Reply (in blue) to Referee #3

We thank the referee #3 for the positive comments and for the detailed review of the paper. Our reply is included after the referee comments.

Mateer et al. (1971) first proposed a Lambertian Equivalent Reflectivity (LER) concept in BUV total ozone retrievals to account for combined spectral dependence of surface, aerosols and cloud reflectance [Mateer, et al., 1971]. The concept works well because ~90% ozone is in the stratosphere, above effective reflecting surface. The simple LER concept with some modifications (e.g. extrapolated LER spectral dependence, effective surface pressure) has been successfully used in heritage (TOMS, GOME, SCIAMACHY) and current (GOME-2, OMI, OMPS, S5P/TROPOMI) stratospheric ozone and other trace gases (e.g., volcanic SO2) BUV retrievals. The need for satellite retrievals of tropospheric ozone and other pollution gases (NO2, SO2, HCHO) in partly cloudy scenes, with peak concentrations in or just above the planetary boundary layer, required modification of the simple LER concept, replacing it with the mixed-LER (MLER) concept: mixing two LER surfaces, one at the ground and the other at the effective cloud pressure, e.g., [Ahmad, et al., 2004; Stammes, et al., 2008]. The MLER approach is currently used in operational BUV pollution gas retrievals (e.g., [Levelt et al., 2018] and references therein). The MLER approach requires a-priori “clear-sky” LER estimate, which can be taken either from concurrent satellite measurements (e.g., OMI geometry-dependent GLER product uses higher-resolution atmospherically corrected MODIS BRDF [Vasilkov et al., AMT 2017]) or from prior measurements (e.g., OMI cloud-cleared climatological LER [Kleipool et al., JGR 2008]). The climatological “clear-sky” LER estimation is less accurate, since it disregards the observational geometry- and time-dependence of surface reflectance. The paper by Loyola et al. presents new geometry-dependent (GE-LER) LER implementation, the "Full Physics – inverse Learning Machine (FP_ILM)" algorithm and the multiple day gridded LER product (G3_LER) derived from the present and previous clear-sky scenes observed by S5P/TROPOMI. In previous LER implementations for ozone retrievals, the LER values were derived at non-absorbing wavelengths (e.g., 340nm and 380nm for Nimbus-7 TOMS) and spectrally interpolated to the ozone and SO2 retrieval windows. The important advantage of the new GE-LER retrieval is that it is retrieved in the same spectral fitting window used by ozone retrieval (325-335nm), thus does not require spectral extrapolation. This is the first simultaneous retrieval of both ozone and LER in this spectral window. The G3_LER can be applied to existing S5P aerosol, clouds and trace gas algorithms by replacing climatological clear-sky LER with the new G3_LER product. I recommend publishing the paper with clarifications and technical corrections and releasing the new S5P GE_LER and gridded G3_LER products for community evaluation.

We include now references to Mateer et al. and Ahmad et al. in the Introduction.

General comments

1) The name “full physics” is misleading, because the forward radiative transfer model used for NN training does not include important physical processes, such as , aerosols and inelastic (RRS) scattering;

The goal is to retrieve the surface properties under clear-sky conditions, therefore the RTM simulations don’t consider modelling of aerosols or clouds.

The impact of using RSS in the forward simulation for the GE_LER retrieval in the ozone fitting window is negligible. We add the following in Section 4.1 “The mean difference in GE_LER retrievals based on LIDORT-RSS and VLIDORT is in the range of 5e-5 for SZA<75° and 3.5e-4 for larger SZA”.

2) acknowledge that BRDF effects on trace gas retrievals cannot be modeled exactly using forward RTM with Lambertian surface. Estimate the ozone errors due to Lambertian surface assumption (GE_LER or simple LER) using BRDF supplement available in VLIDORT RTM.

The following sentence is included at the end of Section 4.1 “The BRDF effects on the ozone fitting window are well modelled using the GE_LER approximation, the difference in the total ozone retrieved using VLIDORT and VLIDORT-BRDF simulations is in the order of 0.5 DU or 0.2%”.

3) Provide more details about GE_LER algorithm:
a. Do you assume that GE_LER is wavelength independent within DOAS fitting window?

Correct, we listed this assumption in Section 2.3.

b. Give reference to the machine learning (NN) software and explain selecting optimal NN topology used in the algorithm training.

We use the MATLAB neural network Toolbox. The following explanation is included in Section 4.1 “Different NN topologies were tested using one, two, and three hidden layers”.

c. Clarify whether the RTM with Lambertian surface or with BRDF model was used for training?

As already indicated in Section 4.1, we use the VLIDORT model with Lambertian surface.

d. Explain which cloud masking algorithm was used in creating G3_LER clear-sky daily map

We add the following explanation in Section 4.3 “”we use the S5P OCRA and the VIIRS/SNPP (flying in constellation with S5P) cloud fractions fc for identifying clear-sky measurements.

e. Fig. 1– clarify that “simulated features” are DOAS ozone slant columns and polynomial closure coefficients.

Fig. 1 is the general scheme for the FP_ILM training phase. The particularities for each GE_LER step (e.g. VLIDORT used as forward model, NN used as machine learning, DOAS used as feature extraction) are described in Sections 2.1 to 2.4.

f. Fig. 2 – clarify that “extracted features” are DOAS ozone slant columns and polynomial closure coefficients.

Fig. 2 is the general scheme for the FP_ILM retrieval phase. The “extracted features” used in each case are algorithm dependent, for example for the GE_LER retrieval we use the DOAS results and for the SO2 layer height retrieval we use principal components.

4) Clarify what are effects of UV-absorbing aerosols (dust or smoke) on GE_LER?

Absorbing aerosols can induce GE_LER values lower than the actual surface LER. As already mentioned in Section 4.3, in the future we plan to use the S5P absorbing aerosol index for filtering the affected measurements.

5) Clarify that the neural network is trained on synthetic clear-sky spectra, but applied to the TROPKMI measurements over mixed, partly cloudy scenes (equation 5).

The GE_LER retrieval is applied to all TROPOMI measurements. Equation 5 indicates only how we compute the effective surface height in case of cloud contamination.

6) Compare TROPOMI GE_LER retrievals with the traditional LER retrievals at 340nm, where ozone absorption is negligible. Add TROPOMI simple LER340 map to Figure 10.

In chapter 4 we include a new section describing the comparison with GOME-2 and OMI LER.

7) Publicly release G3_LER data set for community evaluation.

The retrieved GE_LER and the G3_LER used for each single TROPOMI ground pixel will be included in the operational S5P total ozone product. All operational S5P products are open and free available. We will discuss with ESA/EU the possibility of disseminating the G3_LER total ozone daily maps in the same way as the operational S5P products.

Technical comments

Table 2 is not mentioned in the text.
reference added in Section 4.2

P1, 12: with a significant[ly] lower spatial resolution . . .
corrected

13: satellite viewing [geometry] dependencies
added

P2,

1: are mayor [major] error sources – clarify that the surface reflectance has larger influence on boundary layer trace gases retrievals and much less on the mid-and upper-tropospheric constituent retrievals.
corrected and clarification added.

13: significant[ly] lower spatial resolution
corrected

18: (b) the effect of surface reflectance anisotropy [is]
corrected

20: Retrieval of [Lambertian] effective scene albedo has been used in total ozone algorithms from nadir and limb – add pioneering reference: Mateer et al., 1971.
corrected. Reference to Mateer et al. added two sentences before.

22: - add references to heritage TOMS ozone, e.g., Bhartia et al., 1996 McPeters, et al., 1998.
- and OMI ozone references, e.g., McPeters, et al., 2015 or Veefkind, et al., 2006.
added references to Bhartia (TOMS) and McPeters (OMI)

24: from other [higher spatial resolution] satellite sensors
added

28:" needed for computing LER from [and] BRDF may not be fully compatible" – need clarification: In Vasilkov et al., [2017] LER is calculated from the RT model simulated TOA radiance in a standard way, which is fully compatible with OMI cloud and NO2 retrievals. However, MODIS BRDF product may use different RT assumptions.
modified to "needed for computing MODIS BRDF may not be fully compatible"

P3,

16: errors could be large and [multi-dimensional interpolations are] time consuming. .
modified to “the interpolation/extrapolation in this multi-dimensional space are computational expensive, and the interpolation/extrapolation errors could be significant”

21: During the last years we [Recently] we developed an approached called . . .
modified

22: applied for retrieving [ozone] profile shapes . . .
added

P4,

4, . . . the surface properties - clarify what properties? Did you use RTM with Lambertian surface for training or did you use RTM with BRDF model? Specify, which land/ocean BRDF model/dataset was used for training ?
clarification added “Lambertian surface properties”

15 resolution to resolve [absorbing] features
added

16 usually contains [hyperspectral] radiances at a high-dimensional space
added

17 . . .avoiding the effects of the curse of dimensionality ? – clarify
sentence deleted

27 Explain where does the GE_LER information come from (i.e., equation (3))?
at the end of Section 2.1 (same page as equation (3)) it is already indicated that surface properties Ae are the source of the GE_LER

P5,

19 . . . effective scene approximation - add reference ([Mateer et al., 1971, Coldewey-Egbers et al., 2005])
added

21 whereas a [clear-sky] LER is needed
added

22 GE_LER retrieved under clear sky conditions – explain cloud masking algorithm
explanation included

24, Fig 3 . . . based on the [GE_]LER data from previous days – Clarify if the GE-LER map instrument and viewing geometry specific?
The sentence after this already explains that the G3_LER map should include the viewing geometry dependencies. The GE_LER is instrument specific as it is based on L1 measurements of a given instrument.

25-26 (BRDF) effects, as it is based on radiative transfer model simulations using the actual viewing geometry – clarify did you use RTM with Lambertian or BRDF surface? What surface BRDF model/dataset (if any) was used in creating training spectral dataset?
RTM with Lambertian surface is used, see also reply to comment P4/4.

P6,
2 fitting a polynomial of clear-sky LERs averaged as function of ð˙IIJC . – Please, clarify: -
sentence reformulated as follows: “the dependency on the solar zenith angle can be characterized by fitting a polynomial (or exponential) function over clear-sky LERs sorted as function of θ”

should BRDF function also depend on solar and azimuthal angles in addition to satellite view angle?
- Provide examples (add figure) of the clear sky LER(theta) for land and water surfaces.
this explanation is added “solar zenith angel dependencies can be ignored when combining GE_LER data from Sun-synchronous satellites over the same position because the angle of sunlight upon the Earth's surface is consistently maintained. Likewise relative azimuth angle dependencies are negligible in the UV”

17 synthetic UV spectra – clarify that spectra were simulated assuming Lambertian surface, no aerosols and no inelastic RRS effects.
see reply to General comment 1)

19 ozone [profile?] climatology
added

24 Figure 4 shows the optical densities difference – clarify definition of the optical density and the OD difference. Explain why is Figure 4 necessary?
25 ... albedo of 0.05, 0.3, 0.6, and 0.9 [,which] correspond to water,.. – not clear how [ozone?]

optical density is related to the surface albedo?
clarification added “optical densities of the DOAS polynomial in Equation (2)”
Fig. 4 nicely illustrate how the optical densities of the DOAS polynomial change for different conditions

28 higher [longer?] wavelength.
corrected

P7,
1, Fig 4 . . . optical density increases when the viewing zenith angle decreases – please, explain. The ozone optical density is proportional to the slant column ozone amount, which should decrease when the viewing zenith angle decreases. . . . for all cases, the optical density increases along the wavelength region –Explain why is this important?
clarification added “optical densities of the DOAS polynomial

3 . . .is reorganized according to (3) – clarify the meaning of equation (3) an reorganization algorithm
sentence reformulated to “The simulation results from (3) are reorganized by grouping as input the DOAS polynomial coefficients and ozone slant column, the viewing geometry, and surface height”

5 . . . using a NN with a topology of 9-20-8-2-1, - provide reference to the NN software used and how the optimal topology has been selected?
see reply to General comment 3b

10, Fig.5 . . .represents the inverse function [of the synthetic dataset] in a very precise way – this does not guarantee similar accuracy when applied to the real satellite measurements.
we agree

Figure 6(a) title and color bar show “E_LER” – change to GE_LER
Figure 6(b) – explain cloud fraction stripes over Antarctica?
The cloud stripes over Antarctica are an artefact of the S5P v1 cloud retrieval algorithm that is based on OMI cloud-free composites and scan angle corrections. The S5P v2 of the cloud algorithm solves this issue.

20 In the case of clear-sky (ð˙IS ¸Sð ´ ˙IS´ R˘ ≤ 0.05) the GE_LER represents the surface albedo – clarify if GE_LER represents hemispherical albedo or directional BRF ?
clarification added “hemispherical surface albedo”

25 the TROPOMI clear-sky GE_LER and OMI LER climatology – Add comparison with the

OMI/TROPOMI simple LER at 340nm in Table 2.
26 summarized in Figure 7. - in Table 2?
In chapter 4 we include a new section describing the comparison with GOME-2 and OMI LER.

P8,
1 . . . aggregating normalized [GE_]LER from the couple of days. – these retrievals are obtained under different viewing geometries. - Couple of days may not be sufficient to obtain cloud-free observations over certain locations. - Explain how GE_LER are normalized and what viewing geometry does the aggregated G3_LER map correspond to?
sentence reformulated.
explanation added "normalized to the central detector pixel (nadir)"

10 . . . averaged as function of the viewing zenith angle. – BRDF depends also on solar zenith and relative solar azimuthal angles. Why is this dependence ignored?
see reply to P6, 2

Fig. 8 Why is sun-glint is not visible for the water surface GE_LER and "hot spot" is not visible for the land GE_LER ?
What would GE_LER look like for a cloud-free sun-glint region?
as already explained in the second sentence of 4.3, measurements affected by sun-glint are not used in the G3_LER

Fig. 9(a) – what viewing geometry does the aggregated G3_LER map corresponds to? Reduce upper scale or use logarithmic scale to better show LER variability for snow-free regions.
nadir, see also reply to P8, 1

Clarify wavelength for the OMI climatological LER.
"(335 nm)" added

Fig 9 caption: the ma[j]or differences
corrected

Fig 10. Add comparison with the TROPOMI simple LER map at 340nm (negligible ozone absorption)
TROPOMI LER at 340 nm is not available

25 associated to [with] the coarse resolution

26 most important[ly]
corrected

p9,
5 what is even wors[e]
corrected

11 reduced from -2.53 ± 2.46% using OMI LER to 0.78 ± 3.49% using TROPOMI G3_LER - why did the standard deviation increase?
it is a typo, the correct value should be 2.49

P12,
11 Loyola, D., et al.: The near-real-time total ozone retrieval algorithm from TROPOMI onboard Sentinel-5 Precursor, Atmos.Meas. Tech. Discuss., in preparation, 2019. –provide complete citation
done