Developments in the KNMI retrieval of NO$_2$ from OMI

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The KNMI DOMINO NO2 product

DOMINO: combined retrieval-assimilation system

Based on TM (stratospheric) forecast (not analysis)
Developments NO2 retrieval algorithm

- **DOAS spectral fitting**
- **Air-mass factor improvements:**
  - Use of TM5 model
  - O2-O2 cloud retrieval
  - Error modelling update
Improve solar reference spectrum

Jos van Geffen et al, AMT, 2015

Update of high-resolution solar spectrum:
- better representation of
  OMI ITF (now $\lambda$-dependent)
- better Ring-spectrum and
  $I_0$-corrected reference spectra

New solar spectrum improves effective $\lambda$-calibration

RMS of fit: -17%
$\text{NO}_2$ slant columns: -6%

Other reference spectra otherwise identical to OMNO2A
Improve $\lambda$-calibration window to map $I$ to $I_0$

Identify $\lambda$-calibration window that minimizes RMS/NO$_2$ fit error

Best results for 409-428 nm
Previously: 408-423 nm

RMS of fit: -32%
NO$_2$ slant columns: -13%
Improve other reference spectra

\( \text{NO}_2 \): still Vandaele et al. [1998] but with new ITF
\( \text{O}_3 \): Bogumil et al. [2000] instead of obscure WMO-1975
\( \text{H}_2\text{O} \): HITRAN 2012 instead of HITRAN-2004
\( \text{O}_2-\text{O}_2 \): Now included!
\( \text{LQW} \): Now included!

**Stronger amplitude in new \( \text{NO}_2 \) cross section!**

RMS of fit: -30%
\( \text{NO}_2 \) slant columns: -11%
Including liquid water

Fit results for cloudy pixels are not affected much when including liquid water absorption.

Including liquid water absorption in the NO$_2$ fit is a good idea.

More realistic O3

Strong feature for clear water pixel!
Summary of the spectral fitting improvements

*Jos van Geffen et al, AMT, 2015*

Reduction of $1.0 - 1.3 \times 10^{15}$
Discrepancy between DOMINO v2 and limb sensors

A reduction of $0.4-0.5 \times 10^{15}$ molec.cm$^{-2}$ would largely resolve the discrepancies with limb sensors, *Belmonte Rivas et al.*, 2014
Developments: KNMI OMI/TROPOMI NO2 product

Developments NO2 retrieval algorithm

- DOAS spectral fitting
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A new model for (TROP)OMI NO₂ retrievals

DOMINO v1 and v2: based on TM4 at 3° × 2°
DOMINO v3: will be based on TM5 at 1° × 1°

Motivation:
• TM5 is benchmarked (Huijnen et al., 2010)
• Parallel code: allows 1° × 1°
• Extended chemistry (CB05 scheme)
• Employs up-to-date emission inventories
• Improved stratospheric NO₂:
  use of ODIN HNO₃ climatology

New TM5-mp version available since early 2015
(Philippe Le Sager, Jason Williams, KNMI)
Impact on the stratosphere

White areas: negatives

With TM5: 27% fewer negatives
Increasing resolution to $1° \times 1°$

Better resolved a priori profile shapes lead to a better understanding of pollution gradients observed from space.
DOMINO with TM5 at $1° \times 1°$ vs. at $3° \times 2°$

Increase of the urban-to-rural contrast!
Developments NO2 retrieval algorithm

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Systematic error in $O_2$-$O_2$ cloud pressures

- Retrieved $O_2$-$O_2$ slant column depends on atmospheric temperature profile

$$I(\lambda) = I_0(\lambda) \exp \left( -\int_{z_c}^{Z_{TOA}} m(z,\lambda) n_{O_2}^2(z) \sigma_{O_2-O_2}(\lambda) \, dz \right)$$

- LUT for $O_2$-$O_2$ based on fixed AFGL mid-latitude summer $T$-profile
- $O_2$-$O_2$ slant columns require $T$-correction since ‘true’ $T$ profile may differ strongly from mls-profile

Acknowledgment: Johan de Haan
Impact on NO$_2$ retrievals of O2-O2 improvement

Higher clouds $\rightarrow$ more screening $\rightarrow$ lower AMFs
Refined error modelling

Update of error modelling inputs:
cloud fraction error, albedo error, profile error, stratosphere error, slant column error

Table 3: The effect of the improved DOMINO error parameterization. The first column states the region defined by the boundaries given in column two. Column three give the average tropospheric NO$_2$ column for that region for 20-30 October 2004 in 10$^{15}$ molec./cm$^2$, column four gives the old error in 10$^{15}$ molec./cm$^2$, and column five gives the new error in 10$^{15}$ molec./cm$^2$. Column six gives the relative change in the average error: $100 \times \frac{e_{V_{tr},new} - e_{V_{tr},old}}{e_{V_{tr},old}}$.

<table>
<thead>
<tr>
<th>Region</th>
<th>Coordinates</th>
<th>$V_{tr}$*</th>
<th>$e_{V_{tr},old}$</th>
<th>$e_{V_{tr},new}$</th>
<th>$e_{V_{tr},new}$/$e_{V_{tr},old}$</th>
<th>Relative change</th>
</tr>
</thead>
<tbody>
<tr>
<td>World</td>
<td>-180,-180-60,80</td>
<td>0.52</td>
<td>0.67</td>
<td>0.58</td>
<td>-13%</td>
<td></td>
</tr>
<tr>
<td>Eastern US</td>
<td>-90,-60;35,45</td>
<td>4.57</td>
<td>4.10</td>
<td>2.69</td>
<td>-34%</td>
<td></td>
</tr>
<tr>
<td>China</td>
<td>85,125;30,40</td>
<td>3.45</td>
<td>2.31</td>
<td>1.77</td>
<td>-23%</td>
<td></td>
</tr>
<tr>
<td>Europe</td>
<td>-20,45;35,65</td>
<td>2.07</td>
<td>2.07</td>
<td>1.41</td>
<td>-32%</td>
<td></td>
</tr>
<tr>
<td>The Netherlands</td>
<td>4,7;51,53.5</td>
<td>7.53</td>
<td>5.47</td>
<td>3.84</td>
<td>-30%</td>
<td></td>
</tr>
<tr>
<td>London</td>
<td>-1,1;51,52</td>
<td>8.87</td>
<td>7.22</td>
<td>4.32</td>
<td>-41%</td>
<td></td>
</tr>
<tr>
<td>Barcelona</td>
<td>2,3;41,42</td>
<td>6.40</td>
<td>3.06</td>
<td>2.09</td>
<td>-32%</td>
<td></td>
</tr>
</tbody>
</table>

To give a simple representation of the error, we fit a linear slope for the error in the tropospheric NO$_2$ column as a function of the tropospheric NO$_2$ column. The data (points and bold line) and fit (dashed line) for the old (black) and new (blue) error parameterization are shown in Figure 22. The relation found for the old parametrization is:

$$e_{V_{tr}} = 0.66 V_{tr} + 0.45 \times 10^{15} \text{ molec./cm}^2.$$  

While the new error parameterization is characterized by:

$$e_{V_{tr}} = 0.42 V_{tr} + 0.45 \times 10^{15} \text{ molec./cm}^2.$$  

This error quantification has a larger slope but smaller constant part than the relation reported by Boersma et al. (2011) for DOMINO v2:

$$e_{V_{tr}} = 0.25 V_{tr} + 1.00 \times 10^{15} \text{ molec./cm}^2.$$  

The intercept of the error curve with the y-axis is determined by errors in the slant column, the slope is mainly related the AMF error. Even though our relation is only based on 10 days of data, it provides a relevant representation of errors in DOMINO to compare to Boersma et al. (2011) since our method is based on propagated errors and their associated tropospheric NO$_2$ columns.
Effect of aerosols

DOMINO: implicit correction for aerosols through cloud retrieval
*Patricia Castellanos et al, AMTD 2015*

14,000 collocated OMI-CALIOP clear-sky pixels

Provides measured information on:
- Type
- Loading (AOD)
- Aerosol height (ALH)

Allows to compare explicit aerosol correction to previous implicit correction approach
Effect of aerosols

Patricia Castellanos et al, AMTD 2015

1. Implicit aerosol correction via eff. cloud fraction works well (avg diff < 10%)
2. Implicit correction fails for situations high absorbing aerosol loads → Explicit AMFs are 20-50% higher
3. Explained by absence of abs. aerosol in retrieval cloud model

Outlook:
- Improve flagging!
- Consider explicit aerosol correction for clear sky pixels based on globally available satellite observations - OMI AOT, OMI type, CALIPSO extinction profile (climatology)

Talk by Julien Chimot, Wednesday
OMI, TROPOMI, QA4ECV

- Preparing for DOMINO-v3 re-processing of OMI
- Preparing the TROPOMI NO2 algorithms
  - Near-Real Time
  - Assimilation-Retrieval
- Preparing for QA4ECV reprocessing of NO2 for multiple sensors
  - IUP-Bremen, BIRA, Mainz, KNMI
  - Study all aspects of retrievals
    - (DOAS settings, AMFs, Stratosphere)
  - Define optimal settings

Talk Alba Lorente, Wednesday
Activities 2015: technical aspects

✦ Embedding of the DOMINO modules in the MPI-parallel TM5 code
✦ Generalising the interfaces to improve portability
  • Near-Real Time (file based)
  • Daily offline, reprocessing (Assimilation-Retrieval)
✦ Code “clean-up”

A working version is available
Ongoing: review of settings, optimisation
Conclusions: DOMINO-2 ➔ DOMINO-3

- Improved NO$_2$ slant columns are smaller by 1.0-1.3 $10^{15}$ molec.cm$^{-2}$ with 30% lower fitting residuals
- Coupled DOMINO to TM5-mp (2015 version)
- Improved resolution for a priori profile leads to increases over hotspots (+20%) and stronger contrast urban-rural
- Temperature-correction for cloud pressures relevant over polluted areas

(TROP)OMI NO$_2$ team