Atmos. Meas. Tech. Discuss.,
doi:10.5194/amt-2019-143-AC1, 2019

Atmospheric Measurement Techniques
Discussions

Interactive comment on "A neural network radiative transfer model approach applied to TROPOMI's aerosol height algorithm" *by* S. Nanda et al.

S. Nanda et al.

nanda@knmi.nl

Received and published: 11 July 2019

Reviewer comment (general): This work is novel and interesting. The proposed algorithm produces results that have comparable accuracy to line-by-line models while achieving three orders of magnitude speed-up in computational efficiency. This makes it possible to increase the throughput of TROPOMI aerosol retrievals and possibly enable operational retrievals for all pixels in each TROPOMI orbit. The computational speed-up also opens up the possibility of including more physics in the forward model. The usage of three neural network models is an interesting idea. It takes advantage of the fact that correlations between input parameters and different forward model outputs

are different. The paper should be published, but only after the comments (see below) are dealt with.

Author's response: Thank you for taking the time to review this manuscript. The goal of this research project was to develop a faster aerosol layer height retrieval algorithm, while keeping in mind the possibility of including more details into the model in the future.

Reviewer comment (specific 1): Line 14, page 1: "eligible for retrieving aerosol layer height". Is this because of clouds? If this is the case, say so.

Author's response: The rough estimate of 3% of total eligible pixels for retrieving aerosol layer height needs to be updated following new analyses of 56 TROPOMI files over Europe containing 7.3 million pixels. The selection criterion was a UV Aerosol Indices above 0.0, of which 6.1% of all pixels considered over Europe. TROPOMI's UV Aerosol Index values are one index point lower than UV Aerosol Indices from other indices.

Changes to the manuscript: The new sentence now reads the following:

'With TROPOMI recording approximately 1.4 million pixels within a single orbit, a rough estimate based on a minimum UV Aerosol Index of 0 indicates that at least six percent of all pixels over an area as large as Europe will be eligible for retrieving aerosol layer height. This number can go beyond 50,000 pixels per orbit in many cases, placing a steep requirement on the computational infrastructure to process all possible pixels from a single orbit.'

Reviewer comment (specific 2): Lines 26-28, page 1: The previous sentence suggests that the method utilized line-by-line calculations to generate training data set. Do the authors mean that line-by-line calculations are not used in the “operational" retrieval that utilizes neural networks? The authors also need to say more to distinguish their method from that used by Chimot et al. and Loyola et al.

Reviewer comment (specific 3): Line 33, page 1 – Line 1, page 2: It is not clear what the difference is from the existing neural network approaches. Is it that Optimal Estimation is used? "using artificial neural networks to improve the computational speed of RT calculations" is very vague and general; isn't that common to all neural network approaches?

Author's response: The work by Chimot et al. utilise the DISAMAR radiative transfer model to compute synthetic OMI measurements of the slant column density in the O_2-$O2$ absorption band, which is a part of the feature vector in the neural network models in their implementation of retrieving aerosol layer height. Chimot et al. do not use any line-by-line calculations in their operational retrievals.

The aerosol layer height algorithm that is the subject of this paper follows a similar philosophies to Chimot et al. as well as Loyola et al, with important differences.

- With respect to Chimot et al. the paper discusses using DISAMAR to generate synthetic spectra for training a neural network model, the difference being that while Chimot et al. prefer to retrieve aerosol layer height as the output of their trained neural network model, whereas the neural network model in the paper outputs the top-of-atmosphere oxygen A-band spectra in the forward model. These neural-network-model-calculated top-of-atmosphere oxygen A-band spectra are then utilised by an optimal estimation scheme, which outputs a retrieved aerosol layer height value.
- With respect to Loyola et al, the neural network models both compute top-of-atmosphere spectra, with the difference being that the KNMI aerosol layer height neural network retrieval algorithm has two other neural network models for the

derivatives of the spectra with respect to the state vector parameters aerosol optical thickness and aerosol layer height, whereas Loyola et al. train their neural network models only for the sun-normalised radiances (section 4.4, https://www.atmos-meas-tech.net/11/409/2018/amt-11-409-2018.pdf)

Changes to the manuscript:

- Adjusted text to ‘Chimot et al. (2017) describe an approach using a radiative transfer model to generate OMI slant column densities of the O_2-$O2$ band at 477 nm for different aerosol optical depths (among other input parameters) to train several artificial neural network models that directly retrieve aerosol layer height. Operationally, their neural network models use the MODIS aerosol optical depth at 550 nm product and retrieved OMI slant column densities, thereby entirely foregoing line-by-line calculations and significantly speeding up the retrieval algorithm.’.
- Amended the final paragraph of section 1 to ‘The work of Chimot et al. (2017) and Loyola et al. (2018) bring to light the efficacy of artificial neural networks in satellite remote sensing of oxygen absorption bands for retrieving properties of scattering species in the atmosphere. This paper discusses a method inspired by Chimot et al. and Loyola et al. to retrieve aerosol layer height from oxygen A-band measurements by TROPOMI. While Chimot et al. directly retrieve aerosol layer heights from their neural network models, the operational algorithm in this paper utilises neural networks to calculate top-of-atmosphere radiances in the forward model. This is subsequently used by an optimal estimation scheme to retrieve aerosol layer heights. Similarly while Loyola et al. derive top-of-atmosphere sun-normalised radiances only for their cloud property retrieval algorithm, the method in this paper has dedicated neural network models that calculate the Jacobian as well as the top-of-atmosphere sun-normalised radiances.’.

Reviewer comment (specific 4): Line 8, page 2: Add the following references:

Timofeyev et al., 1995; Sanghavi et al., 2012; Geddes Bösch, 2015; Colosimo et al., 2016; Davis et al., 2017; Xu, et al., 2017; Zeng et al., 2018

Colosimo, S. F., V. Natraj, S. P. Sander, and J. Stutz (2016), A sensitivity study on the retrieval of aerosol vertical profiles using the oxygen A-band, Atmos. Meas. Tech., 9(4), 1889–1905, doi:10.5194/amt-9-1889-2016.

Davis, A. B., O. V. Kalashnikova, and D. J. Diner (2017), Aerosol layer height over water from O2 A-band: mono-angle hyperspectral and/or bispectral multi-angle observations, Preprint, doi:10.20944/preprints201710.0055.v1.

Geddes, A., and H. Bösch (2015), Tropospheric aerosol profile information from high resolution oxygen A-band measurements from space, Atmos. Meas. Tech., 8(2), 859–874, doi:10.5194/amt-8-859-2015.

Sanghavi, S., J. V. Martonchik, J. Landgraf, and U. Platt (2012), Retrieval of aerosol optical depth and vertical distribution using O2 A- and B-band SCIAMACHY observations over Kanpur: A case study, Atmos. Meas. Tech., 5(5), 1099–1119, doi:10.5194/amt-5-1099-2012

Timofeyev, Y. M., A. V. Vasilyev, and V. V. Rozanov (1995), Information content of the spectral measurements of the 0.76 μm O2 outgoing radiation with respect to the vertical aerosol optical properties, Adv. Space Res., 16(10), 91–94, doi:10.1016/0273-1177(95)00385-R.

Xu, X., Wang, J., Wang, Y., Zeng, J., Torres, O., Yang, Y., et al. (2017). Passive remote sensing of altitude and optical depth of dust plumes using the oxygen A and B bands: First results from EPIC/DSCOVR at Lagrange-1 point, Geophys. Res. Lett., 44, 7544–7554, doi:10.1002/2017GL073939.

Zeng, Z.-C., V. Natraj, F. Xu, T. J. Pongetti, R.-L. Shia, E. A. Kort, et al. (2018), Constraining aerosol vertical profile in the boundary layer using hyperspectral measure-

ments of oxygen absorption, Geophys. Res. Lett., 45, doi:10.1029/2018GL079286.

Author's response: Agreed.

Changes to the manuscript: Amended the first sentence of section 2 that discusses previous work done for retrieving vertical information of aerosols using passive space-borne measurements of the oxygen A-band to 'The TROPOMI aerosol layer height is one of the many algorithms that exploit vertical information of scattering aerosol species in the oxygen A-band (Timofeyev et al., 1995; Gabella et al., 1999; Corradini and Cervino, 2006; Pelletier et al., 2008; Dubuisson et al., 2009; Frankenberg et al., 2012; Wang et al., 2012, Sanghavi et al., 2012; Sanders and de Haan, 2013; Hollstein and Fischer, 2014; Geddes Bösch, 2015; Sanders et al., 2015; Colosimo et al., 2016; Sanders and de Haan, 2016; Davis et al., 2017; Xu, et al., 2017; Zeng et al., 2018; Nanda et al., 2018b)'

Reviewer comment (specific 5): Line 24-26, page 4: "The polarized . . . 760 nm".

- First order scattering also has a polarization effect. Presumably, the authors mean that they ONLY compute the first order polarization. If so, please state that.
- What is "small"? $< 5\%$? $< 1\%$? This statement is potentially untrue. If true, values for how small is small must be given, with proof. In the continuum and in weak lines, the second order effects might be large.

Reviewer comment (specific 6): Lines 27-28, page 4: There is a contradiction here. If the exclusion is not advised, the effect cannot be small. The authors should simply state that they ignored this for computational reasons. Besides, the whole point of using neural networks is to speed up calculations. Why not use them for speeding up Raman calculations too, or at least use lookup tables for Raman effects?

Reviewer comment (specific 7): Lines 29-30, page 4: "From preliminary . . . significantly".

Quantify this statement, and ideally provide a figure to illustrate the effects.

Author's response:

- Polarisation is ignored in the sense that for retrieving aerosol layer heights DISAMAR only computes the first element of the Stoke's vector in the radiation fields. The exclusion of higher order Stoke's vector elements has not shown to be a significant source of error.
- The affect of ignoring Rotational Raman Scattering (RRS) in the forward model results in errors in the final retrieved aerosol layer heights. However, as clarified by Sanders and de Haan (2016) who have retrieved aerosol layer height using the same radiative transfer model while including and excluding RRS, this error is significantly less in comparison to other model errors. Because the inclusion of RRS has resulted in a significant increase in time required by the line-by-line radiative transfer model and ignoring it does not yield large errors (from synthetic experiments), it has been historically excluded in the KNMI aerosol layer height retrieval algorithm.

With regards to the reviewer's suggestions to use lookup tables for the Raman effects or potentially incorporating an artificial neural network solution for including RRS into the forward model calculations, the authors appreciate these ideas very much. However, since the goal of this paper is to create a model that replicates the existing TROPOMI aerosol layer height algorithm, RRS is ignored for the sake of comparison and benchmarking. In the future, this may be a serious consideration by the TROPOMI Level-2 algorithm development team.

Finally, the authors acknowledge the confusion in this paragraph. The sentence 'RRS

can alter the line depths in the $O2$ A-band, but this effect is small', is not complete. The authors meant to state that the effect of excluding RRS on the retrieved aerosol layer height is small. The changes to the manuscript will reflect this. With regards to the reviewer's comments on quantifying the statement, the authors have chosen to include a citation to Sanders and de Haan 2016, which is the Algorithm Theoretical Basis Document of the TROPOMI ALH retreival algorithm. This discusses the rationale behind excluding RRS from computations.

Changes to the manuscript: To address the questions raised by the reviewer, the following amendments have been done to Section 2.2, paragraph 3 of the manuscript.

- 'As the Rayleigh optical thickness is low at 760 nm, DISAMAR only computes the monochromatic component of light by calculating the first element of the Stoke's vector. The exclusion of higher order Stoke's vector elements of the radiation fields has not shown to be a significant source of error (Sanders and de Haan, 2016).'
- 'While this exclusion of RRS is not advised by literature (Sioris and Evans, 2000; Vasilkov et al. 2013), preliminary experiments by Sanders and de Haan (2016) have ascertained that the errors in the retrieved aerosol layer height resulting from ignoring RRS of the oxygen A-band in the forward model are significantly smaller than the effect of other model errors. Due to this, the KNMI aerosol layer height retrieval algorithm has historically ignored calculating RRS cross sections.'

Reviewer comment (specific 8): Lines 30-31, page 4: Although it is true that retrievals are typically performed under "cloud free" conditions, optically thin cirrus clouds need to be accounted for since they are almost always present.

Author's response: It is indeed correct that optically thin cirrus clouds need to be accounted for as they are almost always present in the scene. Currently however, there are no implementations in the algorithm to incorporate cirrus cloud properties into the radiative transfer calculations. The operational TROPOMI algorithm utilises a VIIRS cloud mask to flag potential pixels with clouds.

Changes to the manuscript: Added the following sentence: ‘While optically thin cirrus layers are a known source of error in the retrieved aerosol layer height, currently there are no implementations to tackle this problem. Instead, TROPOMI incorporates information from the VIIRS instrument to detect the presence of clouds in the measured scene.’

Reviewer comment (specific 9): Lines 1-8, page 5: What are the effects of these approximations on the retrieved results? It seems that many of these simplifications are not needed because of the use of neural networks. Also, if only single scattering is used, calculation of ANY phase function is trivial and not time consuming. Considering the fact that the authors aim to produce an operational retrieval algorithm, these simplifications seem unwarranted and restrictive.

Author’s response: It is indeed correct that the simplifications are unwarranted and restrictive for a retrieval algorithm that incorporates a fast neural network approach to replace a radiative transfer model. However the goal of the paper is to replicate (as much as possible) the operational algorithm that uses online line-by-line calculations, which incorporates these approximations to reduce computational time. Finally, the paper compares the retrieved aerosol layer heights from both operational algorithm implementations in order to establish an acceptable agreement between the neural network approach to the online line-by-line approach. This is the first benchmark of the neural-network-augmented retrieval algorithm, subsequently leading to further improvements in the future in line with the reviewer’s recommendations.

The affects of these approximations are discussed in detail by Sanders and de Haan

(2016), which is the Algorithm Theoretical Basis Document of the TROPOMI aerosol layer height algorithm. The amendment in the manuscript will reflect their work.

Changes to the manuscript: Added the following final paragraph after the mentioned simplifications.

‘These simplifications in the DISAMAR forward model are a necessity for the line-by-line aerosol layer height algorithm, owing to its slow computational speed. In contrast, a neural network model is significantly faster. While the speed of the neural network model encourages increasing the complexity of the model, for a comparative study the neural network models are trained to replicate, as best as possible, the line-by-line version. Once this is achieved, the improvement of the algorithm will be an iterative endeavour.’

Reviewer comment (specific 10): Table 2, page 8: What does "varied" mean for the aerosol layer thickness? Is the aerosol layer thickness part of the feature vector? If not, how is it handled?

Author’s response: Aerosol layer thickness is not a part of the feature vector. It is a part of the training data set, and the aerosol layer pressure thickness varies between 50 hPa and 200 hPa. Currently, there is no call by the neural network model to the aerosol layer thickness. This shall be implemented into a future release.

Changes to the manuscript: Amended the table entries in Table 2 for aerosol layer thickness. The remark column now reads ‘varied but excluded from feature vector’, whereas the limits now read ‘50 hPa - 200 hPa’.

Reviewer comment (specific 11): Line 8, page 8: “a choice of 500,000 Disamar generated spectra”

How are these spectra generated? It is not clear how the choice is made.

Author's response: The amendment will reflect the clarification of spectra generation.

Changes to the manuscript: Changed the sentence 'Following testing and scrutinizing forward model calculation accuracy, a choice of 500,000 Disamar generated spectra is finalised as the size of the training data set.' to the following.

'The number of spectra generated for the training set was determined by training different models with different number of spectra in the training set ranging from 1,000 to 600,000. In general it was observed that incorporating more data resulted in a better neural network model. In order to test the trained neural network model, a choice of 500,000 spectra were selected, and 100,000 spectra were set aside for the test set. These spectra were generated using Disamar with model parameter ranges described in Table 2 and Figure 1.'

To that extent, the following line is removed from Page 6, line 3-5, as there is an incorrect reference to the correct table.

'Finding the most optimal neural network configuration requires a test data set which in this case contains 100,000 scenes outside the training data set. These test data follow the same input model 5 parameter distributions as described in Figure 1 and Table 1.'

Reviewer comment (specific 12): Lines 20-22, page 9: Need more quantitative error information, like for the derivative with respect to tau. Also, what does continuum (3d) mean?

Reviewer comment (specific 13): Lines 23-24, page 9: "these parts . . . cross sections"

Why do low oxygen absorption cross sections lead to low aerosol information content?

Author's response: The following amendment to the text clarifies the role of oxygen

absorption cross sections and aerosol information content.

Changes to the manuscript: The following change has been added to the text in the final lines of the final paragraph of section 3.2.

'The neural network model for the derivative of the reflectance with respect to τ and z_{aer} perform well in general for parts of the spectrum with large oxygen absorption cross sections, where the value of the derivatives are high (indicating a higher amount of information content from those specific wavelength regions). Errors in the deepest part of the R-branch between 759 nm and 762 nm and the P-branch between 752.50 nm and 765 nm, do not exceed more than 3% for $\text{NN}_{\text{K}_{\text{zaer}}}$. The same can be said for NN_{K_τ}, which displays errors in the range of 1% in the same wavelength region. For wavelengths outside of the deepest parts of the R and P-branch, the relative errors are large, and exceed 10% easily. However, the relative errors are calculated as the absolute value of the difference between the true spectrum and the neural network calculated spectrum, divided by the true spectrum. These values can be very large when the value of the true spectrum is very small, which is the case for the derivatives outside the deepest part of the R and P branches. The consequence of these errors in a retrieval scenario from synthetic and real spectra are discussed in the following section.'

Reviewer comment (technical):

Line 19, page 1: correlative → correlated

Line 20, page 1: Hasekamp and Butz (2008) → (Hasekamp and Butz, 2008)

Line 19, page 4: in → on

Line 25, page 5: an → a

Line 17, page 7: differentiation which → differentiation, which

Line 2, page 8: selected TROPOMI → selected to represent TROPOMI

Line 6, page 8: an → and

Line 7, page 8: isn't a → is no

Line 14, page 8: legible → physical

Line 12, page 9: were trained → was trained

Line 18, page 9: to → of

Line 20, page 9: remove "more than"

Line 23, page 9: at → in

Line 24, page 9: with respect → compared

Line 16, page 10: less than → by less than; remove "approximately"

Line 23, page 10: less than → less by

Line 29, page 10: were → was

Table 3 caption, page 11: an → and

Line 13, page 11: agreements, they primarily departed in the → agreement, they primarily differed for the

Line 16, page 11: departure, different → bias, differing

Line 17, page 11: departure → bias

Table 4 caption, page 11: disamar → Disamar

Figure 1 caption, page 14: available → shown

Figure 2 caption, page 15: A schematic → Schematic

Figure 4, page 17: need x axis label for (a), x and y axis labels for (b), correct x and y

axis labels for (c), y axis label for (d), correct y axis label for (d)

Figure 5 caption, page 18: A histogram → Histogram; plotting → plotted

Figure 6 caption, page 19: A histogram → Histogram

Figure 7 caption, page 20: A MODIS → MODIS; remove "the" before "ocean"; remove "either"; cloud mask, or by a land-sea mask → cloud mask or land-sea mask

Figure 8 caption, page 21: represents the difference → Difference

Figure 9 caption, page 21: Figre (a) directly compares retrieved aerosol layer heights from the two methods. Figure (b) provides a histogram of the difference between these retrieved heights from Disamar and NN. The difference is defined as zaer(Disamar) - zaer(NN). Figure (c) compares these differences with TROPOMI's operational absorbing aerosol index product (x axis). → (a) Retrieved aerosol layer heights from the two methods; (b) Histogram of the difference between retrieved heights from Disamar and NN. The difference is defined as zaer(Disamar) - zaer(NN); (c) Differences compared to TROPOMI's operational absorbing aerosol index product (x axis).

Author's response: Agreed.

Changes to the manuscript: Amended the document as requested by the reviewer.

Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2019-143, 2019.