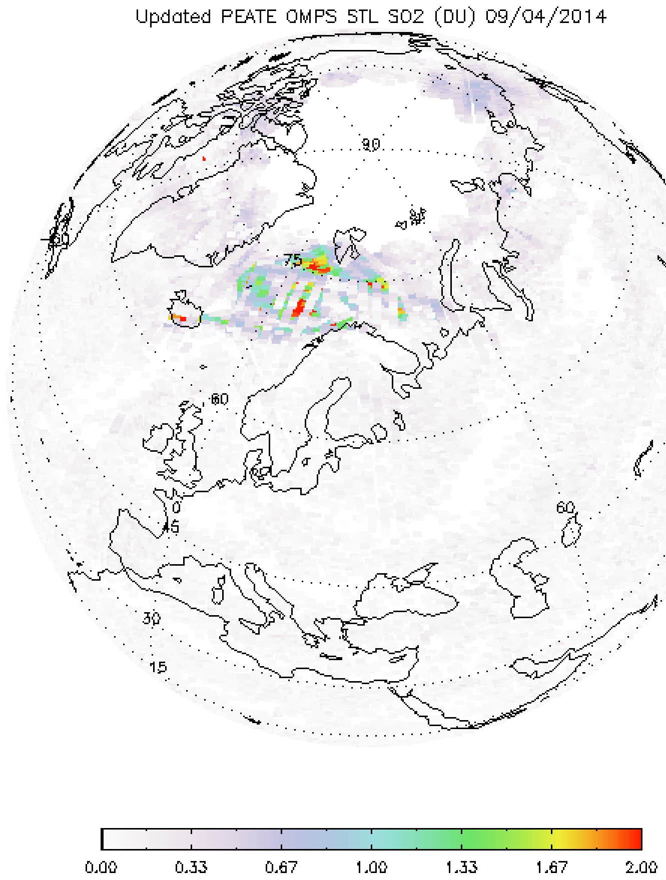


From Star LFSO2

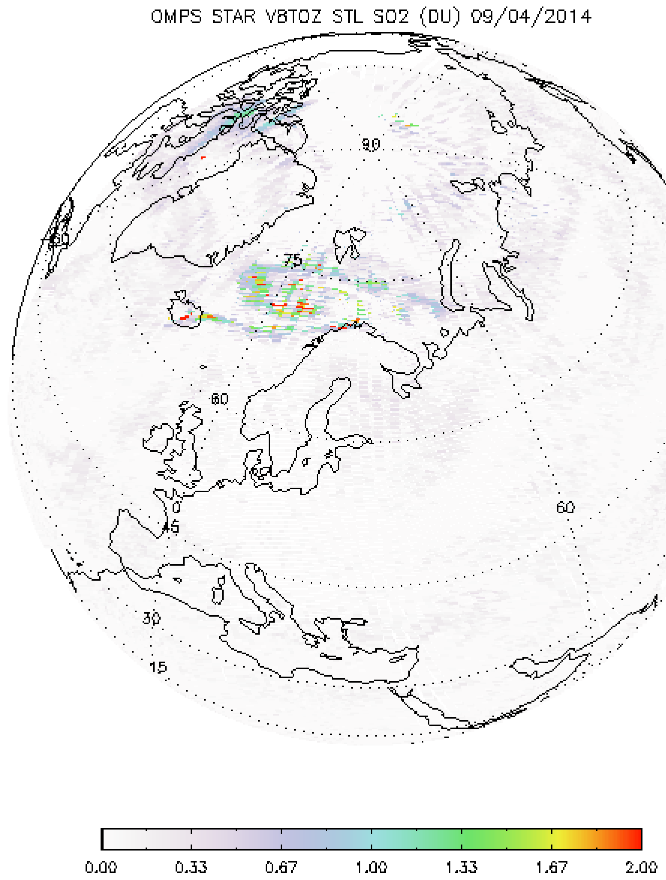


Example-1:
Iceland Bardarbunga volcano eruption

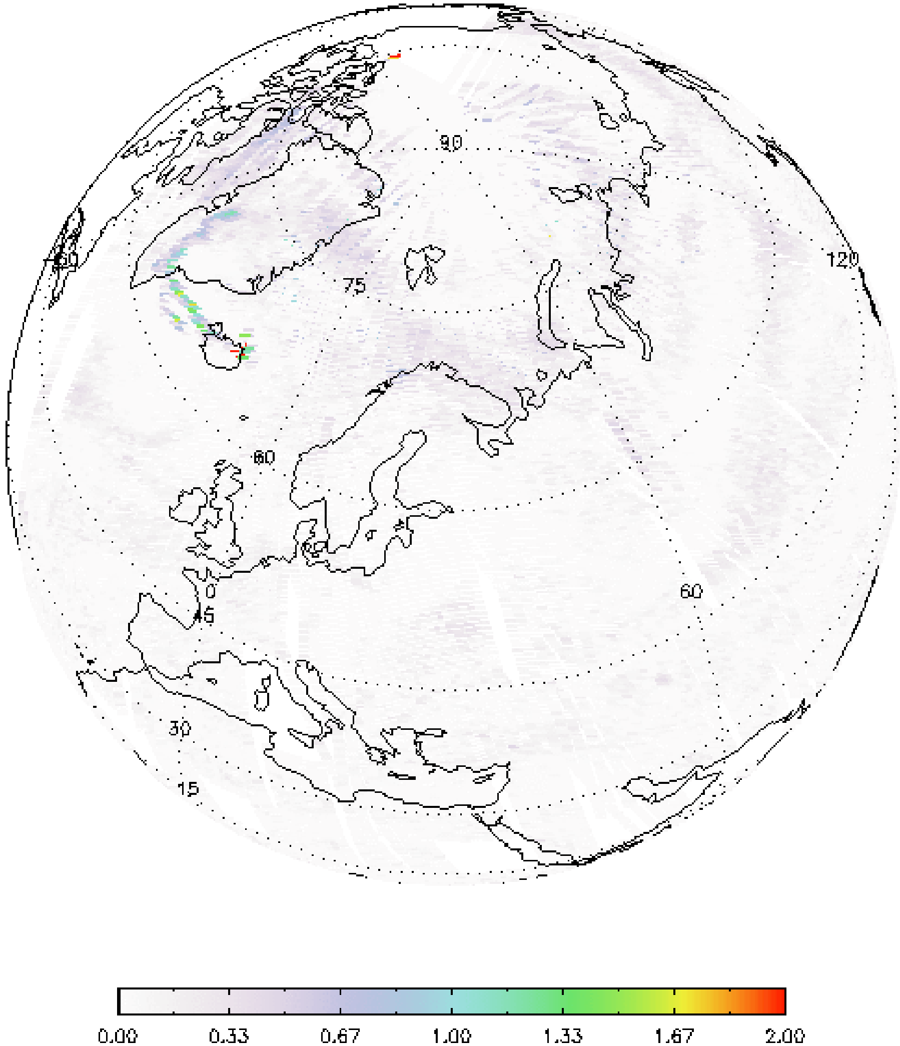
PEATE algorithm's product



STAR products



OMPS STAR V8TOZ STL SO2 (DU) 09/01/2014



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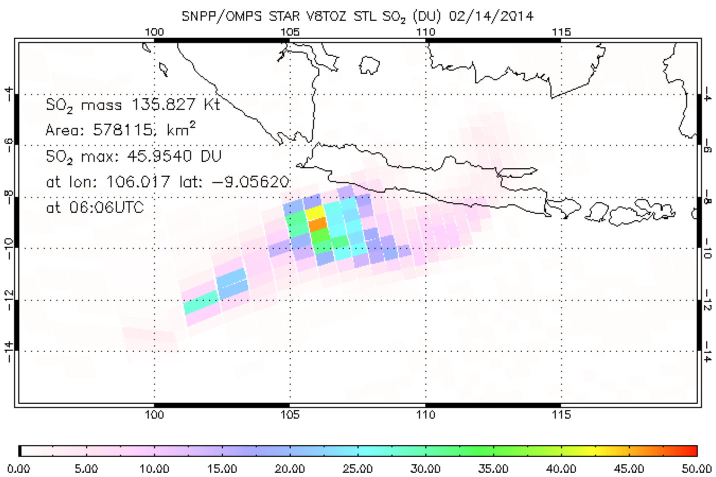
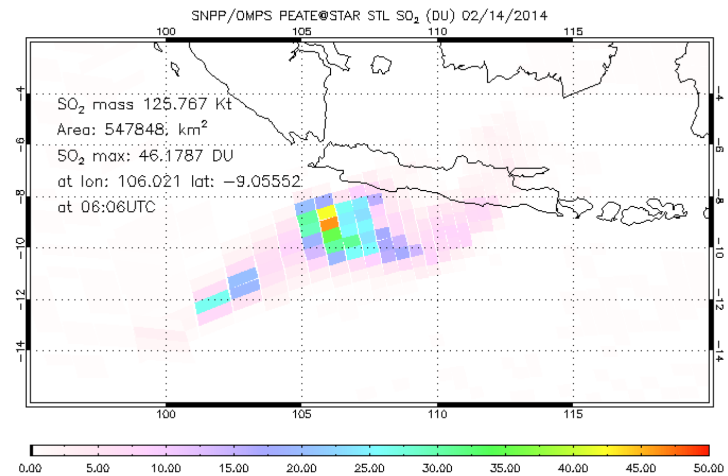
Example-2:
Indonesia Kelud volcano eruption
February 14, 2014

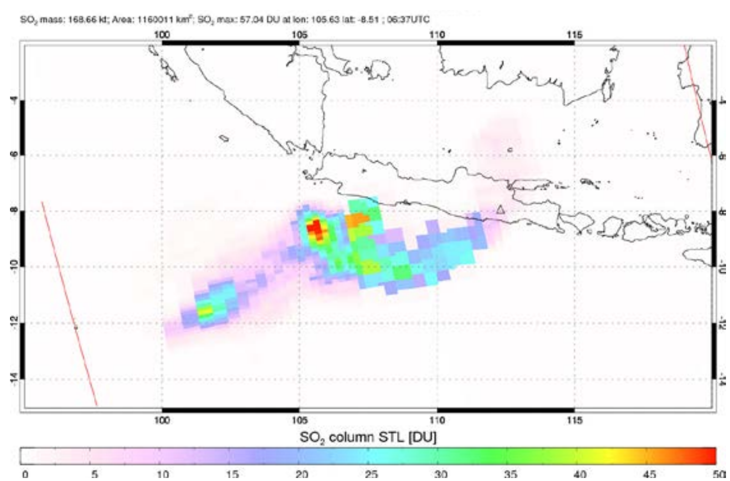
STAR V8+NMSO2



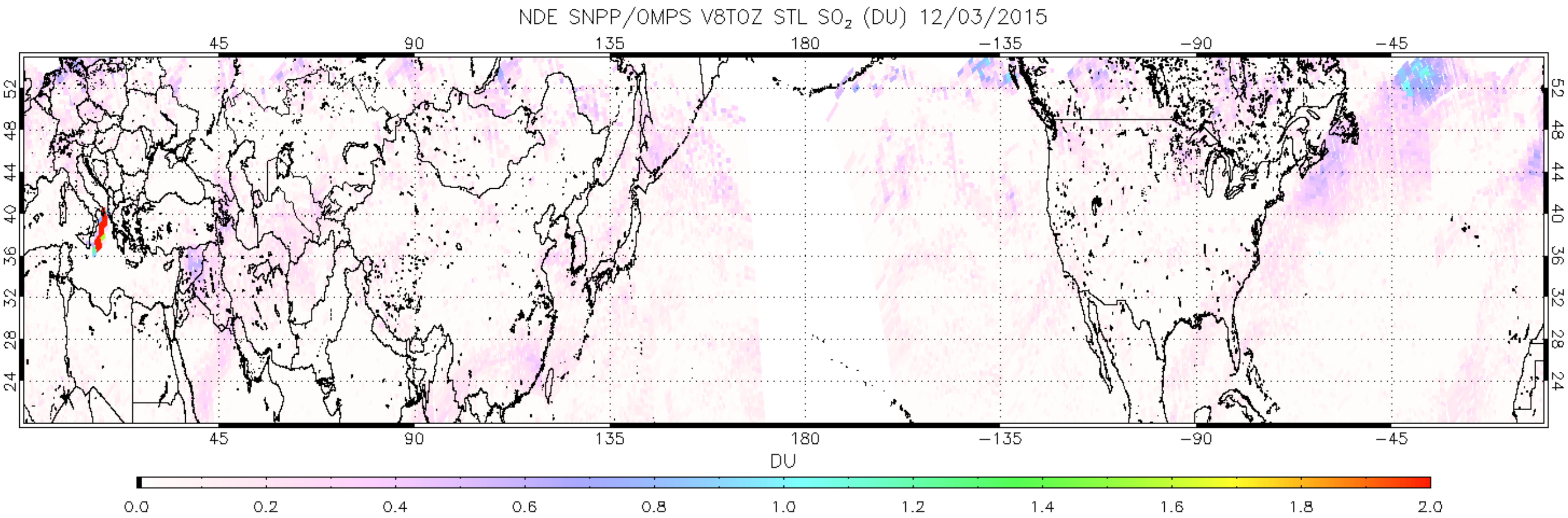
STAR/PEATE updated original



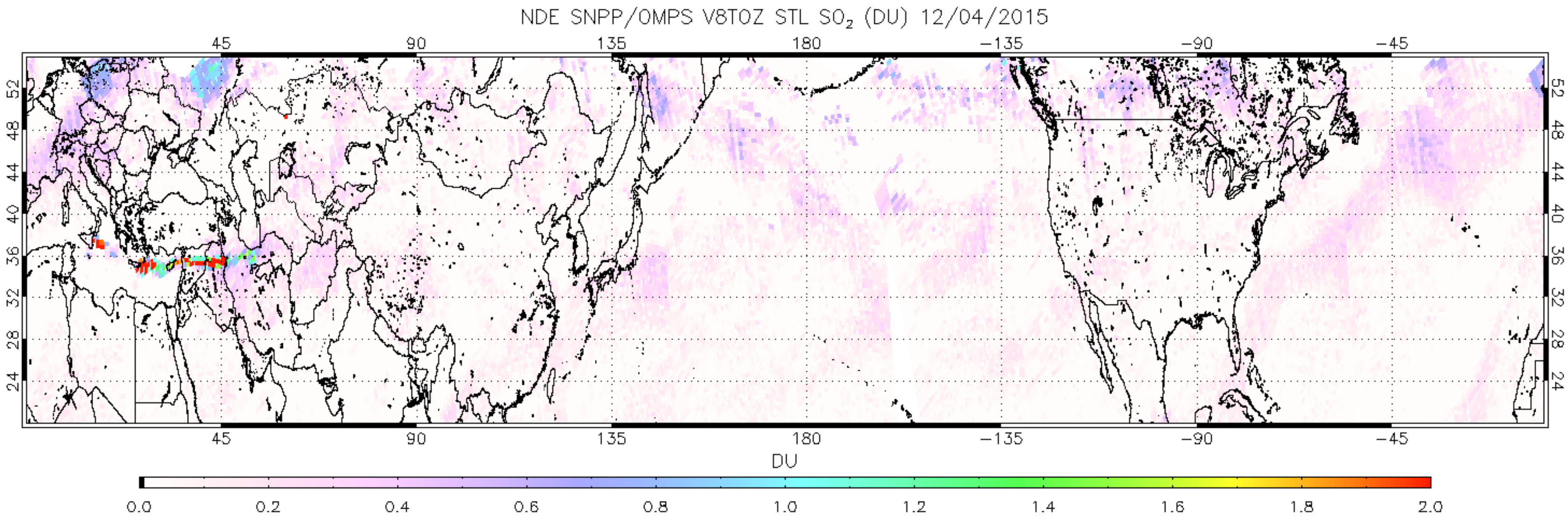
Provided by NASA PEATE



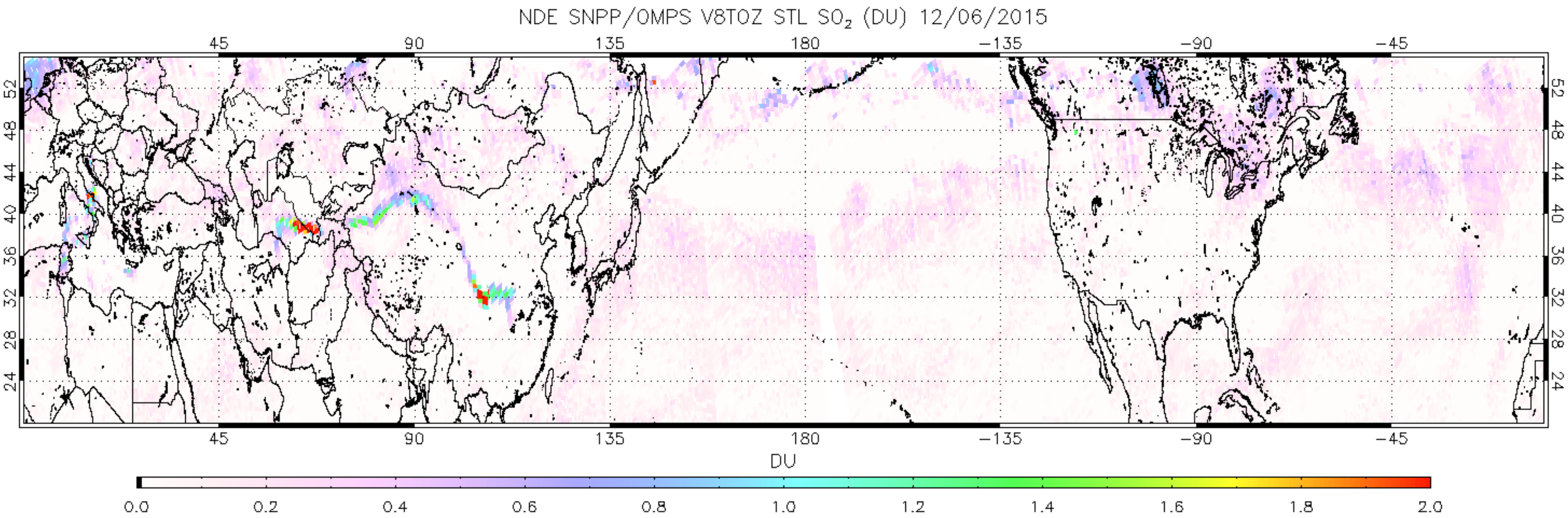
Example 3-1: Sicily Volcano eruption and transportation



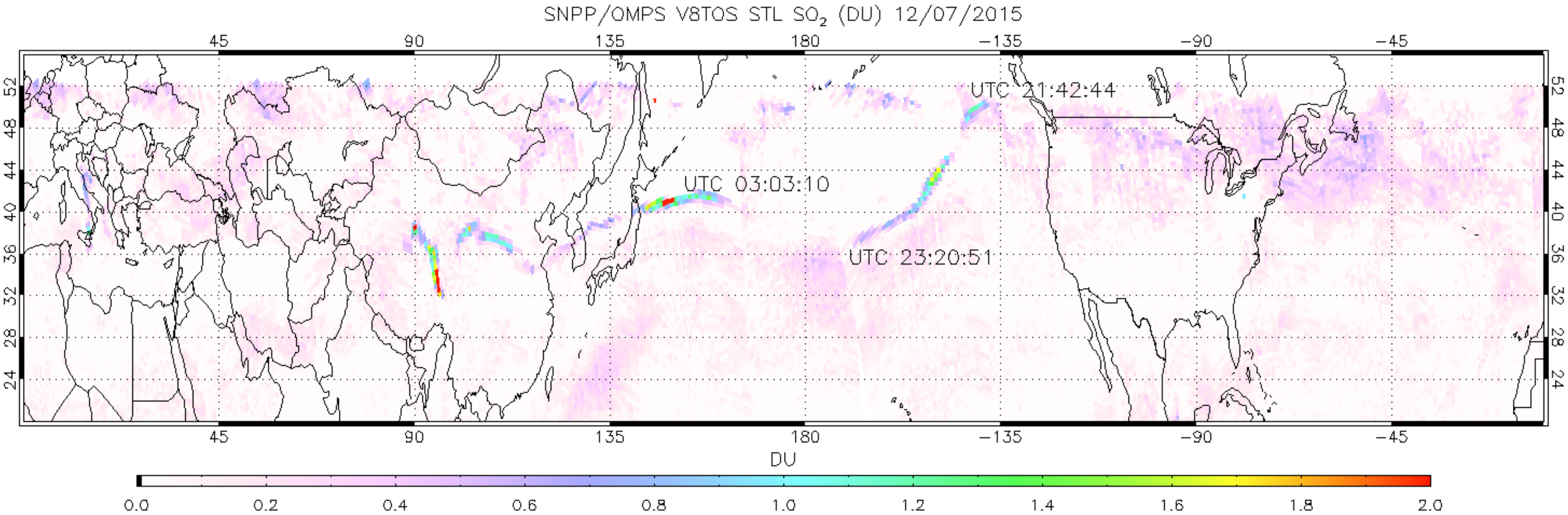
Example 3-2: Sicily Volcano eruption and transportation



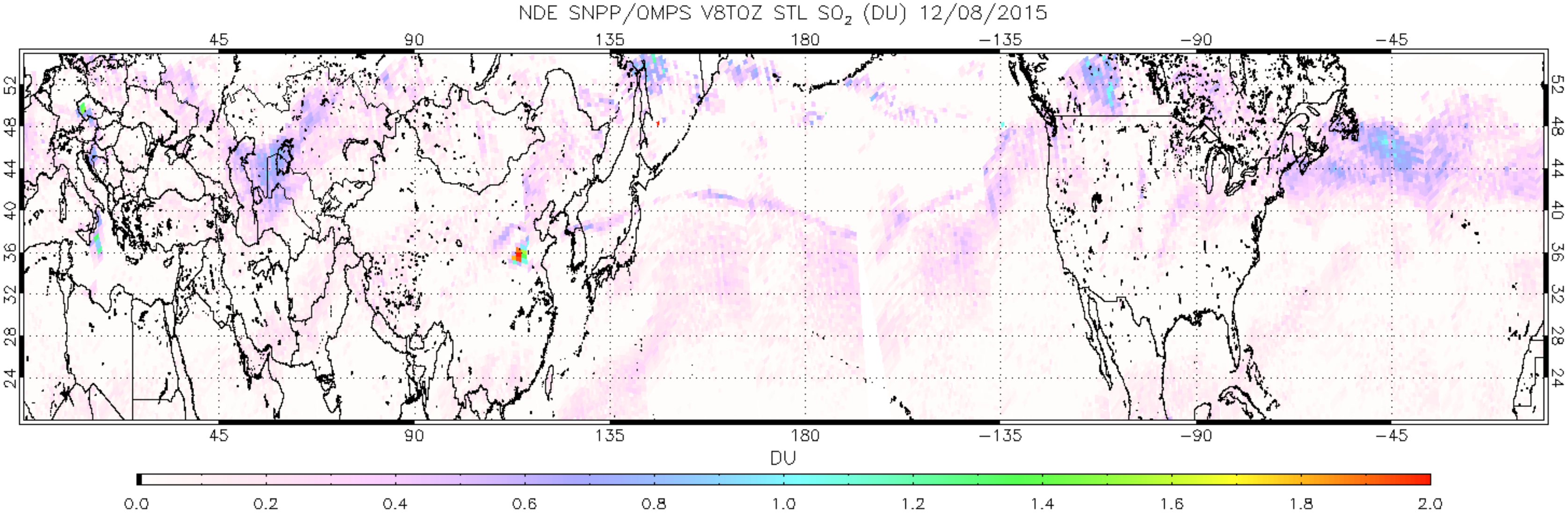
Example 3-3: Sicily Volcano eruption and transportation



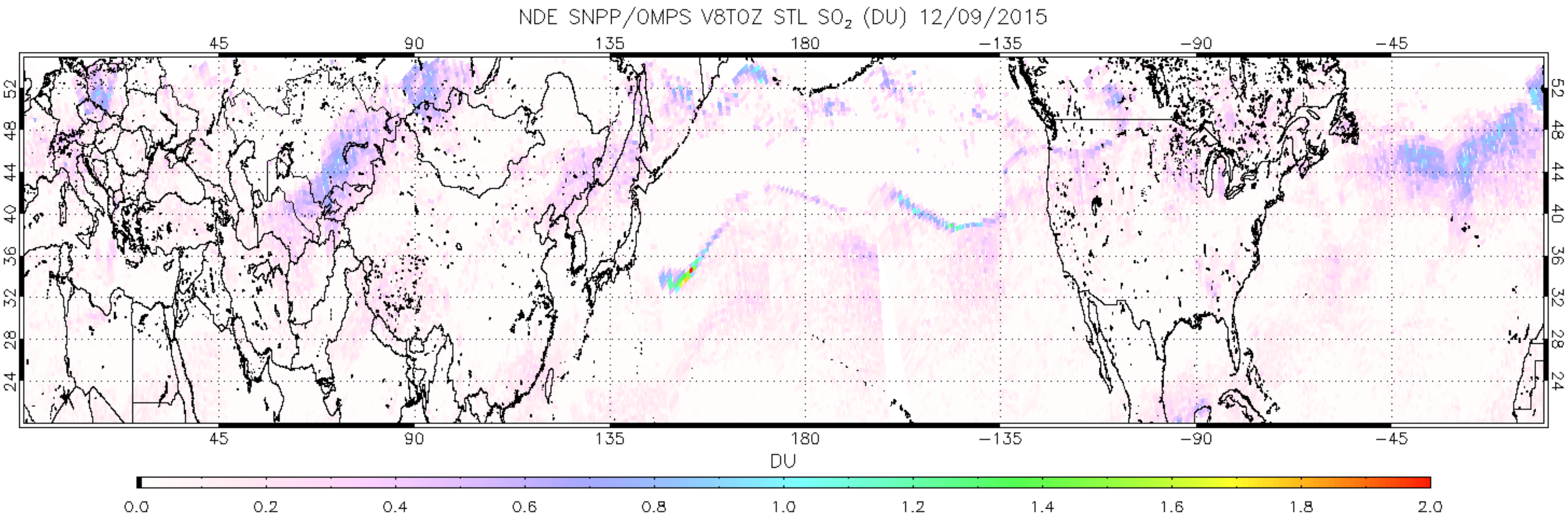
Example 3-4: Sicily Volcano eruption and transportation



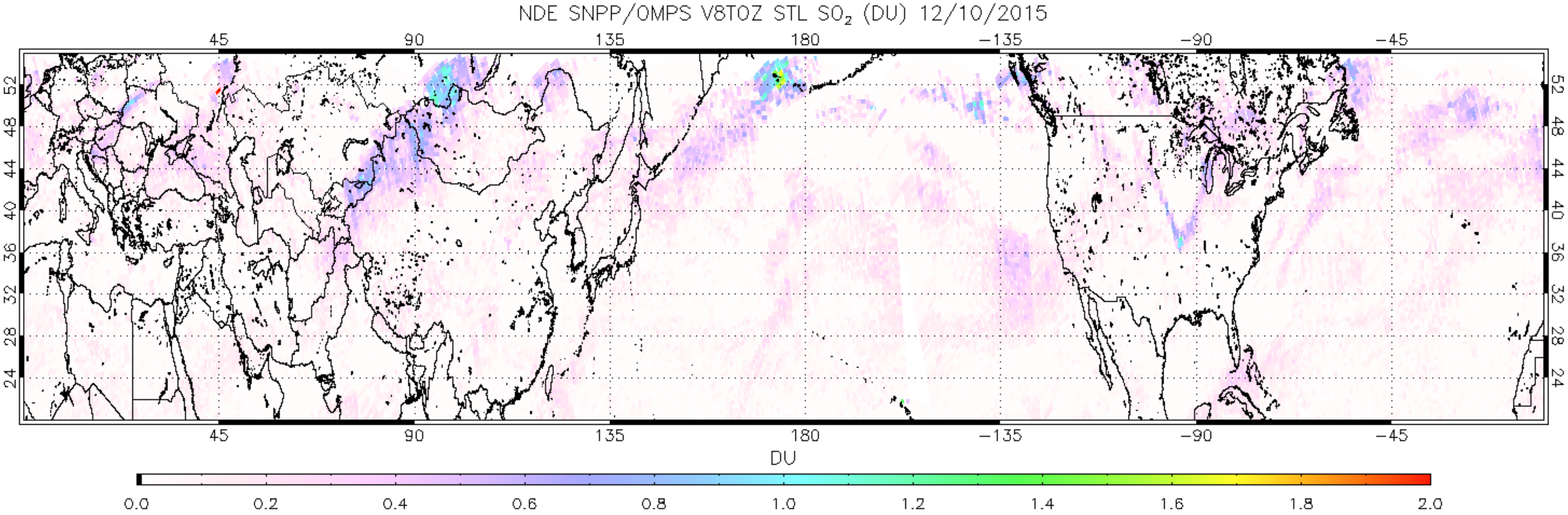
Example 3-5: Sicily Volcano eruption and transportation



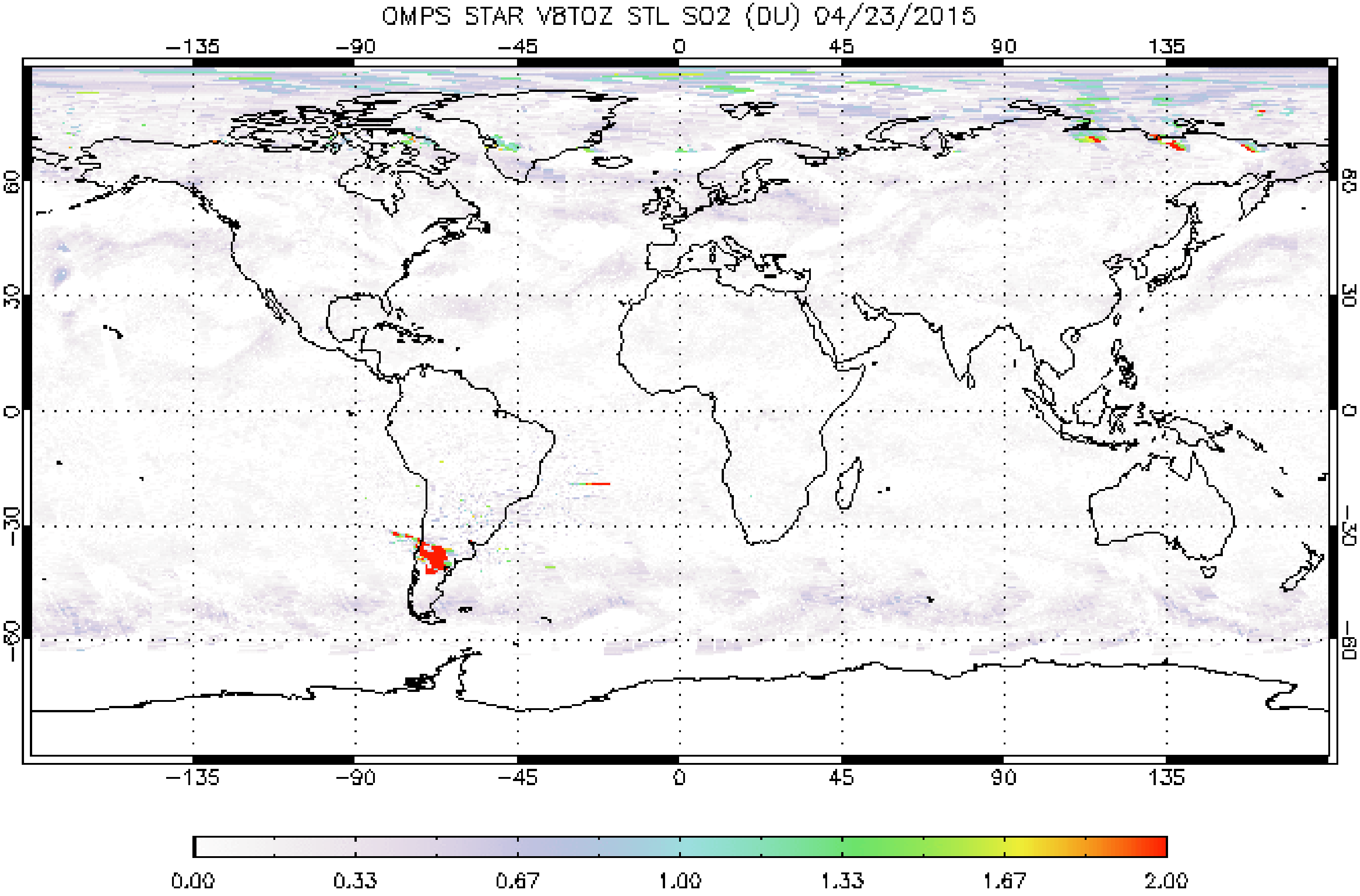
Example 3-6: Sicily Volcano eruption and transportation



Example 3-7: Sicily Volcano eruption and transportation



Example 4: Chile Calbuco volcano 4/23/2015 to 5/04/2015



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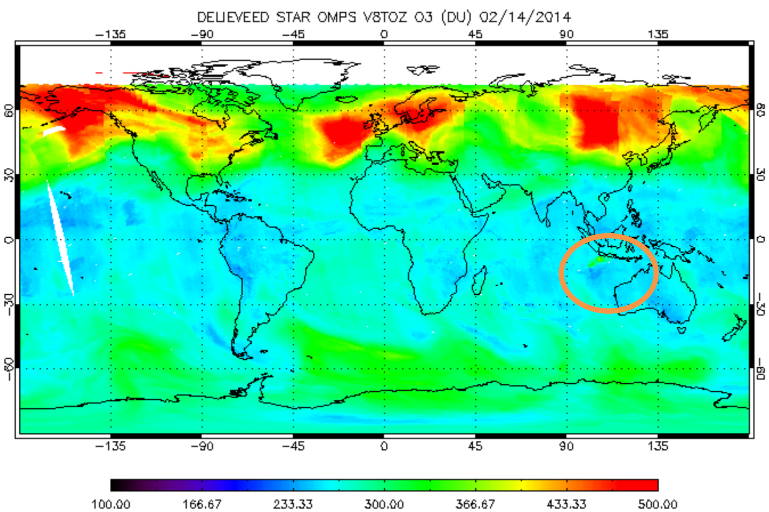
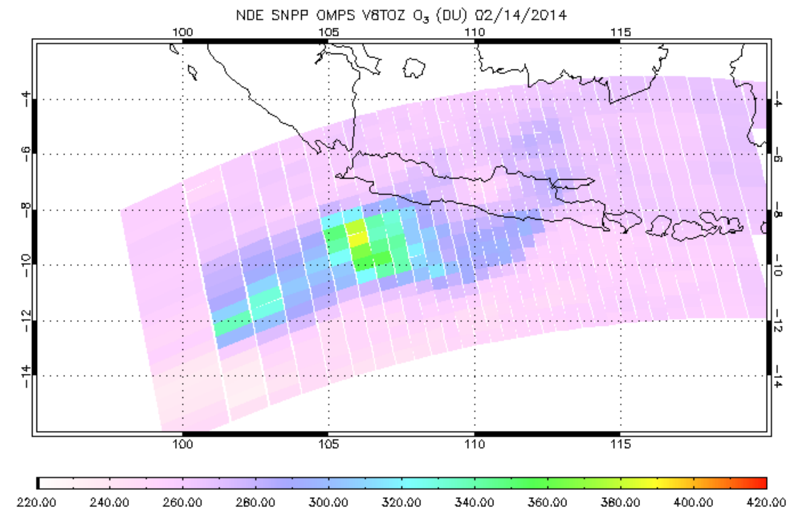
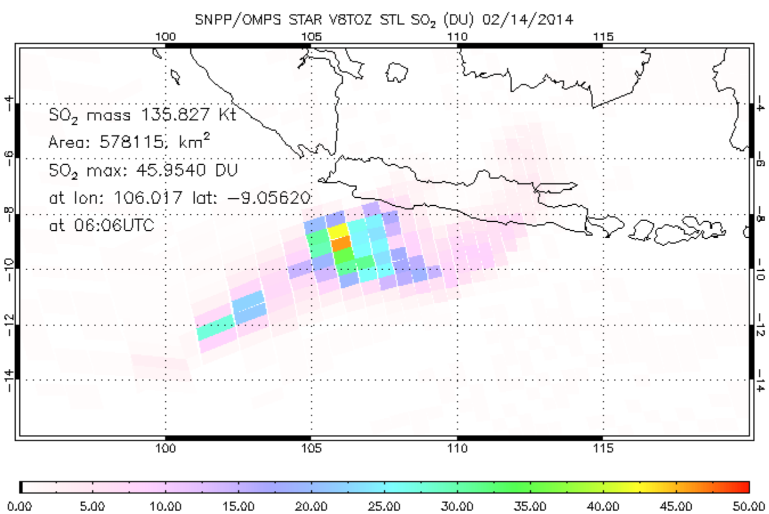
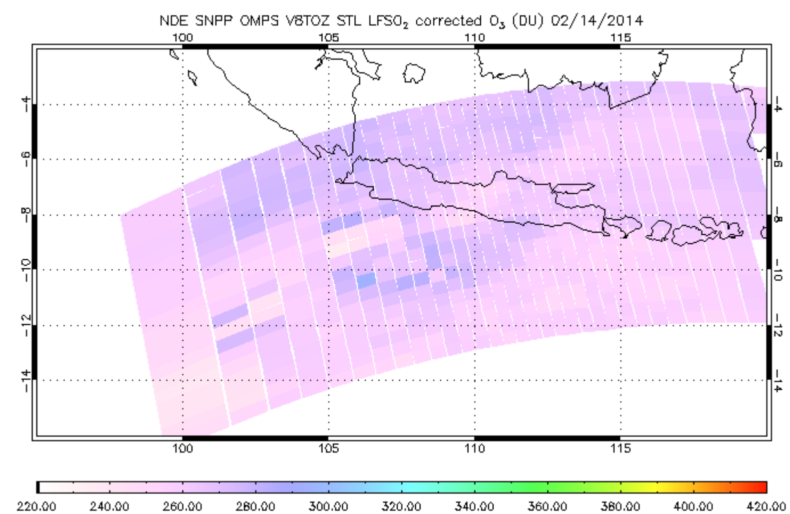
Example-5: Ozone correction by assuming SO_2 in STL for Indonesia Kelud volcano eruption case

February 14, 2014









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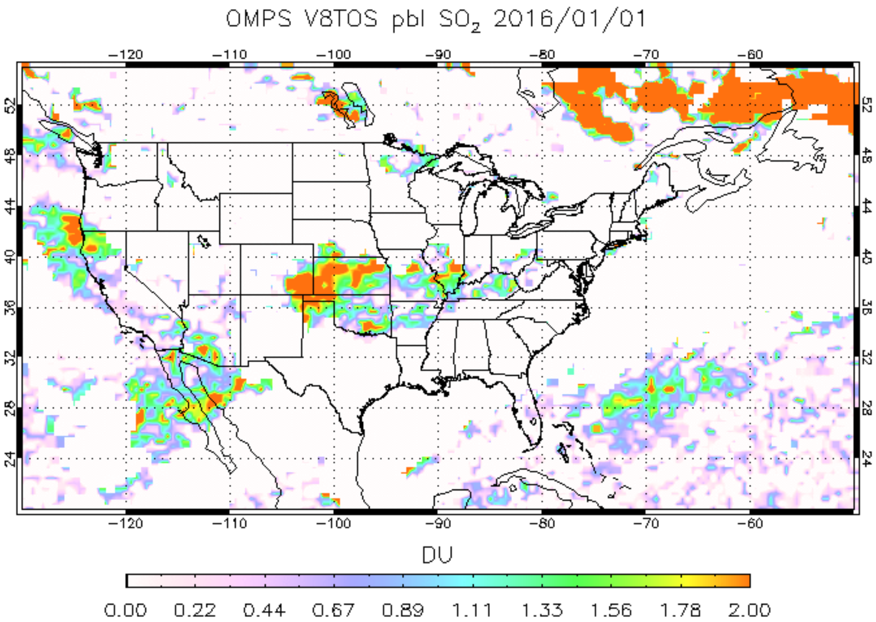
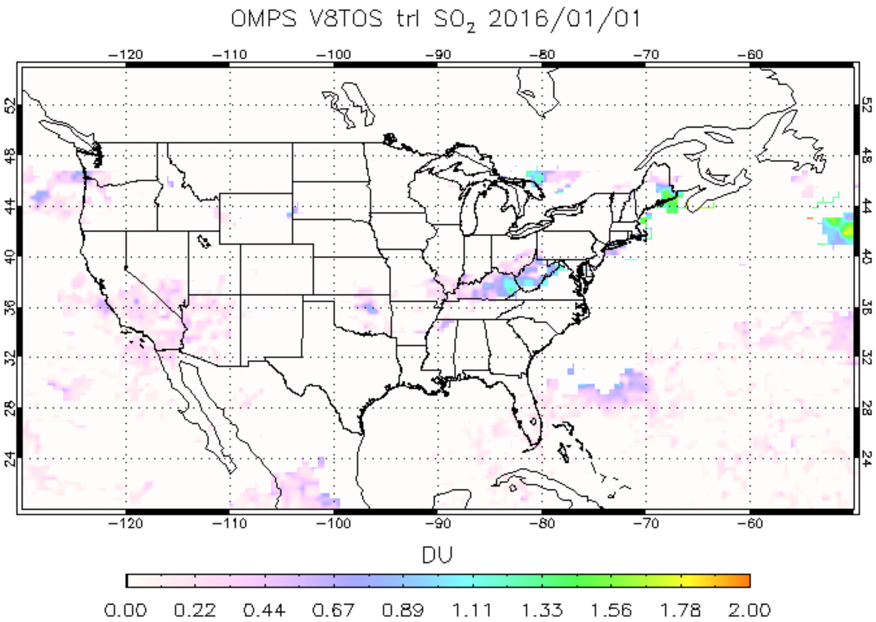
Daily PBL and TRL SO_2 maps over the US January to June 2016





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Summary

1. A 15-granule implementation provide a reliable alert to volcanic SO_2 cloud.

2. LFSO2 retrieval provides a total column O_3 correction when thick SO_2 appears in the atmosphere.

3. Provide accurate SO_2 total column amount for V8TOZ product.

4. Shown that OMPS Nadir Mapper possesses high sensitivity to monitor SO_2 as a pollutant in the atmosphere.