

We thank referee#1 and referee#2 for their questions and suggestions. Here, we provide a description of our answers, corrections and modifications to the manuscript. Apart from trivia and minor changes, corrected as well, the new text added in the manuscript is reported in red.

Referee#1

The authors should explain how the following changes from GOME-2 to UVNS would affect the ozone data, e.g. the increase of retrieval throughput of near surface ozone due to the lower frequency of cloud contamination within field of view of satellite observation. “UVNS will have a higher signal-to-noise ratio (SNR) than GOME-2, a much finer horizontal resolution but a factor 2 coarser spectral resolution.”

We agree that it is useful to explain the gain expected by each instrumental improvement. We add the following text:

A finer resolution will increase the number of surface ozone retrievals, decreasing the number of cloudy pixels with CLF > 0.3. A finer (coarser) spectral resolution will increase (decrease) the retrieval vertical sensitivity to ozone. A higher SNR will improve the quality of the retrieval, leading to a higher vertical sensitivity and a smaller error. For better exploiting IASI-NG+UVNS, we have designed a constrain matrix accounting for the capability of the new sensors. As done by **Cuesta et al. (2013)**, we have adjusted the constraints to keep a similar retrieval error to IASI+GOME-2 and enhance the sensitivity between the surface and 3 km.

The authors should add the actual spectral resolution used in the simulation/retrievals in the list of differences in nominal specifications since the spectral resolution is one of key parameters that determine the sensitivity of observation. The parameter of spectral sampling alone is not enough for this purpose.

The spectral resolution is already present in Table 2. However, we agree that it should be placed next to the spectral sampling to be clearly visible. We re-ordered the table.

Please add in maps of a priori ozone field and estimated uncertainty of near surface ozone to help in showing the performance of joint IASI/GOME2 retrievals catching the spatial distribution of near surface ozone.

We do agree with referee#1 that maps of a-priori values and surface ozone estimated uncertainties would be useful to show the performances of IASI-GOME2 retrieval algorithm, with respect to single band retrieval methods. However, the «philosophy» of this article has been (from the

beginning) to show the improvement of using IASI-NG+UVNS method with respect to IASI+GOME-2 and not to « validate » and corroborate the robustness of IASI+GOME-2 retrieval algorithm and the gain with respect to single-band methods. Also because of the large quantity of images already present in the text (48), if referee and editor agree, we would like to continue to be coherent with this «philosophy» and leave the whole detailed analysis of IASI+GOME-2 product quality to the original paper by Cuesta et al. (2013).

P 1 line 21: lowermost troposphere > lower most troposphere

Changed

P 1 line 28: to observer > to observe

Changed

P 2 line 42: Should “the surface-2km” change to “the surface-3km” since elsewhere in the manuscript always refer to “the surface-3km”?

In this case, we do refer to surface-2km ozone.

P 4 line 134: “(ozone concentration, skin temperature, temperature profile)” > “(ozone concentration and temperature profiles, skin temperature)”

Changed

P 7 line 224: “AKV” > “AVK”

Changed.

P 9 line 279 to 282: “The positive difference of 0.74 DU (7%) that remains between PR*realAVK and real IASI+GOME-2 might be linked to systematic explained underestimation of cloud fraction. overestimation of ozone production in MOCAGE model, coming from the systematic underestimation of cloud fraction.” The sentence is not clear and there is an extra “.” in front of overestimation. Please consider to revise it, e.g., “The positive difference of 0.74 DU (7%) that remains between PR*realAVK and real IASI+GOME-2 might be due to systematic underestimation of cloud fraction since the systematic underestimation of cloud fraction could lead to overestimation of ozone production in MOCAGE model, coming from the systematic underestimation of cloud fraction (reference therein).”. Please add the reference(s) on the relationship between cloud fraction and ozone production, if there is. Or,

perform a brief sensitivity study on the impacts of cloud fraction on ozone production.

We erase the sentence. We agree with referee#2 that there are many factor that can explain such a small positive difference. It is useless just to mention cloud fraction. However, it is a well-established knowledge that an increase solar radiation increases the photolysis and enhances the production of tropospheric ozone (e.g, Seinfeld and Pandis, Atmospheric Physics and Chemistry, 2006).

P 10 line 294: “smoothed by real AVK” > “smoothed by real AVK (blue)”

Changed.

P 20 Figure 9 and Page 21 Figure 10: Besides showing the color bar with unit of mol/μm³, authors should consider add color bar of ppbv for the convenience of many readers in air quality community.

Referee #2 also suggested this change. However, we already considered this change but the result is not convenient. Using ppbv, the strong vertical gradient of atmospheric density does not allow to see small variations in ozone concentration. It is necessary to multiply ppm * air_density * 10⁻⁶ (i.e., molecules/cm³) to appreciate small vertical gradient of ozone.

P 21 line 541: “9E” > “9°E”

Changed.

Referee#2

The abstract seems to be too long with a long introduction. Please make it concise and only highlight the important points.

We did not made major text changes but we erased several sentences in the first part of the abstract and all the references. Now the abstract is much shorter and concise.

The abstract typically should not have citations.

Changed.

Also, please define acronyms at their first occurrences such as IASI, IASI-NG, GOME-2, EPS-NG, UVNS, a.s.l., in the abstract, and also separately at their first occurrences in the text.

Changed.

L40, L43 and in the text, suggest adding “for signal” after “degree of freedom” as it could be used for signal or for noise.

We added «for signal » the first time we speak about degrees freedom.

L51, it seems to me that ADEOS is not currently working.

Changed. ADEOS erased.

L53, this also applies to global CTMs

Changed.

suggest adding “with adequate vertical sensitivity” after “observed” as UV retrievals can be sensitive to ozone down to below 2-3 km although with reduced sensitivity and retrieved at a much broader altitude range as shown in Liu et al. (2010)

Added.

8. L65, add “to enhance sensitivity to LMT ozone” after “spectral domains”

Added.

I would not call this “for the first time” as the study of Fu et al. (2013), published almost at the same time (slightly earlier), also showed similar capabilities (e.g., surface-700 hPa ozone)

Changed. We erased «for the first time». We explained better in what main differences consists :

Due to the limited spatial coverage of TES (no across-track scanning is performed), this method was analysed in a profile-to-profile basis (Fu et al., 2013). Cuesta et al. (2013) developed a multispectral synergism of IASI (for TIR) and GOME-2 (for UV) spectra capable of observing from space the daily distribution of ozone plumes located below 3 km of altitude, defined here as the lowermost troposphere (LMT). This last multispectral approach (referred to as IASI+GOME-2 and used in the following of this paper) shows a particularly good accuracy (low mean bias near 1% and precision of 16%) and the capacity to observe the horizontal distribution of LMT ozone provided the scanning capacities of both IASI and GOME-2. IASI+GOME-2 allows the observation of LMT ozone due to an altitude of maximum sensitivity for the LMT peaking exceptionally low, on average at 2.2 km height over land (about 800 m below single-band methods), enhancing the degree of freedom (for signal) in the LMT by about 40% with respect to single-band retrievals.

suggest rephrasing to “For practical consideration of computation, OSSEs

typically approximate the pseudo-observations, : : :”

Changed.

The vertical resolution is not a property of radiation transfer models, but the radiative transfer calculations. I suggest rephrasing it to “All the profiles are sampled to 1-km layers in the radiative transfer calculations”

Changed

in Table 1, what is the SNR between 306-325 nm?

The SNR is not reported in the Table because this band window is simply not used in the retrieval algorithm (interface between channel 1 and channel 2, large uncertainties in slit functions).

the sentence “At given altitude (defined by the matrix column), each row shows ” is confusing

and should be rephrased, as both column and row refer to a given altitude and the sentence reads like, “For the given column, each row

Changed

In section 4, it would be very useful to mention other retrieval variables (some of them are interfering) in addition to ozone even it is mentioned in Cuesta et al. (2013).

We added:

The ozone profile (volume mixing ratio) is obtained by inverting the measurement vector (built up by merging together IASI TIR atmospheric radiances with GOME-2 UV earth reflectances) and jointly adjusting the water vapour profiles, offsets for each TIR micro-window, wavelength shifts for the UV radiance and irradiance spectra, multiplicative factors of the ring spectrum, surface albedo multiplicative factors and a factor for cloud fraction used in the UV forward calculations.

the sentence is not accurate as the cloud can enhance ozone sensitivity above clouds, suggest rephrasing to “IASI+GOME-2 retrieval sensitivity to LMT ozone is significantly reduced when CLF > 0.3”

Changed.

I don’t see the need to understand the small mean IASI+GOME-2 and MOCAGE differences as one is based on retrievals (not real data), and the other is based on assimilation of different ozone products, and too many important factors in retrievals, model simulations/assimilations can cause their differences.

We agree. We erased the following sentence: “The positive difference of 0.74 DU (7%) that remains between PR*realAVK and real IASI+GOME-2 might be linked to systematic explained underestimation of cloud fraction. overestimation of ozone production in MOCAGE model, coming from the systematic underestimation of cloud fraction.”

P 17. L363, it is not clear about what you mean by “with a similar gap of 0.8 . . .”

We erased this last part of the sentence.

Table 1 & 2: captions typically are put above tables. Please check the requirements. Table 2

caption, it is good to describe what is R, σ -bias, and RMS in a few extra words. The gains for different columns are likely calculated inconsistently, please consistently use the IASI-GOME-2 as the reference point. The gain for the last one should be $(1.55-1.77)/1.77=-12.4\%$

Changed with corrected values. We made a mistake comparing data with the results of a specific day instead of averages values reported in Table. We apologise for this error and we really thank referee#2 for its attention and care in reviewing the article.

In the 3rd row of Figure 5, there are no significant differences in the linear regression slope between black and red. Typically, you want to show how well your pseudo observations can capture the pseudo-reality or pseudo-reality with AVK (typically in validation). I think that it is better to show the PO (y-axis) vs (PR or PR*AVK). The slope for PO vs PR*AVK should be much closer to 1. This is also the case for Figure 12. Also in the 4th row, the standard deviation between PO and PO*AVK is much larger for the IASI-NG+UVNS (1.47 DU) than that of IASI+GOME2 (0.74), suggesting that the retrieval precision is worse for IASI-NG+UVNS. It is good to mention this and give an explanation.

Changed. We agree that this information is more interesting and we changed the images as suggested by the referee. We report here the new figures in.

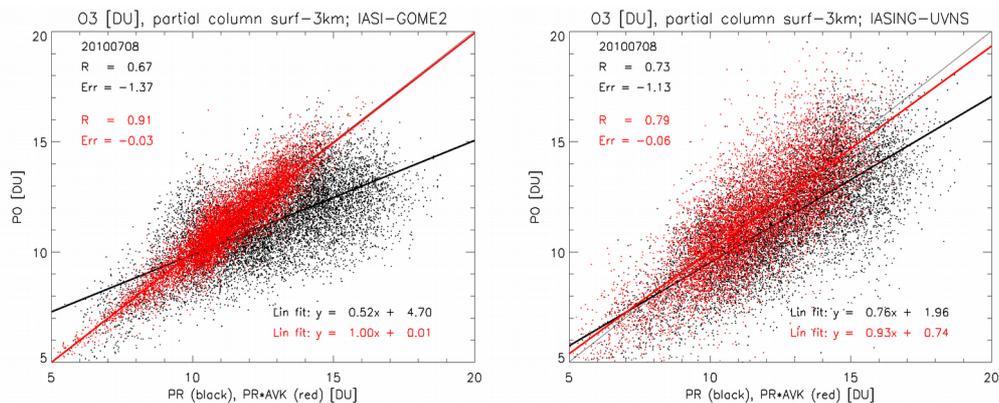


Figure 5

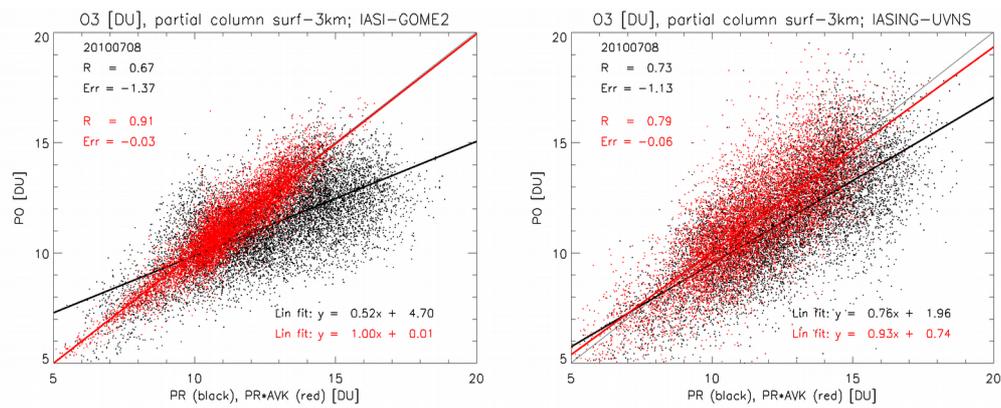


Figure 12

We also added new text

In chapter 3:

The constraint of the retrieval algorithm allows to define which parameter, between vertical sensitivity and retrieval error, is more improved. For better exploiting IASI-NG+UVNS, we have designed a constrain matrix accounting for the capability of the new sensors. As done by **Cuesta et al. (2013)**, we have adjusted the constraints to keep a similar retrieval error to IASI+GOME-2 and enhance the sensitivity between the surface and 3 km.

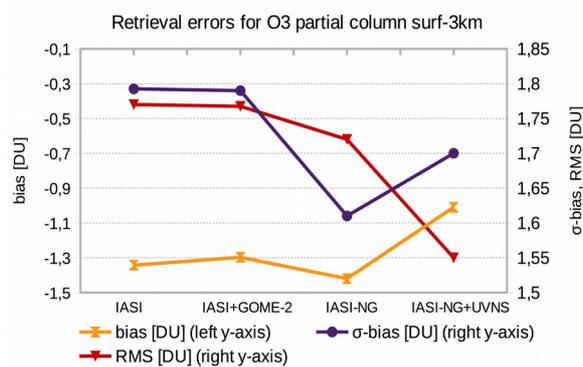
In Chapter 6.2 :

On the other hand, the correlation coefficient between PO and PR*AVK (red) decreases from 0.91 to 0.79 (-13%), as well as the slope of the linear fit slope (from 1 to 0.85, -15%), sing of a larger measurement error for IASI-NG+UVNS than for IASI+GOME-2 (quantified afterwards).

and

The total retrieval error, quantified by the standard deviation of the mean bias, does not vary significantly (from 1.76 to 1.72, -2%) because of the net balance between the decreasing smoothing error (from 1.59 to 1.28, -19%) and the increasing measurements error (from 0.74 to 1.47, +92%). At the same time, the root mean square (RMS) decreases from 1.78 to 1.63 (-8%). These results indicate an overall higher quality of the retrieval (smaller RMS) when using EPS-SG sensor instead of MetOp instrumentation, with a global gain in retrieval accuracy (smaller bias) and an almost constant retrieval precision (slightly smaller σ -bias).

and the RMS has been added to figure 6.



and we also added

The RMS of the PO-PR difference distribution, which is an estimate of the overall retrieval quality combining together accuracy and precision, decreases monotonically from IASI to IASI-NG+UVNS. For what concerns the bias and the σ -bias, results are consistent with the design of the constrain matrix of IASI-NG+UVNS which is less constrained than in IASI, IASI+GOME-2 and IASI-NG algorithms in order to increase the vertical sensitivity to near-surface ozone. This particular choice leads to a higher accuracy and a smaller smoothing error (lower bias) for IASI-NG+UVNS than all other retrieval methods, but also to a larger measurement error that enhances the total retrieval error (σ -bias) of IASI-NG+UVNS with respect to IASI-NG.

In : Chapter 7 (Conclusions)

The IASI-NG+UVNS retrieval algorithm parametrization has been optimized to increase at most the sensitivity in the lowest layers of the atmosphere (as close as possible to human biosphere), rather than decreasing the total retrieval error. Hence, the major gain of using the multispectral synergism of EPS-SG sensors with our retrieval approach concerns DOF-3km and Hmax-3km.

21. Figure 9, I would like to suggest the same thing as the first reviewer, i.e., plotting the data in more conventional units of ppbv.

Referee #1 also suggested this change. However, we already considered this change but the result is not convenient. Using ppbv, the strong vertical gradient of atmospheric density does not allow to see small variations in ozone concentration. It is necessary to multiply ppm * air_density * 10⁻⁶ (i.e., molecules/cm³) to appreciate small vertical gradient of ozone.

The synthetic retrievals show the potential of synergism of combining IASI-NG and GOME-2 for enhancing LMT retrievals. However, real retrievals might not be able to realize all the potentials due to mismatch of IASI-NG and UVNS and the retrieval challenges in TIR or in UV or the combination. Take the UV for example, the signal to noise ratio is assumed to be

1000. In practice, it might be difficult to fit the data well enough to this level. Also there can be strong correlation between surface albedo parameters and ozone in the lower troposphere, reducing the potential such enhancement to LMT ozone retrievals. It might be useful to discuss/mention some of the implementation challenges or future work in the conclusion.

We agree. We added in the conclusion:

It is worth noting that additional challenge will be encountered for real retrievals using high SNR spectra from IASI-NG and UVNS. Indeed, as noise will be lower for such measurements, new sources of errors will be significant (i.e., surface properties accuracy, trace gasses variability). Such additional errors are not considered here and might degrade the capability of the retrieval. Results presented here are then an upper limit of the capability expected for IASI-NG+UVNS multispectral synergism to probe ozone pollution.

Potential of multispectral synergism for observing ozone pollution by combining IASI-NG and UVNS measurements from EPS-SG satellite

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ABSTRACT

Present and future satellite observations offer a great potential for monitoring air quality on daily and global basis. However, measurements from currently in orbit satellites do not allow using a single sensor to probe accurately surface concentrations of gaseous pollutants such as tropospheric ozone. Combining the information of IASI (Infrared Atmospheric Sounding Interferometer) and GOME-2 (Global Ozone Monitoring Experiment-2) respectively in the TIR and UV spectra, a recent multispectral method (referred to as IASI+GOME-2) has shown enhanced sensitivity for probing ozone in the lowermost troposphere (LMT, below 3 km of altitude) with maximum sensitivity down to 2.20 km a.s.l. over land, while sensitivity for IASI or GOME-2 alone only peaks at 3 to 4 km at lowest.

In this work we develop a pseudo-observation simulator and evaluate the potential of future EPS-SG (EUMETSAT Polar System Second Generation) satellite observations, from new-generation sensors IASI-NG (Infrared Atmospheric Sounding Interferometer New Generation) and UVNS (Ultraviolet Visible Near-infrared Shortwave-infrared), to observe near-surface O₃ through IASI-NG+UVNS multispectral method. The pseudo-real state of atmosphere is provided by the MOCAGE (Modèle de Chimie Atmosphérique à Grande Échelle) chemical transport model. We perform full and accurate forward and inverse radiative transfer calculations for a period of 4 days (8-11 July 2010) over Europe.

In the LMT, there is a remarkable agreement in the geographical distribution of O₃ partial columns, calculated between the surface and 3 km of altitude, between IASI-NG+UVNS pseudo-observations and the corresponding MOCAGE pseudo-reality. With respect to synthetic IASI+GOME-2 products, IASI-NG+UVNS shows a higher correlation between pseudo-observations and pseudo-reality, enhanced by about 12%. The bias on high ozone retrieval is reduced and the average accuracy increases by 22%. The sensitivity to LMT ozone is enhanced on average with 159% (from 0.29 to 0.75, over land) and 214% (from

35 0.21 to 0.66, over ocean) higher degree of freedom for signal. The mean height of maximum sensitivity for the LMT peaks at 1.43 km over land and 2.02 km over ocean, respectively 1.03 km and 1.30 km below that of IASI+GOME-2. IASI-NG+UVNS shows also good retrieval skill in the surface-2km altitude range. Unique of its kind for retrieving ozone layers of 2-3 km thickness, in the first 2-3 km of the atmosphere, IASI-NG+UVNS is expected to largely enhance the capacity to observe ozone pollution from space.

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1 Introduction

The retrieval of tropospheric ozone is a major issue for air quality studies. Ground-level ozone is a priority air pollutant, causing approximately 22,000 excess deaths per year in Europe (**Amann et al., 2005**). Current (e.g., Meteorological Operational Satellites, MetOp; Earth Observing System Aura, EOS-Aura) and future (e.g., EUMETSAT Polar System Second Generation, EPS-SG; Meteosat Third Generation Sounder, MTG-S) satellite observation systems offer a great potential for monitoring air quality on daily and global basis. Because of their global coverage every day, they can be used in synergy with global or regional Chemical Transport Models (CTMs) for full data assimilation (e.g., **Coman et al., 2012**) or inter-validation (e.g., **Zyryanov et al., 2012**). Recent spaceborne instruments as the Infrared Atmospheric Sounding Interferometer IASI (**Clerbaux et al., 2009**) and the Global Ozone Monitoring Experiment-2 GOME-2 (**EUMETSAT, 2006**), both onboard MetOp satellites, offer a daily global coverage appropriate for monitoring pollution. Their ground resolutions are relatively fine, with four 12 km-diameter pixels spaced by 25 km (at nadir) for IASI and 80×40 km² ground pixels for GOME-2.

Both TIR and UV observations are able to provide vertical information on ozone concentration. UV sounders were traditionally used for the stratosphere but recently also for the troposphere (e.g. **Liu et al., 2010**) and TIR sensors are particularly sensitive to tropospheric ozone, down to the lower troposphere (below 6 km of altitude, **Eremenko et al., 2008**). However, it has been shown that using spaceborne observations from one spectral domain (either TIR or UV), only ozone down to 3-4 km of altitude at lowest may be observed with adequate vertical sensitivity (**Foret et al., 2014**). Recent studies combine the information on ozone distribution from radiance measurements of different spectral domains to enhance sensitivity in the LMT. Numerical studies (**Landgraf and Hasekamp, 2007; Worden et al., 2007**) showed a significant improvement in the sensitivity to retrieve ozone in the lowest 5 km of the troposphere combining TIR and UV measurements respectively from TES (Tropospheric Emission Spectrometer) and OMI (Ozone Monitoring Instrument) sounders (both onboard Aura satellite).

65 More recently, new retrieval approaches have shown the capability to derive ozone profiles from the multispectral synergism from real TIR and UV satellite measurements. **Fu et al. (2013)** combined measurements from TES (for TIR) and OMI (for UV) sensors and founded a clear improvement in retrieval sensitivity and vertical resolution in the troposphere as well as a sensitivity and accuracy enhancement below 700 hPa, compared with either instrument alone. **Due to the limited spatial coverage of TES (no across-track scanning is performed), this method was analysed in a profile-to-profile basis (Fu et al., 2013). Cuesta et al. (2013) developed a multispectral synergism of IASI (for TIR) and GOME-2 (for UV) spectra capable of**

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observing from space the daily distribution of ozone plumes located below 3 km of altitude, defined here as the lowermost troposphere (LMT). This last multispectral approach (referred to as IASI+GOME-2 and used in the following of this paper) shows a particularly good accuracy (low mean bias near 1% and precision of 16%) and the capacity to observe the horizontal distribution of LMT ozone provided the scanning capacities of both IASI and GOME-2. IASI+GOME-2 allows the observation of LMT ozone due to an altitude of maximum sensitivity for the LMT peaking exceptionally low, on average at 2.2 km height over land (about 800 m below single-band methods), enhancing the degree of freedom (for signal) in the LMT by about 40% with respect to single-band retrievals. IASI+GOME-2 uses two radiative transfer codes, KOPRA (Karlsruhe Optimized and Precise Radiative transfer Algorithm) and VLIDORT (Vector Linearised Discrete Ordinate Radiative Transfer). The inversion algorithm is integrated in the inversion module KOPRAfit. It uses a Tikhonov-Phillips-type altitude dependent regularisation that optimizes sensitivity to LMT (Eremenko et al., 2008), maximizing the degree of freedom (DOF) of signal and minimizing the total retrieval error simultaneously.

Incoming satellite missions are expected to carry new-generation instrumentation capable to provide more accurate observations of tropospheric composition closer to the surface. This is the case of IASI-NG (Infrared Atmospheric Sounding Interferometer New Generation) and UVNS (Ultraviolet Visible Near-infrared Shortwave-infrared) spectrometers both onboard EPS-SG satellite which is expected to be launched in 2022 on a polar-orbit, similar to MetOp. UVNS instrument is part of the ESA mission Sentinel-5 payload, dedicated to monitoring the composition of the atmosphere for Copernicus Atmosphere Services. The advent of these new-generation sensors may allow significant advances in LMT ozone sensing and air quality monitoring. This enhancement needs to be accurately quantified in order to prepare air quality monitoring systems for these future satellite products.

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2 Purpose and strategy

The objective of this work is to provide a quantitative assessment of the potential of upcoming new-generation space-based observing systems for monitoring ozone pollution. In particular, we investigate the performance of the multispectral synergism of IASI-NG (for TIR emitted spectra) and UVNS (for UV backscattered radiances) measurements. IASI-NG will have half of IASI radiometric noise and a factor 2 finer spectral resolution (see Table 1). UVNS will have a higher signal-to-noise ratio (SNR) than GOME-2, a much finer horizontal resolution but a factor 2 coarser spectral resolution. To estimate the performances and errors associated to IASI-NG+UVNS, we adapt the existing IASI+GOME-2 retrieval approach to the technical specifications of IASI-NG and UVNS (Table 1). Hereafter, this method will be referred to as IASI-NG+UVNS.

We set up a Pseudo-Observation Simulator (POS) which is part of an Observing System Simulation Experiment (OSSE). OSSEs are specific type of sensitivity analysis used to quantify the expected added value of an Observing System (OS). They have been largely used to analyse the gain of future satellite

missions on trace gases monitoring (**Edwards et al., 2009; Claeysman et al., 2011; Zoogman et al., 2011**)
110 and are generally composed of three elements: a nature run, a pseudo-observation simulator and an
assimilation run. The nature run defines the pseudo-real state of the atmosphere for the experiment
(**Masutani et al., 2010**). The pseudo-observation simulator generates the pseudo-retrievals. It calculates and
inverts the spectra as it would be done by the observing system, simulating OS performances and errors. The
assimilation run consists in the assimilation of pseudo-retrievals into a new model simulation, different and
115 independent from the nature run.

In this work, we only focus on the first two steps of a typical OSSE: the nature run and the simulator of
synthetic retrievals, while the assimilation run is left to a further and future research effort. Pseudo-reality is
generated by the chemical transport model MOCAGE (MOdèle de Chimie Atmosphérique à Grande Échelle)
that simulates physical and chemical processes of atmospheric gasses and aerosol including clouds (e.g.,
120 **Josse et al. 2004, Marécal et al. 2015**). For practical consideration of computation, OSSEs typically
approximate the pseudo-observations by means of a predefined parametrization of the averaging kernels
(AVK) that describe the retrieval method sensitivity to true vertical profiles of atmospheric species. If this
procedure allows to avoid full radiative transfer calculations and costly computational time, approximated
averaging kernels with no (or limited) scene-dependence may fail to replicate the variability of the full
125 radiative transfer calculations (**Sellitto et al., 2013b**); complex scene-dependent parametrizations of AVK
(**Worden et al., 2013**) may represent a more useful cost-benefits compromise in case of
multispectral/multi-instrument observing systems. In order to avoid these approximations, we perform full
and accurate forward and inverse radiative transfer calculations, but for a limited time period of 4 days.

We pay particular attention to set-up and run the simulation experiment with a high degree of reliability.
130 Indeed, systematic biases in the key parameters of the model control sensitivity and lead to unrealistic
performances of the satellite product. This is particularly true for parameters such as cloud fraction, surface
temperature and temperature profiles. The consistency of pseudo-reality and POS with respect to real data
and existing sensor products is analysed and validated in terms of absolute magnitude and spatial variability
of a number of atmospheric variables (ozone concentration and temperature profiles, skin temperature) and
135 diagnostic parameters (degree of freedom and altitude of maximum sensitivity of the retrieval algorithm).

In the following paragraphs, we present the methodology used to set up the simulation experiment: the nature
run, the forward radiative transfer calculations and retrieval scheme of the OS simulator. Then, we carry out
a statistical analysis of MOCAGE pseudo-reality with respect to real IASI+GOME-2 measurements and
quantify retrieval errors and sensitivity for IASI+GOME-2 and IASI-NG+UVNS. Finally, we compare
140 pseudo-observations of surface-3 km ozone partial columns of the two observing systems.

3 Nature run and pseudo-observation simulator

The pseudo-reality is defined by the MOCAGE model (run at CERFACS laboratory), that provides vertical
145 profiles of atmospheric state and composition variables on hourly basis. It uses 47 sigma-pressure hybrid

levels up to 5 hPa (approximately 35 km of altitude) with a vertical resolution that increases from 150 m (lower troposphere) to approximately 1 km (stratosphere) and a horizontal resolution of 0.2×0.2 degrees. The same model configuration that provides operational air quality forecasts over Europe (**Marécal et al., 2015**) has been used for this study. We simulate LMT ozone pollution events over Europe, from 8 to 11 July 2010.

150 Real ozone data, from surface network stations (AIRBASE), the Laboratoire d'Aérologie (LA) IASI product (**Barret et al. 2011, Dufour et al., 2005**) and MLS (Microwave Limb Sounder) V4.2 retrievals have been assimilated into MOCAGE simulation to improve the accuracy of the modelled ozone fields at the surface, in the free troposphere and in the stratosphere. The assimilation is performed hourly using a 3D-Var algorithm, described in **Jamouillé et al. (2012)**.

155 To simulate the multispectral retrievals from IASI+GOME-2, we select the two model grid points that are closest to IASI and GOME-2 ground pixels respectively. For each point, KOPRA (for TIR) and VLIDORT (for UV) radiative transfer codes calculate the spectra, as observed by the satellite sensors, issued from radiation emitted, scattered (only UV) and absorbed by the surface and the atmosphere between 0 and 60 km of altitude. All the profiles are sampled to 1-km layers in the radiative transfer calculations. As the

160 MOCAGE model top is set at 35 km of altitude, we complete the atmospheric vertical information between 30 and 50 km with data from a global MOCAGE simulation, run at coarser resolution and with model top at 0.1 hPa (**Emili et al., 2014**), and with climatological profiles above 50 km.

Radiometric random noise for IASI and GOME-2 is added to the raw spectra before their ingestion into the retrieval algorithm. For TIR, the nominal noise standard deviation is taken from literature as 20 nW/(

165 $\text{cm}^2\text{cm}^{-1}\text{sr}$) (**Eremenko et al., 2008**). Therefore, we added a noise of 13 nW/($\text{cm}^2\text{cm}^{-1}\text{sr}$) roughly accounting the reduction of noise due to apodization. For UV, noise is estimated for each wavelength using Muller matrix radiance response elements (**Nowlan et al., 2011; Cai et al., 2012**). The signal-to-noise ratio for GOME-2 is equal to 32, for wavelengths between 290 and 306 nm, and equal to 350 between 325 and 340 nm. Spectra are then ingested into the IASI+GOME-2 retrieval algorithm, that assumes no error in

170 co-localization of TIR and UV measurements: each IASI spectrum (12 km-diameter pixel) is matched with the co-located GOME-2 spectrum ($80 \times 40 \text{ km}^2$) within a distance of 1 degree, without any averaging. IASI+GOME-2 retrievals are calculated at the IASI ground resolution and processed independently for each IASI pixel.

Partial cloud cover and aerosols are not explicitly modelled in KOPRA, but their effects in the IASI spectra

175 are partially compensated by offsets for each TIR micro-window (**Eremenko et al., 2008; Dufour et al., 2010**). In the UV spectra calculations, pixels with partial cloud cover are treated as a mixture of clear sky and cloudy scenes according to the independent pixel approximation (**e.g., Cai et al., 2012**). For more details on IASI+GOME-2 multispectral method refer to **Cuesta et al. (2013)**

The IASI-NG+UVNS retrieval method uses the same procedure as IASI+GOME-2, accounting for some

180 differences in the specifications of the new instruments with respect to the existing ones that are summarized in Table 1 (for more information, visit <https://directory.eoportal.org/web/eoportal/satellite-missions>). Note

that for UVNS, only the UV-2 spectral channel is considered as the pixel resolution of the UV-1 is much coarser.

185 UVNS will have a higher SNR than GOME-2 but only half of its spectral resolution. IASI-NG noise and spectral resolution will be approximately the half and a factor 2 finer than those of IASI, respectively. While IASI-NG will have the same spatial resolution as IASI and hence the same footprint (as MetOp and EPS-SG will fly on a similar polar orbit), UVNS will have a spatial resolution of 7.5 km which is much higher than that of GOME-2. **A finer resolution will increase the number of pixels with ozone retrievals, decreasing the number of cloudy pixels with CLF > 0.3. A finer (coarser) spectral resolution will increase (decrease) the**

190 **retrieval vertical sensitivity to ozone. A higher SNR would improve the quality of the retrieval, leading to a higher vertical sensitivity and a smaller error. For better exploiting IASI-NG+UVNS, we have designed a constrain matrix accounting for the capability of the new sensors. As done by Cuesta et al. (2013), we have adjusted the constraints to keep a similar retrieval error to IASI+GOME-2 and enhance the sensitivity between the surface and 3 km of altitude.**

195 To simulate real IASI-NG+UVNS retrievals, we use the closest UVNS measurement with respect to IASI-NG pixel centre.

	IASI (MetOp-B)	IASI-NG (EPS-SG)	GOME-2 (MetOp-B)	UVNS (EPS-SG) UV-2 channel
Radiometric noise	20 nW/(cm ² cm ⁻¹ sr)	10 nW/(cm ² cm ⁻¹ sr)	-	-
Spectral resolution	0.50 cm ⁻¹	0.25 cm ⁻¹	0.22-0.28 nm (λ=290-306 nm) 0.24-0.30 nm (λ=325-340 nm)	0.5 nm (λ=300-370 nm)
Spectral sampling	0.25 cm ⁻¹	0.125 cm ⁻¹	0.12 nm	0.15 nm
SNR	-	-	32 (λ=290-306 nm) 350 (λ=325-340 nm)	1000 (λ=300-370 nm)
Spatial resolution	12 km-diameter pixel spaced by 25 km at nadir	12 km-diameter pixel spaced by 25 km at nadir	80×40 km ²	7.5×7.5 km ²

200 Table 1. Differences in nominal specifications of IASI-NG and UVNS (EPS-SG) with respect to IASI and GOME-2 (MetOp-B). For UVNS, only the UV-2 spectral channel is considered.

4 Inversion algorithm and ozone retrieval

205 As previously mentioned, the inversion algorithm of IASI+GOME-2 is an altitude dependent Tikhonov-Phillips regularization method for satellite nadir measurements (Cuesta et al., 2013). It is

integrated in the KOPRAfit module and optimized for lowermost tropospheric ozone observations. The constrain matrix and parameters are optimized to maximize the degree of freedom and minimize the error in the LMT, retaining a sufficient accuracy in the upper troposphere and in the stratosphere (Cuesta et al., 2013). Three different ozone a priori profiles, derived from climatological values of McPeters et al. (2007), are selected depending on the pseudo-real tropopause height (TH). We use a mid-latitude a priori (30°-60° N) for TH between 10 and 14 km, a tropical a priori (20°-30° N) for higher TH and a polar (60°-90° N) for TH lower than 10 km. The ozone profile (volume mixing ratio) is obtained by inverting the measurement vector (built up by merging together IASI TIR atmospheric radiances with GOME-2 UV earth reflectances) and jointly adjusting the water vapour profiles, offsets for each TIR micro-window, wavelength shifts for the UV radiance and irradiance spectra, multiplicative factors of the ring spectrum, surface albedo multiplicative factors and a factor for cloud fraction used in the UV forward calculations.

We provide here a quantitative tool to analyse and quantify the error budget associated to each algorithm. If the inversion occurs in an incrementally linear regime, we can consider that the *total error* of a constrained least square fit method is separated into three components (Rodgers, 2000): 1) a *measurement error*, which is random and due to instrumental limitations; 2) a *smoothing error*, which is due the specific retrieval techniques and to the limited sensitivity of the radiance measurements to the vertical distribution of the considered gas; 3) a *systematic error*.

The KOPRAfit module provides the averaging kernel (AVK) matrix of the inversion, describing the vertical sensitivity of retrievals to true profiles. For a given column, each row shows the fractional height-resolved part of information for the retrieval that comes from the observed spectrum, while the remaining fraction comes from the a priori. The peak value of each AVK column indicates the height of maximum sensitivity to true profiles for the selected altitude. If we integrate the AVK over the rows (i.e., over the different altitudes), we can deduce the height of maximum sensitivity (Hmax) of the retrieval. In the following, we will be interested in the altitude of maximum sensitivity of LMT ozone retrievals, between the surface and 3 km of altitude (Hmax-3km). According to Rodgers (2000), the trace of AVK matrix gives the DOF, a scalar quantity indicating the number of independent pieces of informations within a measurement. For the LMT, the DOF of ozone partial columns is obtained from the trace of AVK up to 3 km (DOF-3km). It is an easy and direct parameter to quantify the vertical sensitivity of each retrieval.

An example of real IASI+GOME-2 retrievals is provided in Figure 1, that shows O₃ partial columns (top image) integrated between the surface and 3 km a.s.l. (O3-3km), DOF-3km (middle) and Hmax-3km (bottom) for the 8 July 2010. White gaps indicate a lack of values due to the presence of relatively high cloud cover (>30%), unavailability of satellite data or invalid retrievals. The DOF-3km map indicates that O3-3km estimates are closer to true profiles over land, where DOF-3km is higher (0.28) than over ocean (0.22), because of a stronger thermal contrast (i.e., the temperature difference between the surface and the lowest atmospheric layer). DOF and Hmax are the two diagnostic parameters that will be used in this work to quantify the sensitivity of a retrieval method.

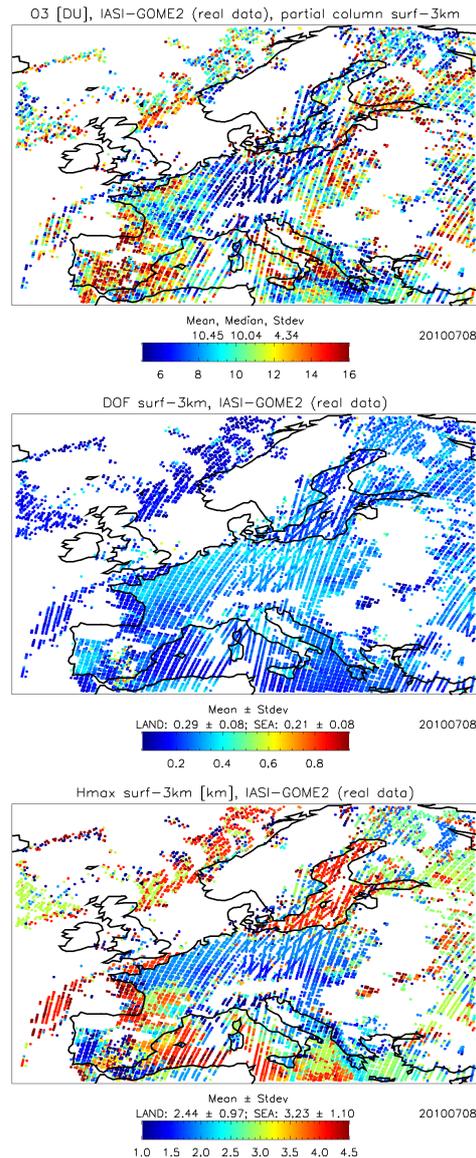


Figure 1. Real IASI+GOME-2 retrievals for the 8 July, 2010. Maps of O3-3km [DU] (top image), DOF-3km
 250 (middle), Hmax-3km [km] (bottom). White areas indicate a lack of measurements due to the presence of relatively high cloud fraction (>30%), unavailability of satellite data or invalid retrievals.

The convolution of the pseudo-reality with the AVK matrix (generally referred to as AVK-smoothing) gives
 255 an estimate of what retrievals would be without accounting for instrumental limitations (radiometric noise). The *smoothing error* is directly linked to the difference between AVK-smoothed pseudo-reality and pseudo-reality. It can be estimated from the standard deviation of the frequency distribution of this difference. The *measurement error* (i.e. due to radiometric noise) can be estimated from the standard deviation of the difference between pseudo-observations and AVK-smoothed pseudo-reality.

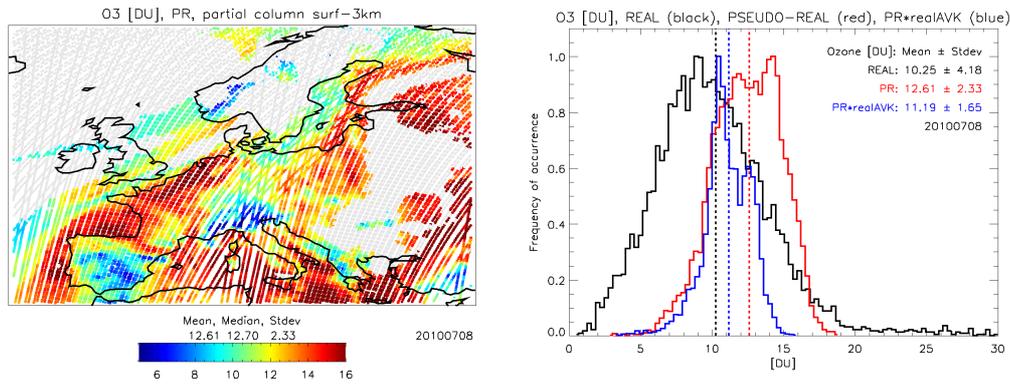
260 Finally, the difference between pseudo-observations and pseudo-reality (bias) gives an estimates of the inversion algorithm accuracy. Its standard deviation (σ -bias) quantifies the *total error* which is an estimate of the algorithm precision.

265 **5 MOCAGE pseudo-reality**

In a first analysis, we observed that MOCAGE strongly underestimates the cloud fraction (CLF), that never exceeds a value of 0.3. Therefore, we have estimated an empirical conversion from MOCAGE cloud fraction to more realistic values used as inputs of the pseudo-reality. We then compared the MOCAGE cloud fraction with GOME-2 apriori values, given from an external algorithm called FRESCO (Koelemeijer et al., 2001),
270 for the whole 8-10 July time period. As IASI+GOME-2 retrieval sensitivity to LMT ozone is significantly reduced when $CLF > 0.3$, such cloudy pixels are excluded. For those pixels with $CLF < 0.3$, we defined two correction factors that minimize the differences in CLF frequency distribution and mean CLF, between the two datasets. The corrected cloud fraction is calculated as $CLF = 20.70 \times (CLF_{mocage})^{1.2}$, where CLF_{mocage} represents the original CLF given by MOCAGE. We assume the presence of only low clouds
275 with cloud top pressures above 700 hPa.

As previously mentioned, a more realistic representation of ozone horizontal variability is obtained by assimilation of real ozone data into MOCAGE. To test the reliability of pseudo-real ozone concentration, we compared O3-3km from MOCAGE with real IASI+GOME-2 retrievals. Figure 2 (left) shows the map of model O3-3km data for the 8 July 2010. Light-grey indicates where cloud fraction is larger than 0.3. For
280 consistency with Figure 1, we only show those MOCAGE pixels that would have been selected by IASI+GOME-2 algorithm on that day (i.e., co-located and near-simultaneousness with IASI and GOME-2 footprint at the time of MetOp overpass).

The normalized frequency distributions of Figure 2 (right) show an overall consistence between MOCAGE outputs and IASI+GOME-2 retrievals, in terms of O3-3km magnitude and spatial distribution. MOCAGE
285 (red) seems to overestimate the regional mean O3-3km (black) by 2.16 DU (21%). This difference is mostly due to the reduced sensitivity of IASI+GOME-2 retrievals to ozone below 3km of altitude. If we account for this effect, smoothing the PR by real AVK ($PR \cdot realAVK$, blue), the resulting O3-3km distribution shows an average value much closer to real data. A positive bias of MOCAGE at the LMT is also shown by Zyryanov et al. (2012). The larger standard deviation of IASI+GOME-2 than MOCAGE outputs might be due to the
290 radiometric noise of real satellite measurements and to the naturally higher variability of real data than for model simulations.

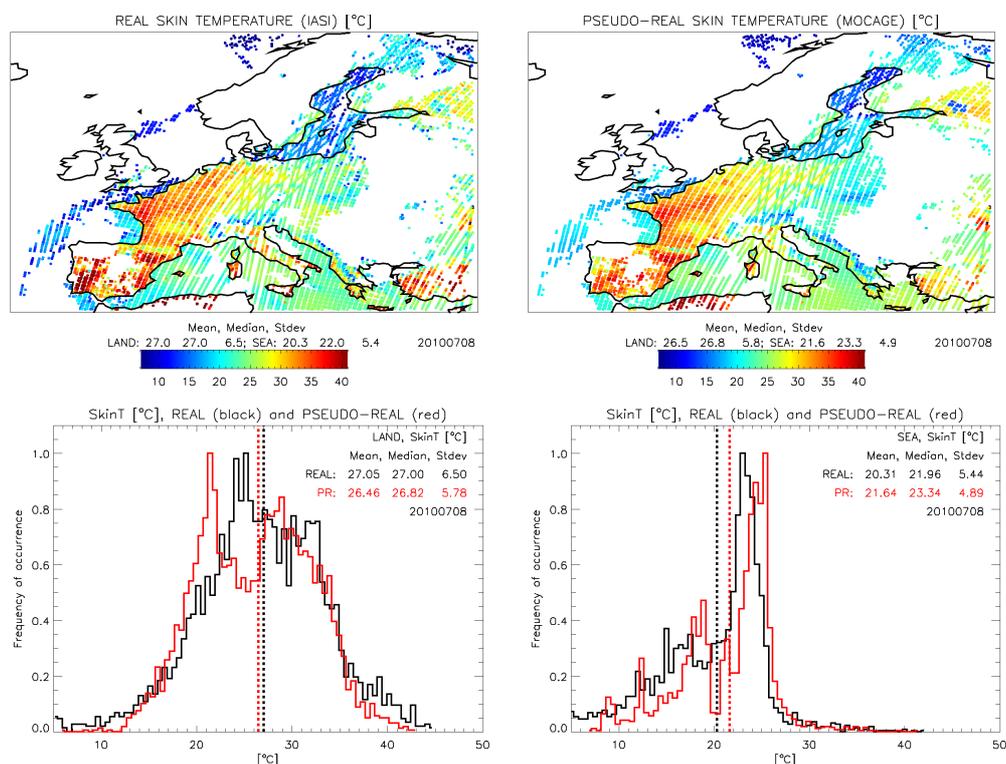


295

Figure 2. MOCAGE simulation for the 8 July, 2010. (left image) Map of pseudo-real O3-3km [DU]. For consistency with Figure 1, we consider only those MOCAGE pixels that would have been selected by IASI+GOME-2 retrieval algorithm on that day. (right image) O3-3km [DU] normalized frequency distributions of real IASI+GOME-2 measurements (black), pseudo-real MOCAGE data (red) and PR
 300 smoothed by real AVK (blue). Dashed lines show mean O3-3km [DU] values of each distribution.

The analysis of pseudo-reality was also performed by comparison of surface temperatures (T_s) from MOCAGE and retrievals, using IASI real spectra within the IASI+GOME-2 algorithm. Figure 3 shows maps of T_s derived from real IASI measurements (top left) and model simulations (top right) for the 8 July 2010,
 305 together with the histogram of their normalized frequency distribution over land (bottom left) and over ocean (bottom right). We consider only those pixels with skin temperature in the 5-45 °C range, where the absolute T_s difference between real measurements and MOCAGE is lower than 10 °C. Histograms of Figure 3 clearly indicates that MOCAGE (red) overestimates on average the ocean surface temperature and underestimates
 310 land surface temperature with respect to IASI data (black). This is true for the whole 8-10 July time period and the mean difference between real and MOCAGE T_s is equal to -1.42 °C (ocean) and +0.67 °C (land). Further analysis also shows that MOCAGE overestimates the atmospheric temperature profile in the first 6 km of altitude. For the whole period, the mean difference between real and MOCAGE temperature is equal to -2.69 (0-1km), -1.41 (1-2km), -1.51 (2-3km), -1.14 (3-4km), -0.88 (4-5km) and -0.51 (5-6km) °C. These
 315 values have been used to modify MOCAGE temperatures before running radiative calculations and inversion algorithms, in order to consider realistic thermal contrasts for pseudo-reality. It should be mentioned that this work of nature run calibration against real observations and especially for meteorological variables (important for the retrievals) is mandatory to get a realistic pseudo-reality. We believe that it is one important strength of this work to have taken care of these aspects that are often not really tackled in OSSE studies.

320



325 Figure 3. (top) maps of Ts, from real IASI measurements (left) and MOCAGE simulation (right) before
 330 correction, for the 8 July 2010. For consistency with IASI data, we consider only those MOCAGE pixels that
 would have been selected by IASI+GOME-2 retrieval algorithm on that day. (bottom) histograms of Ts
 normalized frequency distributions for real data (IASI, black) and pseudo-real outputs (MOCAGE, red), over
 land (left) and ocean (right). Dashed lines indicate the mean value. We consider only those pixels with skin
 335 temperature in the 5-45 °C range and where the absolute Ts difference between real measurements and
 MOCAGE is lower than 10 °C.

6 Results

335 After the correction of MOCAGE cloud fraction and temperature fields toward more realistic values, we
 have used MOCAGE atmospheric profiles to simulate TIR radiances and UV reflectances by KOPRA and
 VLIDORT respectively. We then added radiometric random noise to raw spectra and processed the simulated
 spectra by IASI+GOME-2 and IASI-NG+UVNS inversion algorithms. Retrievals are provided at the IASI
 ground resolution. Statistics of retrieval sensitivity and LMT ozone partial columns are presented in the
 340 following paragraph.

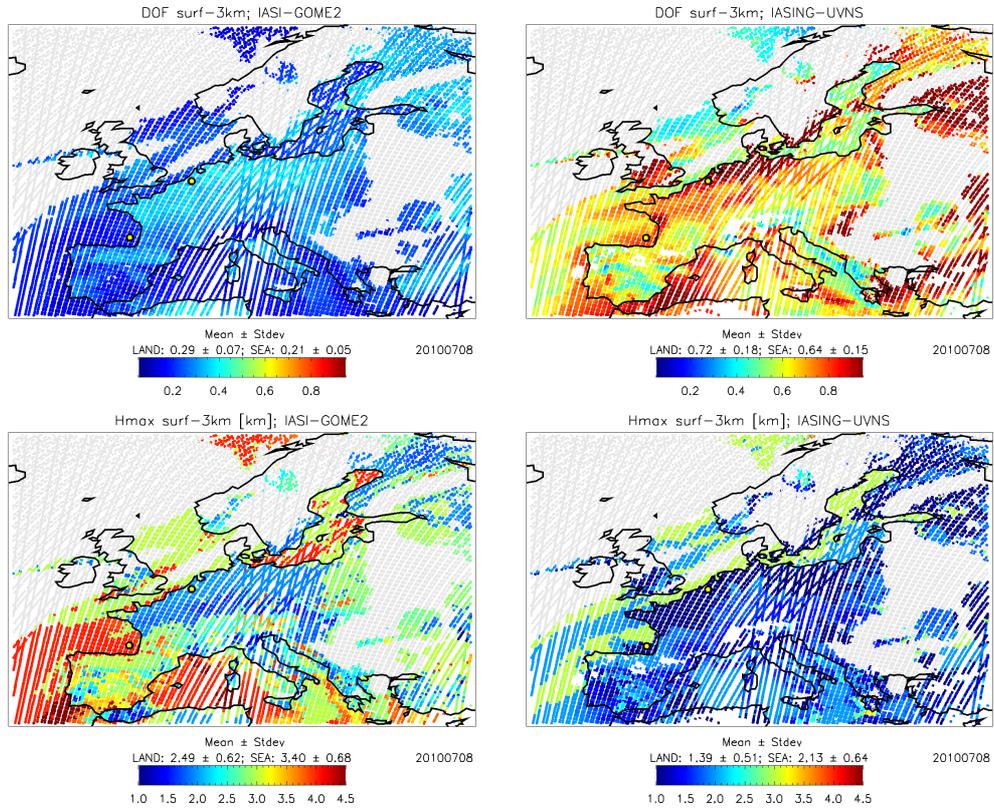
6.1 Retrieval sensitivity

As previously mentioned, multispectral retrieval sensitivity is quantified in terms of lowermost tropospheric
345 DOF and Hmax. The first row of Figure 4 shows DOF-3km maps from IASI+GOME-2 (left) and
IASI-NG+UVNS (right). To test the general consistency of retrieval performances between the POS and
reality, pseudo-real DOF-3km and Hmax-3km from IASI+GOME-2 (Figure 4) are compared with real
satellite products (Figure 1). We already observed that the MOCAGE geographical distribution of O3-3km is
realistic over Europe (Figure 1 and Figure 2). Figure 4 also shows that pseudo-real and real retrievals from
350 IASI+GOME-2 are consistent in terms DOF-3km (first row) and Hmax-3km (second row) for both
magnitude and spatial variability. On average, the regional DOF-3km is equal to 0.29 ± 0.07 (over land) and
 0.21 ± 0.05 (over ocean) for the synthetic retrievals and to 0.29 ± 0.08 (over land) and 0.21 ± 0.08 (over ocean)
for the real case. The peak of maximum sensitivity in the LMT is equal to 2.49 ± 0.62 km (over land) and
 3.40 ± 0.68 (over ocean) for the synthetic retrievals and to 2.44 ± 0.97 km (over land) and 3.23 ± 1.10 km (over
355 ocean) for the real case. Results are consistent (within statistical uncertainties) with real IASI+GOME-2
sensitivity values obtained by **Cuesta et al. (2013)** over the same region for the 19-20 August 2009. They
find a DOF-3km of 0.34 ± 0.04 (land) and 0.23 ± 0.04 (ocean), and a Hmax-3km of 2.20 ± 0.50 (land) and
 3.42 ± 0.59 (ocean).

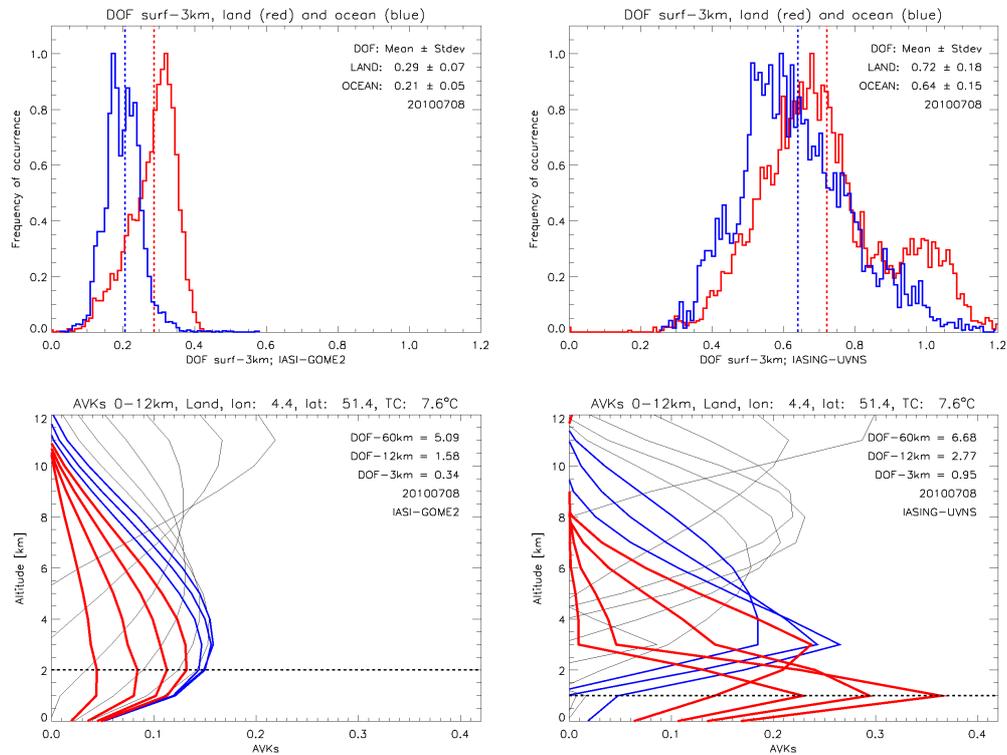
The IASI-NG+UVNS map of DOF-3km (right) shows an average increase in the degree of freedom at 3km
360 over both land and ocean of about 150% and 200%, respectively with respect to IASI+GOME-2, with mean
values that grow from 0.29 (land) and 0.21 (ocean) with IASI+GOME-2 to 0.72 (land) and 0.64 (ocean) with
IASI-NG+UVNS. Note that IASI-NG+UVNS uses an optimised constraint to enhance sensitivity in the
LMT. Accordingly, with the new spectral method the peak of LMT sensitivity to ozone (Hmax-3km, second
row of Figure 4) decreases on average by about 1.1 km over land (from 2.50 to 1.41 km) and 1.27 km over
365 ocean (from 3.40 to 2.13 km). Sensitivity differences between land and ocean are strong for IASI+GOME-2
and are also present in IASI-NG+UVNS retrievals, because of the different thermal contrast which is greater
over land. The third row of Figure 4 shows that normalized frequency distributions of DOF-3km are wider
and shifted to higher values when using new-generation sensors (right image) for both land (red) and ocean
(blue). It is remarkable that in several cases IASI-NG+UVNS method shows a DOF-3km ≥ 0.8 (22% of
370 total) and a Hmax-3km ≤ 1.5 km (37% of total).

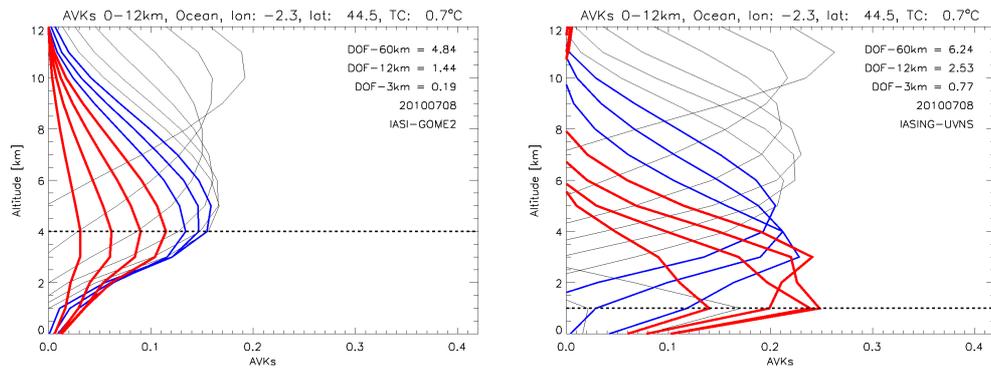
The fourth and fifth rows of Figure 4 report two examples of AVK vertical profiles at retrieval altitudes of 0,
1, 2, 3 km (red) and 4, 5, 6 km (blue) and 7, 8, 9, 10, 11, 12 km (black) for two specific pixels over land and
ocean (black-yellow spot in maps) with thermal contrast (reported in figure) particularly high and equal to
14.5°C (land) and 5.9°C (ocean). Stratospheric DOF (surface-60 km) is consistently increased with
375 IASI-NG+UVNS, by 1.59 (+31%) over land and 1.40 (+29%) over ocean, and tropospheric DOF
(surface-12km) is increased by 1.19 (+75%) over land and 1.09 (+76%) over ocean. However, the maximum
gain is obtained in the LMT where DOF-3km increases by 0.61 (+179%) over land and 0.58 (+305%) over
ocean. The dotted line indicates the height of maximum sensitivity in the LMT. As expected, IASI+GOME-2
shows better retrieval performances over land (Hmax-3km = 2 km) than over ocean (Hmax-3km = 4 km).

380 The use of IASI-NG+UVNS further decreases Hmax-3km over land and even more over ocean, down to 1 km of altitude in both cases.



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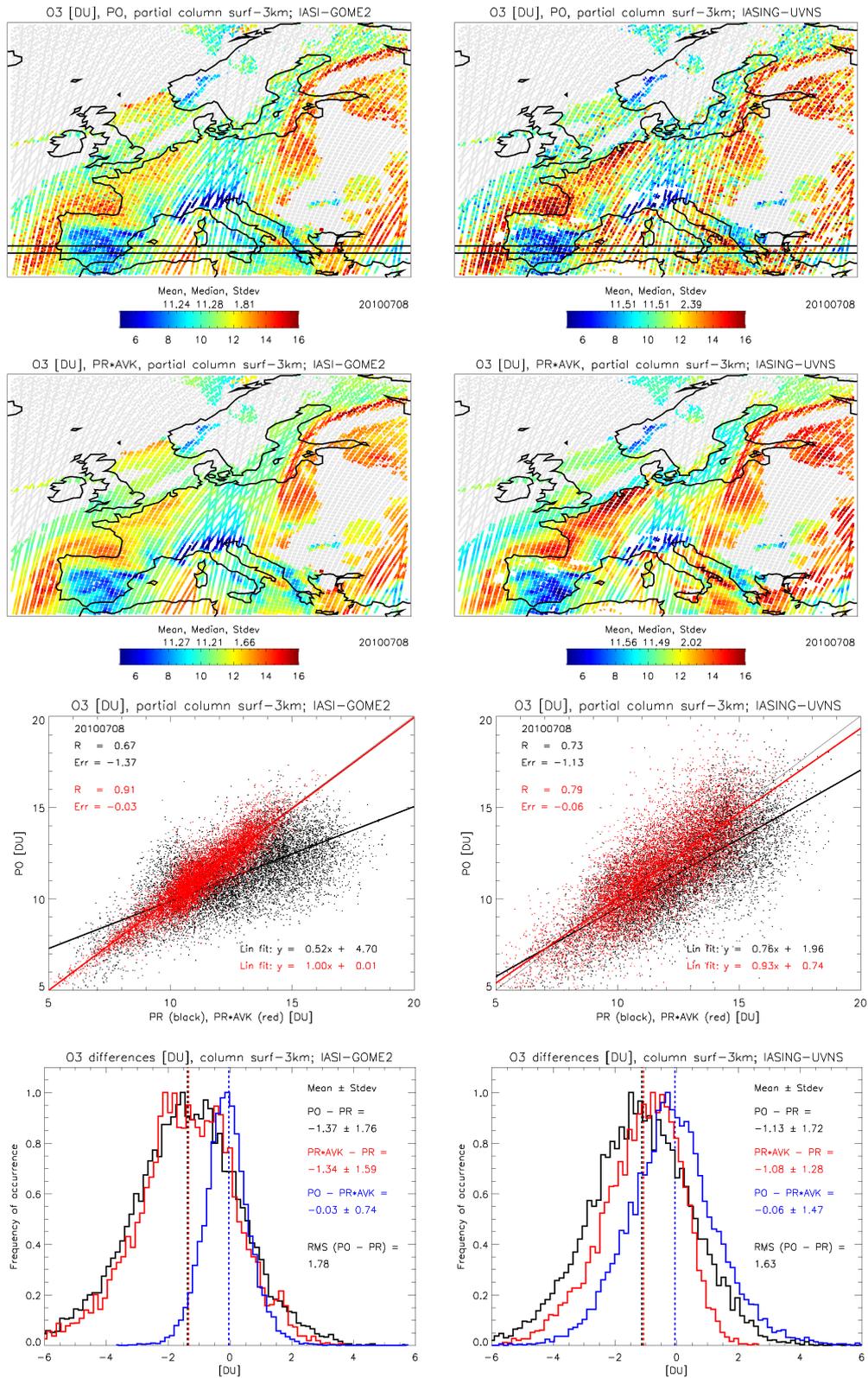
390 Figure 4. IASI+GOME-2 (left column) and IASI-NG+UVNS (right column) data, for the 8 July 2010. (first
row) maps of DOF-3km pseudo-observations (PO), grey colour indicates where CLF is larger than 0.3.
(second row) maps of Hmax-3km from PO. (third row) histograms of DOF-3km normalized frequency
distribution from PO, over land (red) and ocean (blue). (fourth row) AVK vertical profiles at retrieval
altitudes of 0, 1, 2, 3 km (red) and 4, 5, 6 km (blue) and 7, 8, 9, 10, 11, 12 km (black) for a pixel over land
395 (black-yellow spot in the map) in a highly polluted area. Values of DOF-60km, DOF-12km and DOF-3km
are reported in figure. Dashed line indicates the altitude of maximum sensitivity in the LMT. (fifth row) same
as before but over ocean.

400 For the whole time period (8-11 July), averaged values of regional mean DOF-3km and Hmax-3km for
IASI+GOME-2 and IASI-NG+UVNS are presented in Table 2, with real IASI+GOME-2 data reported in
parenthesis next to pseudo-real ones.

405 6.2 LMT ozone retrievals

Figure 5 shows maps of O3-3km pseudo-observations (first row) and AVK-smoothed pseudo-reality (second
row), for IASI+GOME-2 (left) and IASI-NG+UVNS (right). In terms of absolute ozone concentrations, both
IASI+GOME-2 and IASI-NG+UVNS have an overall good agreement with the MOCAGE pseudo-reality.
The two multispectral methods differ by less than 3% in estimating the mean O3-3km value over the whole
410 region. However IASI-NG+UVNS shows a larger spatial variability and capture more efficiently some high
O3-3km values off the coast of Northern Spain, France, Holland, and Mediterranean Basin. This is even more
visible looking at the AVK-smoothed pseudo-reality (Figure 5, second row), where radiometric noise is not
present. O3-km patterns smoothed by IASI-NG+UVNS averaging kernels are closer to MOCAGE product
(Figure 2) because of the stronger sensitivity to true profiles.

415



420

Figure 5. IASI+GOME-2 (left column) and IASI-NG+UVNS (right column) data, for the 8 July 2010. (first row) maps of O3-3km pseudo-observations (PO), grey colour indicates where CLF is larger than 0.3. Black lines indicate the [38N, 39N] latitude band. (second row) maps of O3-3km from AVK-smoothed pseudo-reality (PR*AVK). (third row) scatterplot of O3-3km [DU] from pseudo-observations (y-axis) versus

pseudo-reality (black, x-axis) and AVK-smoothed pseudo-reality (red, y-axis). Linear correlation coefficient, mean error and linear fit equation are reported in figure. (fourth row) histograms of normalized frequency distribution of O3-3km differences [DU] between PO and PR (black), PR*AVK and PR (red), PO and PR*AVK (blue). Mean value and standard deviation of each difference is reported in figure, together with
 430 PO-PR root mean square (RMS).

As a consequence, the correlation between pseudo-retrievals and pseudo-reality is enhanced for IASI-NG+UVNS. Figure 5 (third row) presents the scatterplot of O3-3km pseudo-observations versus
 435 pseudo-reality (black) and AVK-smoothed pseudo-reality (red). With respect to existing instruments (left image), the product of new-generation sensors (right image) are better correlated to MOCAGE data. The correlation coefficient between PO and PR (black) increases from 0.67 to 0.73 (+9%) and the linear fit slope (reported in figure) of the dispersion plot increases from 0.52 to 0.76 (+46%), sign that high O3-3km values (larger than ~8.5 DU) are less underestimated. **On the other hand, the correlation coefficient between PO and PR*AVK (red) decreases from 0.91 to 0.79 (-13%), as well as the slope of the linear fit slope (from 1 to 0.85, -15%), sing of a larger measurement error for IASI-NG+UVNS than for IASI+GOME-2 (quantified afterwards).**

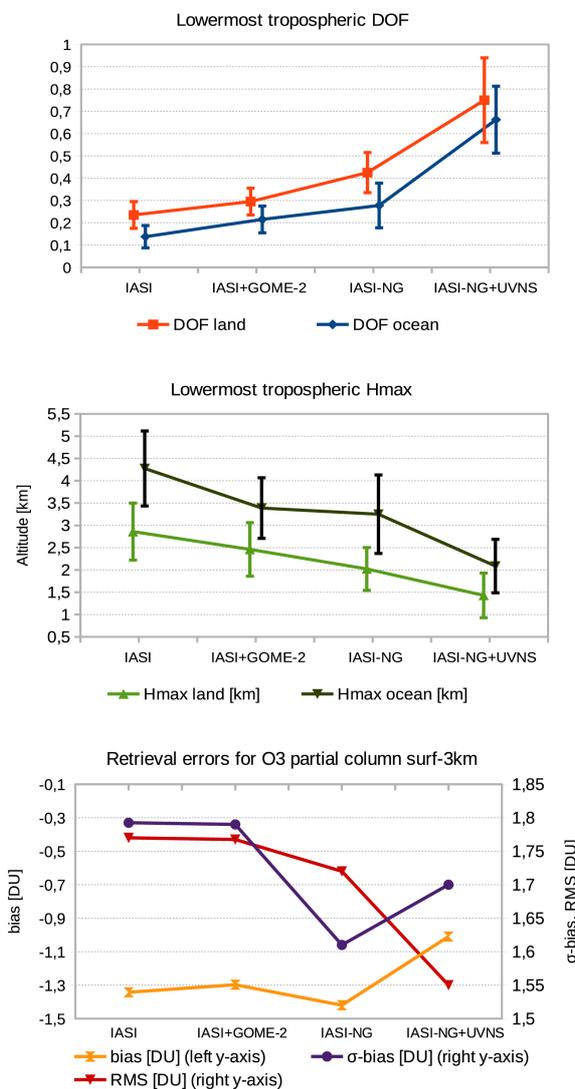
The fourth row of Figure 5 shows the normalized frequency distributions of (pixel-by-pixel) difference in O3-3km between: pseudo-observations and pseudo-reality (PO-PR, black), AVK-smoothed pseudo-reality and pseudo-reality (PR*AVK-PR, red), pseudo-observation and AVK-smoothed pseudo-reality (PO-PR*AVK, blue). With respect to IASI+GOME-2, the IASI-NG+UVNS mean value of PO-PR distribution (retrieval mean bias) decreases from -1.37 to -1.13 (-17%). **The total retrieval error, quantified by the standard deviation of the mean bias, does not vary significantly (from 1.76 to 1.72, -2%) because of the net balance between the decreasing smoothing error (from 1.59 to 1.28, -19%) and the increasing measurements error (from 0.74 to 1.47, +92%). At the same time, the root mean square (RMS) decreases from 1.78 to 1.63 (-8%). These results indicate an overall higher quality of the retrieval (smaller RMS) when using EPS-SG sensor instead of MetOp instrumentation, with a global gain in retrieval accuracy (smaller bias) and an almost constant retrieval precision (slightly smaller σ -bias).**

For the whole time period (8-11 July), Table 2 reports regional means of the linear correlation coefficient R,
 455 between pseudo-observations and pseudo-real data of O3-3km, as well as the bias, the σ -bias and the RMS of the PO-PR distribution, for both IASI+GOME-2 and IASI-NG+UVNS.

	DOF-3km		Hmax-3km [km]		R	Bias [DU]	σ -bias [DU]	RMS [DU]
	land	ocean	land	ocean				
IASI+GOME-2	0.29±0.06	0.21±0.06	2.46±0.60	3.39±0.68	0.65	-1.30	1.79	1.77
(real)	(0.29±0.08)	(0.21±0.08)	(2.51±0.88)	(3.32±1.07)				

IASI-NG+UVNS	0.75±0.19	0.66±0.15	1.43±0.50	2.09±0.60	0.73	-1.01	1.70	1.55
Gain	+159%	+214%	-1.03	-1.30	+12%	-22%	-5%	-12%

460 Table 2. Averaged values (8-11 July 2010) of regional mean degree of freedom in the LMT (DOF-3km),
altitude of maximum sensitivity in the LMT (Hmax-3km [km]), linear correlation coefficient between PR
and PO of O3-3km, together with the mean value (bias [DU]), the standard deviation (σ -bias [DU]) and the
root mean square (RMS [DU]) of PO-PR distribution of O3-3km over Europe. For IASI+GOME-2 (top row)
and IASI-NG+UVNS (bottom row). Real IASI+GOME-2 values of DOF-3km and Hmax-3km are reported
465 in parenthesis next to pseudo-real ones.



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Figure 6. Average values of DOF-3km (top); Hmax-3km (middle); bias, σ -bias and RMS (bottom) of the O3-3km PO-PR distribution from IASI, IASI+GOME-2, IASI-NG and IASI-NG+UVNS, for the 8-11 July 2010 over Europe.

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Figure 6 shows graphically the mean values of DOF-3km (middle), Hmax-3km (middle), bias, σ -bias and RMS (bottom) of the O3-3km PO-PR distribution for IASI+GOME-2 and IASI-NG+UVNS (Table 2), together with these same values for IASI and IASI-NG alone, simulated over the same area and time period.

480 Note in case of IASI alone, the POS seems to overestimate the retrieval performances with a Hmax-3km over land equal to 2.86 ± 0.64 km, which is only 400 m above that of IASI+GOME-2 instead of the 800 m expected by Cuesta et al. (2013). For what concerns DOF-3km and Hmax-3km, IASI+GOME-2 represents a clear improvement to IASI alone, while technical advances of IASI-NG allow retrieval performances even higher than IASI+GOME-2. When IASI-NG is coupled with UVNS, the IASI-NG+UVNS synergism
485 overpasses by far the retrieval skills of all other configurations.

The RMS of the PO-PR difference distribution, which is an estimate of the overall retrieval quality combining together accuracy and precision, decreases monotonically from IASI to IASI-NG+UVNS. For what concerns the bias and the σ -bias, results are consistent with the design of the constrain matrix of IASI-NG+UVNS which is less constrained than in IASI, IASI+GOME-2 and IASI-NG algorithms in order
490 to increase the vertical sensitivity to near-surface ozone. This particular choice leads to a higher accuracy and a smaller smoothing error (lower bias) for IASI-NG+UVNS than all other retrieval methods, but also to a larger measurement error that enhances the total retrieval error (σ -bias) of IASI-NG+UVNS with respect to IASI-NG.

The high quality retrieval skills of IASI-NG+UVNS below 3km of altitude suggest to go deeper in the
495 lowermost troposphere and investigate ozone sensitivity in the surface-2km layer. Figure 7 shows the DOF-2km (top) and the Hmax-2km (bottom) for the 8 July 2010, for IASI+GOME-2 (left) and IASI-NG+UVNS (right). With respect to LMT, the retrieval performances of IASI+GOME-2 degradate sensibly in terms of DOF (0.16 ± 0.05 over land 0.10 ± 0.03 over ocean) as Hmax-2km remains above 2 km of latitude (2.41 ± 0.63 km over land and 3.34 ± 0.68 km over ocean). On the contrary, IASI-NG+UVNS shows
500 still a relatively high DOF-2km of 0.49 ± 0.17 (land) and 0.40 ± 0.15 (ocean) and a Hmax-2km of 1.25 ± 0.48 km (land) and 2.0 ± 0.67 km (ocean), even better than IASI+GOME-2 for the surface-3km partial column.

Averaged over the whole time period, the IASI-NG+UVNS regional mean DOF-2km is equal to 0.52 ± 0.17 (land) and 0.42 ± 0.15 (ocean) with a Hmax-2km of 1.29 ± 0.49 km (land) and 1.96 ± 0.63 km (ocean). As a consequence, the map of O3-2km pseudo-retrievals from IASI-NG+UVNS (Figure 8) is much closer to
505 reality than for IASI+GOME-2. In particular, high ozone values are less underestimated over Holland and the Mediterranean basin (especially off the coast of East Spain and Southern Italy), where low level ozone layers are present.

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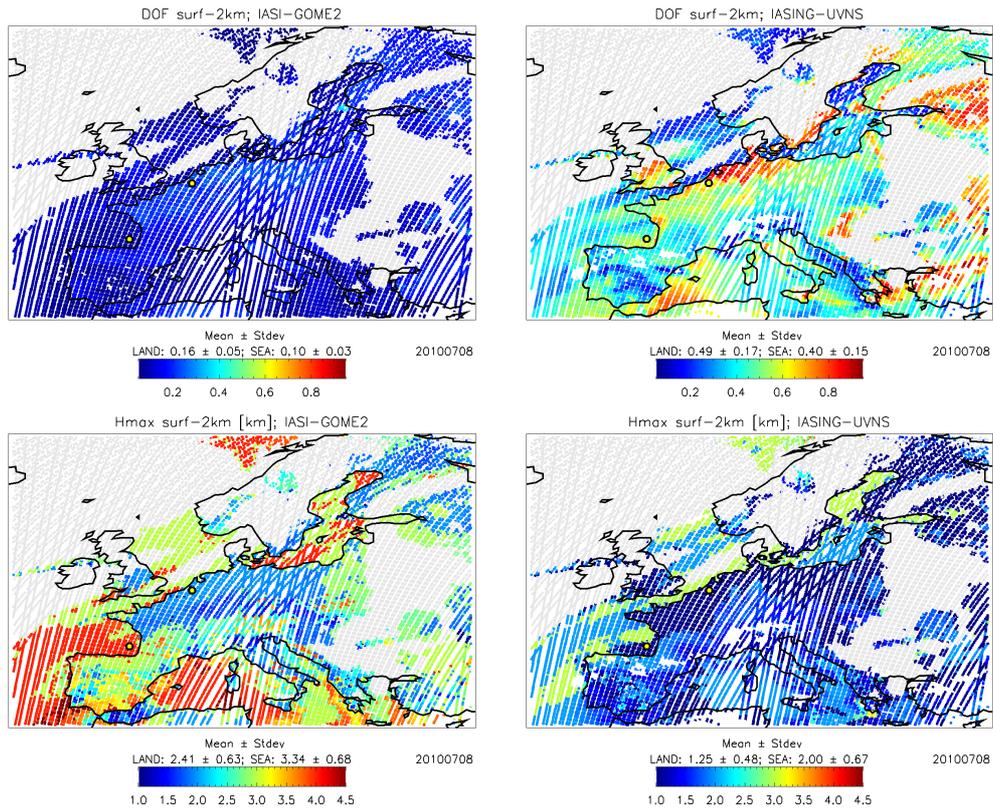
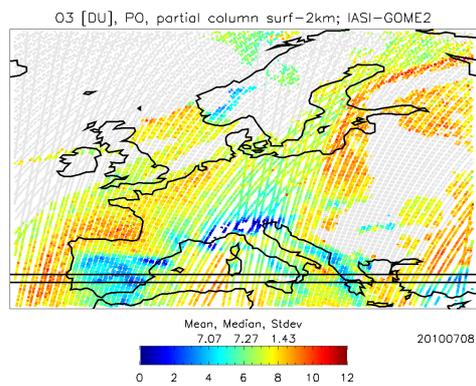
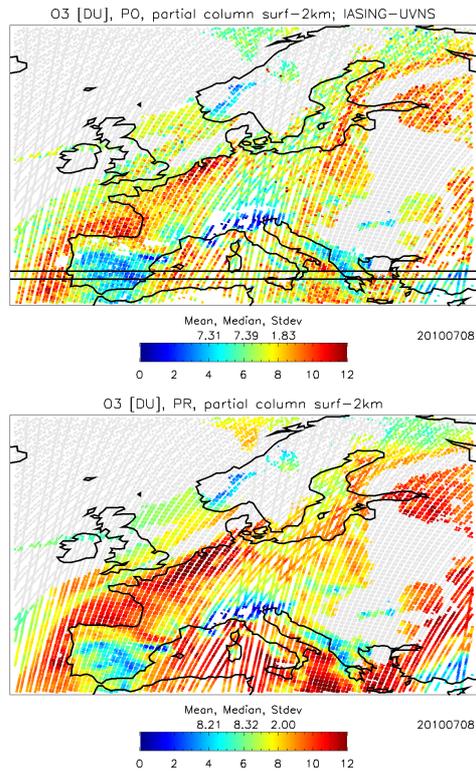


Figure 7. IASI+GOME-2 (left) and IASI-NG+UVNS (right) data, for the 8 July 2010. Maps of DOF-2km (top) and Hmax-2km (bottom) pseudo-observations.

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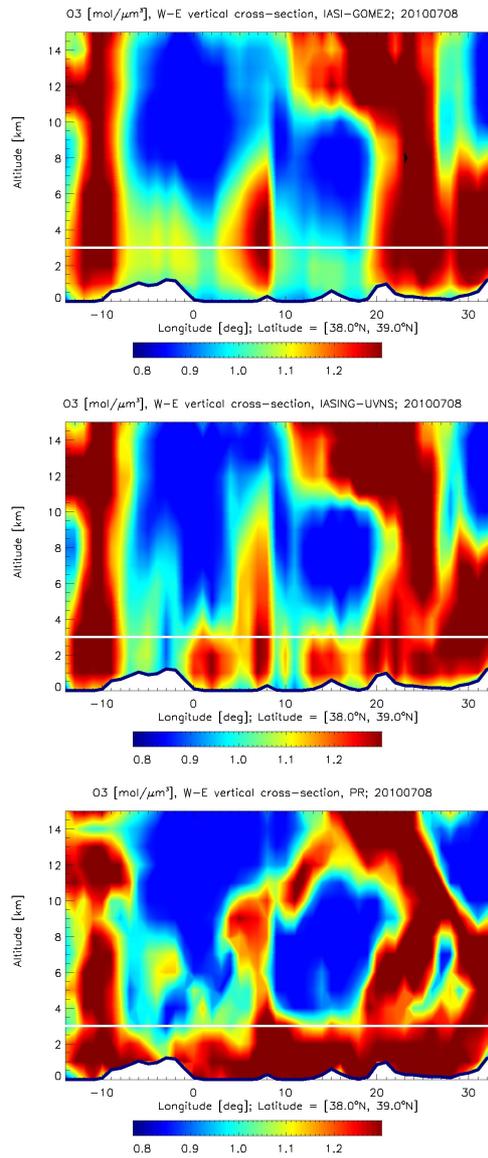
Figure 8. IASI+GOME-2 (top) and IASI-NG+UVNS (middle) pseudo observations of 03-2km and PR (bottom) for the 8 July 2010.

525 **6.3 Capacity of resolving layers**

Along with sensitivity to surface ozone concentrations, vertical resolution of ozone retrievals is the major limitations of such products. Indeed, the mixing of vertical information screens out the origin of ozone and limits for example their capability to improve models when assimilated.

Figure 9 shows a transect of ozone profiles which allows one to compare the capability of each retrieval to resolve ozone layers. It presents the vertical cross-sections of ozone concentration as observed by IASI+GOME-2 (top) and IASI-NG+UVNS (middle), with the corresponding MOCAGE output (bottom). Data are averaged horizontally with a resolution of 1x1 degrees, along the latitude band [38°N, 39°N]. Both retrieval methods show an overall agreement with pseudo-reality for ozone plumes with concentration higher than 1.0 molecules/ μm^3 .

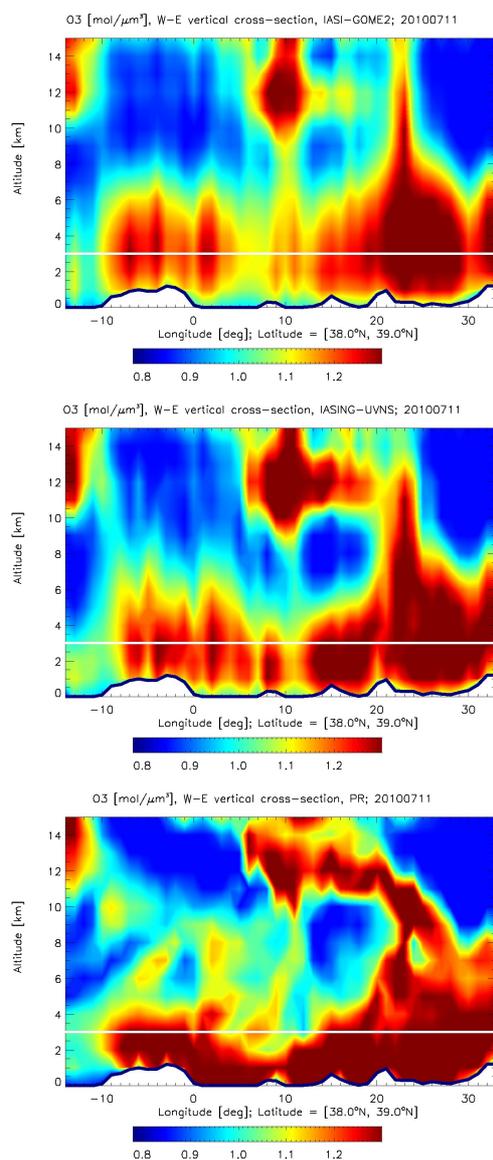
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Figure 9. Cross section of ozone concentration [molecules/ μm^3] in the latitude band [38°N, 39°N] (as shown in Figure 5, first row), from the surface to 15 km of altitude, for the 8 July 2010. Data are averaged horizontally with a resolution of 1×1 degrees. (top) IASI+GOME-2 retrievals. (middle) IASI-NG+UVNS retrievals. (bottom) MOCAGE pseudo-reality. White line indicates an altitude of 3 km.

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Figure 10. Same as Figure 9, but for the 11 July 2010.

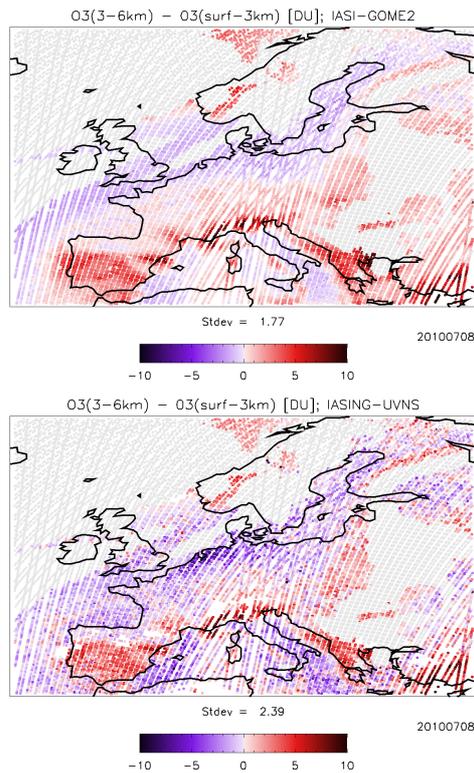
The comparison of IASI+GOME-2 cross-section with the pseudo-real O_3 concentration confirms that IASI+GOME-2 is able to resolve complex vertical ozone distribution in the lowermost and lower troposphere. This is true for the three ozone peaks (red colour) at [14°W, 10°W], [4°E, 8°E] and [20°E, 30°E] or the moderate O_3 concentrations (yellow-green colour) at [12°W, 5°E] and [9°E, 17°E] located below a clean atmosphere. The vertical structures described by IASI+GOME-2 matches well MOCAGE simulations and are consistent with real IASI+GOME-2 product, which is able to observe ozone plumes below 3 km, even if it cannot distinguish whether the ozone plumes are located in the LMT or between 3 and 6km of altitude (Cuesta et al., 2013).

IASI-NG+UVNS shows a finer resolution than IASI+GOME-2, resolving ozone layers of 2-3 km thickness below 3 km of altitude. At [0°E, 5°E] and [8°E, 20°E], ozone concentrations higher than 1.2 molecules/ μm^3

are entirely located in the lowermost troposphere. Even is partially, IASI-NG+UVNS is able to detect the presence of LMT ozone where IASI+GOME-2 fails to detect strong O_3 concentrations.

Same as Figure 9, but for the 11 July 2010, Figure 10 shows the O_3 -3km vertical cross-section in the $[38^\circ N, 39^\circ N]$ latitude band. Again, IASI-NG+UVNS provides more reliable retrievals where ozone concentrations are larger than $1.2 \text{ molecules}/\mu\text{m}^3$, as at $[3^\circ E, 10^\circ E]$ below 4 km (and in particular the peak at $[8^\circ E, 10^\circ E]$ below 2 km) and at $[14^\circ E, 19^\circ E]$ below 3 km. At higher altitudes between 11 and 13 km a.s.l., the 2 km thick ozone layer at $[12^\circ E, 20^\circ E]$ is well resolved by IASI-NG+UVNS but invisible to IASI+GOME-2.

The ability of IASI-NG+UVNS to identify ozone gradient between the 3-6 km and the surface-3km layers is analysed afterwards. Figure 11 shows maps of pixel-by-pixel difference in ozone partial columns between the two altitude bands. Negative values (in purple) indicate where the O_3 concentration is higher in the LMT. The regional standard deviation of the difference is reported in figure, above the colour scale. IASI-NG+UVNS (middle) clearly shows a better agreement with pseudo-reality (bottom) than IASI+GOME-2 (top), especially over Northern France, Holland and Mediterranean basin.



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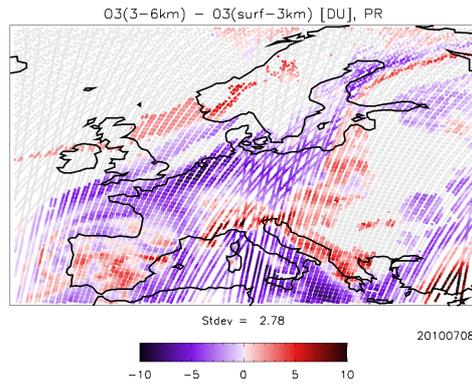


Figure 11. Maps of pixel-by-pixel difference between ozone partial columns [DU] calculated in the surface-3km and 3-6km altitude bands, for the 8 July 2010. Negative values (purple) indicate stronger ozone concentration in the LMT than above. Regional standard deviation (Stdev) value is reported in figure.

The same dataset shown in Figure 11 is analysed in Figure 12 as a scatterplot. On the y-axis we present pseudo-observations, plotted in function of pseudo-reality (black) and AVK-smoothed pseudo-reality (red). Both methods seem to identify correctly those cases where pseudo-real differences are positive, but IASI-NG+UVNS allows to detect also negative values (higher ozone concentration in the LMT than above it) down to -8 DU, while IASI+GOME-2 is limited to -2 DU. In case of EPS-SG sensors, the mean error between pseudo-reality and synthetic retrievals is sensibly less biased by -36%. At the same time, IASI-NG+UVNS shows a larger dispersion in the scatterplot of PO versus PR*AVK, because of a larger measurement error than IASI+GOME-2 (although total error remains similar in both cases).

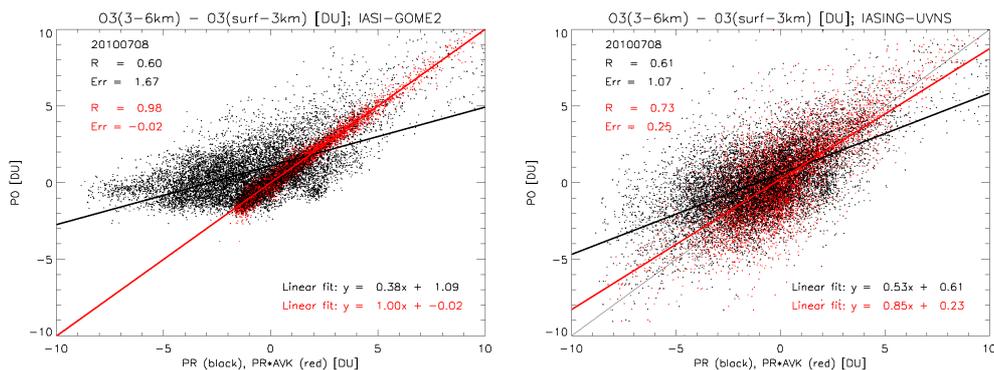


Figure 12. Same data as in Figure 11. IASI+GOME-2 (left image) and IASI-NG+UVNS (right image) pseudo-observations (PO, y-axis) versus pseudo-reality (PR, black, x-axis) and AVK-smoothed pseudo-reality (PR*AVK, red, x-axis). Linear correlation coefficient, mean error and linear fit equation are reported in figure.

7 Summary and conclusion

In this work, we quantify the potential of the synergism for LMT ozone retrieval of combining TIR and UV measurements from the new-generation sensors IASI-NG and UVNS (onboard EPS-SG satellite) with respect to the existing IASI+GOME-2 multispectral method. To achieve this goal, we develop a pseudo-observation simulator. The nature run is generated by the MOCAGE model, where real ozone data from surface network stations, IASI and MLS instruments have been assimilated for a realistic representation of ozone horizontal variability at the surface and the free troposphere. To ensure the highest degree of reliability with respect to the experiment, the pseudo-real atmosphere has been carefully calibrated by a comparison of real data with the POS of IASI+GOME-2. Cloud fraction, skin temperature and temperature profile were empirically corrected in order to obtain realistic sensitivity of the satellite products. This calibration stage of meteorological variables important for retrievals appears as a key point of the methodology and we believe it should systematically be considered in OSSEs. Atmospheric and surface spectra are simulated by KOPRA and VLIDORT radiative transfer codes, performing full and accurate forward and inverse radiative transfer calculations. We analyse and compare pseudo-observations of IASI+GOME-2 and IASI-NG+UVNS from 8 to 11 July 2010 over Europe. Data assimilation analysis in a different chemical transport model independent from MOCAGE is left to a future research work.

Over the whole time period, IASI-NG+UVNS estimates of ozone partial columns, calculated between the surface and 3 km of altitude, are highly correlated to the MOCAGE outputs. With respect to IASI+GOME-2, using new-generation sensors the correlation coefficient between O3-3km pseudo-observations and pseudo-reality increases on average by about 12%, from 0.65 to 0.73, and the retrieval of high ozone values is less underestimated. As a consequence, the retrieval bias is significantly reduced by -22%. In addition, σ -bias slightly decreases by -5%. The bias between PO and PR gives an estimate of the retrieval method accuracy. It is strongly improved mostly because of a higher retrieval sensitivity to true profiles in the lower tropospheric layers (below 2-3km). The σ -bias quantifies the *total error* of the multispectral retrieval and measures the inversion algorithm precision that remains almost constant when migrating from the existing to the new-generation sensor synergism.

The IASI-NG+UVNS retrieval algorithm parametrization has been optimized to increase at most the sensitivity in the lowest layers of the atmosphere (as close as possible to human biosphere), rather than decreasing the total retrieval error. Hence, the major gain of using the multispectral synergism of EPS-SG sensors with our retrieval approach concerns DOF-3km and Hmax-3km. With respect to IASI+GOME-2, the mean DOF-3km of IASI-NG+UVNS increases over both land (from 0.29 to 0.75) and ocean (from 0.21 to 0.66), which is respectively 159% and 214% higher than using present instrumentation. Accordingly, the mean height of maximum sensitivity in the LMT decreases down to 1.43 km over land and 2.09 km over ocean, which is approximately 1.03 km and 1.30 km below that of IASI+GOME-2. In addition,

IASI-NG+UVNS can also provide reliable ozone retrievals below 2 km of altitude, with an average DOF-2km of 0.52 (land) and 0.42 (ocean) and a mean Hmax-2km of 1.29 km (land) and 1.96 km (ocean). It seems to be able to observe ozone layers of 2-3 km thickness and distinguish if ozone plumes are located in the lowermost troposphere or just above it, between 3 and 6 km.

645 It is worth noting that additional challenge will be encountered for real retrievals using high SNR spectra from IASI-NG and UVNS. Indeed, as noise will be lower for such measurements, new sources of errors will be significant (i.e., surface properties accuracy, trace gasses variability). Such additional errors are not considered here and might degrade the capability of the retrieval. Results presented here are then an upper limit of the capability expected for IASI-NG+UVNS multispectral synergism to probe ozone pollution.

650 Nevertheless, IASI-NG+UVNS shows a unique capability to provide high confidence O₃ retrievals in the first 2-3 km of the atmosphere that should significantly improve regional ozone estimates for air quality studies. Further work should assess the potential impact on ozone forecasts, when assimilating this new multispectral product in a chemical transport model independent from MOCAGE.

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