On the potential of a neural network-based approach for estimating XCO2 from OCO-2 measurements

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Abstract. In David et al (2021), we introduced a neural network (NN) approach for estimating the column-averaged dry air mole fraction of CO_2 (XCO2) and the surface pressure from the reflected solar spectra acquired by the OCO-2 instrument. The results indicated great potential for the technique as the comparison against both model estimates and independent TCCON measurements showed an accuracy and precision similar or better than that of the operational ACOS (NASA's Atmospheric CO_2 Observations from Space retrievals – ACOS) algorithm. Yet, subsequent analysis showed that the neural network estimate often mimics the training dataset and is unable to retrieve small scale features such as CO_2 plumes from industrial sites. Importantly, we found that, with the same inputs as those used to estimate XCO2 and surface pressure, the NN technique is able to estimate latitude and date with unexpected skill, i.e. with an error whose standard deviation is only 7° and 61 days, respectively. The information about the date mainly comes from the weak CO_2 band, that is influenced by the well-mixed and increasing concentrations of CO_2 in the stratosphere. The availability of such information in the measured spectrum may therefore allow the NN to exploit it rather than the direct CO_2 imprint in the spectrum, to estimate XCO2. Thus, our first version of the NN performed well mostly because the XCO2 fields used for the training were remarkably accurate, but it did not bring any added value.

Further to this analysis, we designed a second version of the NN, excluding the weak CO_2 band from the input. This new version has a different behaviour as it does retrieve XCO2 enhancements downwind of emission hotspots, i.e. a feature that is not in the training dataset. The comparison against the reference Total Carbon Column Observing Network (TCCON) and the surface-air-sample-driven inversion of the Copernicus Atmosphere Monitoring Service (CAMS) remains very good, as in the first version of the NN. In addition, the difference with the CAMS model (also called *innovation* in a data assimilation context) for NASA Atmospheric CO_2 Observations from Space (ACOS) and the NN estimates are correlated.

These results confirm the potential of the NN approach for an operational processing of satellite observations aiming at the monitoring of CO_2 concentrations and fluxes. The true information content of the neural network product remains to be properly evaluated, in particular regarding the respective input of the measured spectrum and the training dataset.

1. Introduction

There is a growing interest for the monitoring of CO_2 from space. The aim is not so much the atmospheric concentration, which is already known with high accuracy, but rather the CO_2 fluxes. Indeed, there is a need to monitor natural fluxes of CO_2 to better understand their driving factors and to improve land and ocean models. There is also a strong societal requirement to monitor the CO_2 anthropogenic emissions at national and more detailed scales. For these objectives, a series of dedicated instruments have been put in orbit since the Greenhouse Gases Observing Satellite

(GOSAT, Yokota et al., 2009) and the second Orbiting Carbon Observatory (OCO-2 Eldering et al., 2017), launched in 2009 and 2014, respectively, and still operated at the time of writing. This new and evolving constellation is directly supported by Japanese, US, Chinese and European space agencies (CEOS Atmospheric Composition Virtual Constellation Greenhouse Gas Team, 2018).

50 The OCO-3 instrument was launched in 2019 and is flying attached to the International Space Station (ISS) with a focus on the imagery of cities and industrial sites (Taylor et al., 2020). These targets are also the main focus of the CO2M mission under development at ESA.

These missions all use the same general principal to estimate the CO_2 concentration in the atmosphere. They measure the reflected solar light at high spectral resolution, which allows

55 identifying absorption lines whose depth is related to the total amount of gas along the atmospheric path. Atmospheric CO_2 shows a number of such lines close to 1.61 and 2.06 μm so that these spectral regions are targeted. Because the absorption is more intense at 2.06 μm, this measurement channel is often referred to as the *strong-CO₂* (or sCO2) band, whereas the 1.61 μm is the *weak-CO2* (wCO2) band. The line depth is also affected by the surface pressure and the amount of

60 scattering particles in the atmosphere. To identify and account for their contribution, an additional measurement is made around the oxygen absorption band at 0.76 μm (O_2 band). The combination of these measurements makes it possible to estimate the column-averaged dry air mole fraction of CO_2, referred to as XCO2 (Crisp et al., 2004). Note that the MicroCarb instrument, to be launched by CNES in 2022, will have a fourth band at 1.27 μm. This band serves the same purpose as the O_2

65 band; it has the advantage of being spectrally closer to the CO2 bands and the disadvantage of being affected by airglow (Bertaux et al., 2020).

The interpretation of measured spectra in terms of XCO2 is achieved through *full physics* algorithms that explicitly account for the absorption by CO_2, O_2 and water vapor, for scattering in

70 the atmosphere and for non-lambertian reflection on the Earth surface. The modeling must also account for the instrument line shape function and doppler effects. The inversion process is iterative and starts from a prior estimate of all atmospheric parameters. It is very computer-time consuming. The processing of OCO-2 data has shown systematic differences between the measured spectra and those modeled after inversion which led to the development of empirical

75 corrections to the measured spectra (Crisp et al., 2012; O'Dell et al., 2018). In addition, raw XCO2 retrievals show significant biases against reference ground-based retrievals (Wunch et al., 2011b, 2017). These biases, together with the comparison against modelling results, led to the development of empirical corrections to the retrieved XCO2.

The need for empirical corrections to the full-physics algorithms and the considerable computer

80 load motivated us to develop an alternative approach described in David et al. (2021). We used an artificial network technique (NN) which is purely empirical, without the use of any radiative transfer model. Our hypothesis was that the CAMS (Copernicus Atmosphere Monitoring Service) model constrained by surface air-sample measurements provides a fairly accurate estimate of the atmospheric CO_2 concentration, including the growth rate over multiple years (Chevalier et al.,

85 2019; see also Figure 8). Indeed, the seasonal cycle of CO_2 together with the growth rate generate a set of XCO2 samples with a well-known variability. The uncertainties on the modeling (≈1 ppm) are small with respect to the range of XCO2 samples that is available in the multi-year dataset (20 ppm). As a consequence, although CAMS is not the truth, it may be used for supervised learning. Note that other 4D description of the atmospheric composition could have been used for our work.

90 We chose CAMS mostly for practical reasons; the same procedure may be attempted with another modeling dataset.

In practice, we used a series of OCO-2 spectra from a 5 year-dataset for the NN training. We then applied the NN to the observations that were not used in the training and compared their estimates to both the same CAMS model used for the training and also the fully-independent set of Total

95 Carbon Column Observing Network (TCCON, Wunch et al., 2011a) observations. The results indicated an accuracy and precision that were similar, if not better, to that of the ACOS algorithm.

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More recent results challenged our interpretation of the NN skill. In particular, the XCO2 estimates of the NN did not show significant enhancement downwind of large power plants, unlike the product of the NASA Atmospheric CO_2 Observations from Space (ACOS) full-physics algorithm. This is shown in the following together with our interpretation. A new version of the NN resulted from this interpretation, that retains the high accuracy of the first version, while being much more independent from the training dataset.

In the following, Section 2 describes the main characteristic of the NN approach and the training procedure. Section 3 presents the limitation of the first version of the NN, as it shows no innovation with respect to the training dataset. Section 4 describes and justifies a new version of the NN approach. Section 5 discusses the results, suggests directions for improvements, and concludes.

2. Data and method

The NN described in this paper estimates XCO2 from spectra measured by the OCO-2 satellite over land. Most of the analysis is made with the spectra acquired in nadir mode, but we have also developed a version for glint acquisition that is described and commented at the end of section 4. Conversely to the analysis in David et al. (2021) we now use all cross-track footprints. A single NN is used to process all footprints even though the spectral elements of different footprints correspond to different sampled wavelength.

We use spectral samples in the three bands of the instrument (around 0.76, 1.61 and 2.06 μm). They have footprints of ~ 3 km^2 on the ground. In principle, each band is described by 1016 samples but some are marked as bad either because some of the corresponding detectors died at some stage or because of known temporary or permanent issues. We systematically remove 15 spectral samples that are flagged in about 80% of the spectra and 478 pixels in the band edges. Conversely, we do not remove the samples that are affected by the deep solar lines, and we let the NN handle these specific features. Because the information in the spectrum is mostly in the relative depth of the absorption lines, and not in their overall amplitude, we normalize each spectrum by a radiance that is representative of the offline values (i.e. the mean of the 90-95% range for each spectrum). This essentially removes the impact of the variations in the surface albedo and in the solar irradiance linked to the sun zenith angle.

Figure 1 offers a graphical representation of the NN. As input, we use the three band spectra (or a subset, see below), the observation geometry (Sun and view zenith angle: SZA and VZA, and relative Azimuth: AZI). Some versions also use the surface pressure (Psurf) as input. No explicit information is provided to the NN regarding the location or date of the observation. The inputs feed all the neurons of a first "hidden" layer. We use a fully connected neural network, which means that all the neurons are connected to the neurons of the previous and next layer. We have attempted NN versions with a variable number of hidden layers (a single one was used in David et al. (2021)). Each neuron computes a weighted sum of the inputs and derives a single output on the basis of either a sigmoid function or a "rectified linear unit". The loss is derived from the Mean Absolute Error. The weights of the input variables to the neurons are adjusted iteratively with the standard Keras library (Keras Team, 2015) for an optimal agreement between the NN output and a reference.

The NN training is based on OCO-2 radiance measurements (v10r) acquired between February 2015 and December 2019. We make use of XCO2 estimates and the quality control filters of the ACOS L2Lite v9r products: only observations with *xco2_quality_flag*=0 are used. For the validation of the NN estimates, we also use observations with relaxed quality requirements. For versions of the NN that use the surface pressure as input, we use the estimate that is provided together with the OCO-2 data and that is derived from the Goddard Earth Observing System, Version 5, Forward Processing for Instrument Teams (GEOS5-FP-IT) created at Goddard Space Flight Center Global Modeling and Assimilation Office (Suarez et al. 2008 and Lucchesi et al. 2013). The weather model pressures have been adjusted to the sounding surface height.

Our analysis makes use of the CAMS CO_2 atmospheric inversion (Chevallier et al., 2010; version
150   19r1). This product was released in July 2020 and contributed, e.g., to the Global Carbon Budget
2020 (Friedlingstein et al., 2020). It results from the assimilation of CO_2 surface air-sample
measurements in a global atmospheric transport model run at spatial resolution 1.90° in latitude and
3.75° in longitude over the period 1979-2019 and using the adjoint of this transport model. Neither
satellite retrievals nor TCCON observations were used for this modelling. For each OCO-2
155   observation, XCO2 is computed from the collocated concentration vertical profile, through a simple
integration weighted by the pressure width of the model layers. Note that the model layers use
"dry" pressure coordinates so that there is no need for a water vapor correction in the vertical
integration. The XCO2 from CAMS is used both for the training and the evaluation, although using
independent datasets: The "training" dataset is a 3% random sample of the full dataset. The
160   observations that are used for the training are earmarked and not used for further evaluation.

3. Initial results and interpretation

David et al (2021) described a first version of the NN approach to estimate XCO2. In this first
version, the surface pressure was not used as input, and the training was made on observations
acquired during even months, while the validation used observations of the odd months. The results
165   were surprisingly good in that the statistical difference to both the CAMS modeling and the
independent TCCON observations indicated an accuracy similar or better than that of the CAMS
product. Further analysis posterior to the publication were worrisome, however.
First, we found that well-documented local enhancements of XCO2 in the ACOS product (e.g.,
Nassar et al., 2017; Reuter et al., 2019), also referred to as *plumes*, did not show up in the NN
170   product. We analyzed in particular a case over South Africa acquired on August, 31st, 2016 an
illustration of which is provided on Figure A1. Over a distance of ≈100 km, the ACOS product
shows several well identified enhancements of ≈5 ppm, whereas the NN product does not show any
significant pattern. The presence of large coal power plants upwind of the OCO-2 observations
makes the enhancements trustworthy. We found many similar cases where the NN did not display
175   an XCO2 plume where ACOS did. We concluded that the NN did reproduce the seasonal variation
of XCO2 together with the growth rate but was unable to identify small-scale features. Since all
observations are processed independently, we could not interpret this apparent incoherence.
Second, we made an experiment where the training dataset is biased by 1 ppm for the observations
acquired during a single month (within the full period of 50+ months). When applied to the
180   validation dataset, the differences to CAMS show a bias of ≈0.5 ppm but only for the observations
that are within a few weeks of the biased period. This is rather surprising as the observation date is
not an input of the NN. Still, these results provide a clear indication that this version of the NN is
somehow sensitive to the observation date.
To investigate the issue, we developed and trained a new NN with the same inputs, but aiming at
185   estimating the date, latitude and longitude. For the training, we used the true values of these
parameters and we analyzed how the NN was able to make an estimate based on the inputs (the
spectra and the observation geometry). Figure 2 shows the histograms of the errors when applied to
the independent dataset.

The results indicate that the NN approach is able to make a reasonable estimate of the location and
190   date of the observation based on the spectra and the observation geometry. The standard deviation
of the latitude error is on the order of 7° and there is no significant difference with the footprint.
One may expect that this information is largely derived from the observation geometry that changes
with the latitude (both the SZA and the azimuth do). One argument in favor of this hypothesis is
195   that the precision of the longitude estimate is much worse, with a standard deviation on the order of
58°. Indeed, for a given day, the observation geometry is nearly the same for all successive orbits;
thus, there is no information in the observation geometry to estimate the longitude, while there is
such information for the latitude. As for the date, the standard deviation is ≈ 61 days, or 2 months.
Clearly then, in the input data of the NN, there is indirect information about the observation date

and latitude and this was a surprise to us. Indeed, when describing the NN approach in David et al (2021), we argued that the NN had no information on the measurement date, as successive observations from the same day-of-year and location, but different years, were made with the exact same observation geometry.

210 The various histograms of Figure 1 were made using a single (O2) band, a combination of the O2 band with either CO2 band, and all three bands. The most striking difference between the various histograms is for the date estimate. Indeed, the accuracy strongly degrades when the wCO2 band is not included. The combination of O2+wCO2 bands leads to a much better accuracy (a factor of more than 3 on the standard deviation) than that obtained with O2+sCO2. The other differences on
215 the histograms are not as large.

How does the NN gets an indirect information on the observation date, and why is this information somehow contained in the wCO2 band? Our best interpretation is that the weak CO_2 spectrum is sensitive to the upper atmosphere CO_2 concentration that is rather well mixed while increasing regularly in time. The absorption lines in the sCO2 band are much stronger so that their centers are
220 saturated in the spectra. As a consequence, the CO_2 signal is more in the line wings which are more sensitive to the higher pressure (lower altitude) levels. The wCO2 lines are not saturated and the spectrum shape may provide the information for an estimate of the high-altitude CO_2 concentration. We investigated another hypothesis that the wCO2 detector shows an evolution in time, that could be used by the NN to infer the observation date. However, we did not find any indication of such
225 behavior. Thus, at this point, the stratospheric CO_2 hypothesis is physically plausible and is our best hypothesis because of no other. Note however that we have investigated the correlation between the longitudinal anomalies of stratospheric CO_2 in the CAMS model and the error on the date estimate by the NN approach. No such correlation was found. Thus, either our hypothesis is wrong or the description of the longitudinal variations of stratospheric CO_2 in CAMS offer a poor
230 representation of the reality. Both hypotheses are plausible.

These results clearly demonstrate that the input data to the NN provides indirect information on the date and latitude. Atmospheric simulations such as those of CAMS indicate that XCO2 variations are mostly a function of time and latitude. Indeed, on average, the deviations of XCO2 along the
235 longitudes are on the order of 0.5 ppm (standard deviation). They are however larger (≈1 ppm) over the Northern hemisphere where most of the observations analyzed here are acquired. We hypothesize that our first version of the NN, as published in David et al. (2021) obtains a proxy of the latitude and date, and outputs the corresponding CAMS value. Based on the CAMS simulation, we found that the typical uncertainty on the position and date (σ_{lat}=7°, σ_{lon}=58° and σ_{date}= 60 days)
240 leads to a 1-sigma error of 0.91 ppm on XCO2 (difference between the values at the true and perturbated location/date). This value appears consistent with the precision obtained with our first version of the NN. Note however that this statistical difference gets larger when considering locations consistent with the OCO-2 observations that are used here. The important point is that the error increases considerably (a factor of 2) for degraded precisions on the location and date with a
245 different version of the NN that is discussed below.

4. A new version of the neural network

As shown above, the NN appears to use the wCO2 band to derive a proxy of the observation date which makes it possible, together with the proxies of the location, to estimate XCO2 based on the statistical distribution of the CAMS XCO2. To avoid this feature, an option is to not use the
250 information from the wCO2 band. We therefore developed a similar version of the NN but without this band (i.e. only the O2 and sCO2, together with the observation geometry). With this version, the behavior of the NN changes markedly. The most important feature is that the NN now reproduces the XCO2 plumes that are shown by the output of the ACOS algorithm. Two representative examples are shown in Figure 3. These cases demonstrate that the NN does produce
255 XCO2 features that are not in the training database, as we expected. The NN is trained on the

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260   variations of XCO2 caused by the atmospheric growth rate and the surface flux seasonal cycle. It
      identifies signatures in the spectra that relate to the CO_2 atmospheric content. These signatures can
      then be used for an estimate of XCO2, even for situations that are poorly reproduced in the training
      dataset.
      In addition to the change in the band selection, and posterior to the result shown in Figure 3, we
265   made several other modifications to the NN algorithm:
      First, we decided to use the surface pressure from the weather forecast model as an additional input
      to the NN. In David et al. (2021), the surface pressure was an output of the NN model. It was used
      to demonstrate the capability of the NN approach to interpret the spectral shapes in terms of
      atmospheric parameters. Indeed, the estimate of the surface pressure could be compared to an
270   independent estimate from numerical weather analyses which are known to be precise within ≈1 ‰.
      However, the surface pressure may alternatively provide useful information to the NN for the
      interpretation of the spectra, as it does in the full-physics algorithms in the form of a prior estimate
      and also for the derivation of the bias-corrected product.
      Second, we decided to increase the number of NN hidden layers to 5 (instead of 1 in David et al.
275   2021). Our experience indicates that, with a larger number of layers, there is less over-fitting of the
      training spectra, i.e. there is a better agreement between the loss of the training and that of the test
      dataset. An increased number of hidden layers also leads to slightly better performance, in
      particular for the NN that was designed for the land-glint observations (see below).
      Third, we developed a similar approach for the glint cases (still over land). Our initial fear was that
280   it would be more difficult for the NN to handle glint observations because of (i) larger variations in
      the optical path than for the nadir mode and (ii) the doppler effect that may affect the absorption
      line positions on the input spectra. This is why our first attempts focused on the nadir cases, but
      there is a need to also exploit the many observations acquired in glint mode.

285   Figure 4 shows the inter-comparison of the XCO2 estimated from CAMS, ACOS and NN. All
      three datasets are highly consistent, with a statistical difference around 1 ppm and little bias. Let us
      recall that there is no satellite data input to the version of CAMS that is used here, so that it is fully
      independent from ACOS. The 1.06 ppm standard deviation of their differences demonstrates that
      both product precisions are better than this number. CAMS and the NN are not as independent
290   because the latter is trained with the former (but using different space-time locations). Let us stress
      that any bias in CAMS may be transferred to the NN product. Thus, a high agreement between
      CAMS and the NN product is not a demonstration of the latter accuracy. Still, it has been shown
      that the NN retrieves features that are not in CAMS which indicates some independence between
      the satellite product and the model. The standard deviation of their differences is 0.85 ppm. The
295   quadratic difference between NN and ACOS is a strong function of the sCO2 albedo as shown in
      Figure 5: it decreases from ≈1.5 to ≈0.75 ppm as the sCO2 band albedo increases from 0.10 to 0.45.
      A better accuracy of the satellite product with stronger surface albedo is expected as (i) the
      measurement signal to noise gets higher and (ii) the relative contribution of atmospheric scattering
      to the signal decreases. The estimate precision is also a function of the O2 band albedo, but this
300   effect is not as strong and the O2 band albedo shows less variability than that of the sCO2 band.
      Figure 4 also shows that the slope of the best fit of the satellite products against CAMS are small
      but of opposite side with respect to 1. As a consequence, there is a more significant slope deviation
      from 1 (0.97) between the two satellite products.
      Figure 6 provides further information on the differences between the remotely-sensed products and
305   the CAMS estimate. The histograms are close to Gaussian and confirm that NN is closer to CAMS
      than the ACOS counterpart. An interesting feature is that both the NN-CAMS and ACOS-CAMS
      differences depend on the cloud flag (*cloud_flag_idp*), which indicates that this flag has some
      value. The difference between the cloud contamination histogram remains small however, and does
      not deserve to disqualify the observations with a cloud flag of 2. Here, we only use the "definitely
310   clear" and "probably clear" cases (flags of 3 and 2). The population of the lower value cases
      ("definitely cloudy" and "probably cloudy") is much smaller and the histogram for these cases are

not shown, while they show further degradation. It is difficult to elaborate further as the true nature
315   of the cloud contamination in the cases classified as "probably clear" is unknown.

Figure 7 is based on the satellite product innovation, i.e. the difference to the model estimates.
Indeed, one may consider that the model provides current knowledge on the XCO2 distribution,
constrained by surface air-sample measurements and atmospheric transport. The satellite product
320   has the potential to improve this knowledge, but only as much as the difference with the model
estimate. Typical values are around 1 ppm. The interesting result brought by Figure 7 is that the
two satellite estimates are significantly correlated. This provides further evidence that the NN
estimate is not only a reconstruction of the training dataset (CAMS) with some noise. Indeed, when
NN differs from the model, ACOS, the independent satellite product, tends to agree.
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Finally, Figure 8 shows a comparison of the model and remotely-sensed estimates of XCO2 against
the reference retrievals of the TCCON network. Although the OCO-2 satellite platform can be
oriented so that the instrument field of view is close to the surface station, we only use here nadir
data. Indeed, the NN was not trained on the target data and can only be used to process
330   measurements that have been acquired in observation configurations that are similar to those of the
training. We thus have to rely on nadir or glint measurements acquired in the vicinity of TCCON
sites. In the following, we use nadir measurements that are within 5 degrees in longitude and 1.5
degrees in latitude to the TCCON site. For the reference, we average the TCCON estimates of
XCO2 within 30 minutes of the satellite overpass. No attempt was made to correct for the different
335   weighting functions of the surface and spaceborne remote sensing estimates. Statistics per station
are provided in Table 1. The biases vary significantly among stations, although they are generally
less than 1 ppm (in amplitude). Two stations, Pasadena and Zugspitze, show a large negative bias
for both satellite estimates as well as the model. For Pasadena, it may be interpreted as the impact
of the city on the atmosphere sampled by the TCCON measurement, while the atmosphere at the
340   location of the satellite observation (which may be several hundred km away) is less affected.
Zugspitze is a high-altitude site (2960 m), so that the atmospheric column sampled by the
sunphotometer does not have the same vertical representativeness as that of the satellite observation
(in addition to the spatial distance, that is common with other sites). A large negative bias is also
found at Eureka (80.05°N). The fact that the difference with the CAMS model at this site is much
345   larger than for other sites could hint at an issue in the sunphotometer product there. Conversely,
there are large positive biases at Burgos and Ny-Ålesund (78.9°N, very close to the latitude of
Eureka). Since the model and satellite estimates somewhat agree, one may also question the
TCCON calibration at these sites. For other stations, which forms the large majority, the biases are
smaller than 1 ppm and there is a fair consistency between the satellite products in the sense that the
350   sign of their bias is the same in most cases. The range of the difference with TCCON varies among
stations. The best satellite-TCCON agreement is found at the Lamont station which, interestingly,
is also the one with the most coincidences. Excellent agreement is also seen at Darwin, Edwards,
Park Falls and Bremen. The comparison with TCCON does not allow favoring one satellite
estimate versus the other. Focusing on the stations with a large number of observation (25
355   overpasses or more), the NN estimates appears slightly better than ACOS at Darwin, Edwards,
Garmisch, Orléans and Bialystok, while it is the opposite at Saga, Park Falls, and Sodankylä. The
figure (and table) also clearly shows that the CAMS product offers a better agreement with the
TCCON data than any of the satellite estimates in most cases. The high quality of the CAMS
modelling used in this paper, at least over the TCCON site, provides further justification of its use
360   as a training dataset.

We have applied a very similar procedure to the OCO-2 observations acquired in glint mode over
land. An evaluation of the estimate performance is shown in Figure 6, 7, A3 and A4. The
conclusions are very similar to those obtained for nadir. The agreement with CAMS is slightly
365   degraded with respect to the nadir cases (0.92 ppm vs 0.85 for the "certainly clear" observations)

but somewhat closer than that of ACOS (Fig. 6 and S3). The deviations from the model of the two satellite estimates are significantly correlated, and the correlation coefficient is even larger than that
375 derived for nadir observations (0.45 vs 0.39, Figure 7). The comparison with the TCCON estimates leads to the same conclusions as those described above for the nadir cases.

5. Discussion and Conclusion

This paper follows on from David et al. (2021) in which we described a neural network-based technique to estimate XCO2 and the surface pressure from the OCO-2 spectral measurements. An
380 important message is that our interpretation of the results in that earlier study was incorrect. The NN developed in that paper reproduced the statistical variations of the training dataset (CAMS) and was unable to generate features, such as plume from emission hot-spots. Thus, contrary to our claims, the NN method, as presented in that paper, could not be used to process OCO-2 and generate XCO2 estimates with any real value. We have shown here that a NN-based procedure is
385 able to estimate the latitude and date of the observation with a reasonable accuracy. This was unexpected to us as we wrote in David et al. (2021) "Let us recall that the NN input does not contain any information on the location or date of the observation. This is a strong indication that the information is derived from the spectra as the NN does not "know" the CAMS value that corresponds to the observation location". Our interpretation was wrong. In fact, the NN input can
390 somehow be used by the NN for a fairly accurate estimate of the latitude and date. Because most of XCO2 variations are a function of latitude and date, this information could be used by the NN to generate a reasonable estimate, i.e. one that mimics the main variations in the training dataset.
A question remains on the indirect information that is used by the NN to estimate the observation date. The fact that the precision on the date estimate is much better when using a combination of
395 the O2+wCO2 rather than of the O2+sCO2 suggests that the information lies in the wCO2 band. Our best hypothesis is that the wCO2 spectra contains some information on the stratospheric CO_2 whose concentration is well-mixed while increasing regularly with time and implicitly contains, therefore, an information on the observation date. Further testing this hypothesis would require, for instance, the identification of some anomaly in the stratospheric CO_2 (linked to a specific
400 atmospheric circulation) that would show up as a significant error on the date estimate made by the NN. We have not been able to identify such feature.
Despite this initial setback we have continued our analysis on the potential of the NN to process the OCO-2 spectra. A strong motivation relied on the results obtained for the estimate of the surface pressure. Indeed, David et al. (2021) showed that the NN could estimate the surface pressure with
405 an accuracy on the order of 3 hPa. The spatial and temporal variations of the surface pressure, at the scale of the potential accuracies on the date and location, are very much larger than this number, so that the NN estimate cannot rely on this kind of indirect information. This provided a strong indication that the NN method has the potential to extract meaningful information from the spectra itself.
410 We have therefore developed a new version of the NN excluding the wCO2 band from the inputs. In this version, the behavior of the NN is very much different from the earlier version as it generates features that are not in the training dataset. This clearly shows that the NN uses the signature of XCO2 contained in the sCO2 spectra to make an XCO2 estimate. The accuracy of this estimate is similar to the one obtained with the first version of the NN, and similar to that of the ACOS
415 products. This is confirmed by the comparison of the XCO2 estimates against the TCCON retrievals. Another strong argument that the NN XCO2 estimate contains true information and is not only a noisy copy of the training dataset is that the innovations of the two satellite estimates, i.e. the differences to the model data, are significantly correlated (Fig. 7).
Note that we use here a single neural network for the eight footprints of the OCO-2instrument. We
420 analyzed whether the result performance, assessed as the standard deviation of the differences with CAMS, is a function of the footprint. The statistics are very similar for all, except for footprint #2 that shows slightly higher deviation for both the ACOS and the NN satellite products (a difference of ≈0.1 ppm to the mean of ≈1 ppm).

430   These results confirm that the NN technique has a strong potential to process the OCO-2 observations, as well as those from forthcoming missions aiming at the observation of CO_2 from space such as the forthcoming MicroCarb (Pascal et al. 2017) or the CO2M constellation (Sierk et al. 2019). As discussed above, the current version does not use the wCO2 band at all and this may be seen as a loss of useful information. There is therefore a need to select appropriate spectral
435   samples in the wCO2 band rather than discarding them all. It requires improved understanding of the indirect information that is used by the NN to estimate the observation date and location.

The NN technique has two obvious advantages compared to the physical methods that are used to process the OCO-2 observations as well as other instruments with similar objectives: (i) a much
440   smaller computational burden and (ii) no need for a de-bias procedure (O'Dell et al 2018, Kiel et al. 2019). Our implementation still faces remaining challenges, that we discussed in David et al. (2021).

The first challenge is the cloud detection. All the analysis described in this paper relies on the
445 ACOS cloud detection and only the observations identified as "clear" are processed. Our analysis demonstrates the potential of the NN approach but is currently not independent from ACOS. We are currently evaluating independent approaches for the cloud detection. Although the NN described here aims at an estimate of XCO2, we have shown earlier that the same tool can be used for an estimate of the surface pressure with a 1 sigma precision on the order of 3 hPa for clear-sky
450   cases. Numerical weather analyses are actually better than that. Thus, one may use the comparison of the surface pressure estimate from the NN to the numerical weather data for an easy identification of perturbations to the spectra that are linked to cloud or large aerosol contamination. This would allow an easy and rapid quality indicator for the selection of observations that may be used for XCO2 estimates, either using a physics-based algorithm or a NN approach. This idea
455 remains to be evaluated.

The second challenge concerns the absence of a quantitative indication of the amount of information that the NN takes from its prior information (contained in the training database) vs. the amount of information that the NN takes from the measured spectra. For Bayesian full-physics
460   retrievals, these weights are represented by the *averaging kernel* (Rodgers, 1990) that allows a clean comparison of each retrieval with 3D atmospheric models, at least in theory (see the discussion about the practical difficulties in Chevallier, 2015). The NN training targets the CO_2 column with a homogeneous weighting along the vertical but this can hardly be achieved without some contribution from the prior information. This challenge may be evaluated in the future on the
465 basis of radiative transfer simulations.

The third challenge concerns the absence of a quality indicator with the XCO2 estimate. With the physical methods, the spectrum residuals provide an efficient mean to identify cases when no satisfactory agreement can be found between the measured and modelled spectra. With the NN
470   approach, there is no uncertainty associated to each retrieval. Our analysis has shown that the apparent precision (evaluated against CAMS) is a strong function of the surface albedo. There may be other geophysical variables that pilot the uncertainty. To provide precision estimates for each NN-based XCO2 estimate, ensembles of randomized trainings, where uncertain parameters or input/output variables are varied adequately (e.g., Chau et al. 2021), or analytical estimates (Aires et
475 al., 2004) should be explored.

The last challenge concerns the need for a high-quality training dataset, in the context of increasing XCO2. The comparison against the TCCON observations (Figure 8) demonstrates that the CAMS inversion product meets this requirement. In fact, there are strong indications that CAMS remains
480   better than the satellite products, at the very least in terms of global precision. However, because of the atmospheric growth rate of CO_2, the training must be regularly updated. Indeed, with a frozen

Moved down [1]: absence of a quality indicator. With the physical methods, the spectrum residuals provide an efficient mean to identify cases when no satisfactory agreement can be found between the measured and modelled spectra.

Moved down [2]: To provide precision estimates for each NN-based XCO2 estimate, ensembles of randomized trainings, where uncertain parameters or input/output variables are varied adequately (e.g., Chau et al. 2021), or analytical estimates (Aires et al., 2004) should be explored. ¶

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training dataset, the true real-time XCO2 progressively leaves the training range. The NN approach requires a training dataset that is representative of the observation and would then lead to underestimates. For quasi-near-real time data assimilation (e.g., Massart et al., 2016), the training dataset must therefore gradually integrate recent high-quality XCO2 data, but without sacrificing robustness.

As a final remark, we call for caution. We have been tricked by the NN ability to generate a consistent description of the atmospheric XCO2 in our first analysis. It is difficult to ensure that we are not tricked again. The source of the information that leads to a fairly accurate estimate of the date, when using the weak CO2 band, remains unclear. As a consequence, although it is demonstrated that the new version of the NN generates structures that are not in the training dataset, there may be biases in the CAMS modeling that have a significant influence on the NN product.

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Code/Data availability
The codes used in this paper and the CAMS model simulations are available, upon request, from the author. The OCO-2 and TCCON data can be downloaded from the respective websites.

Author contributions
FMB designed the study. PC and LD developed the codes and performed the computations. All authors shared the result analysis.

Competing interests
The authors declare no competing interests.

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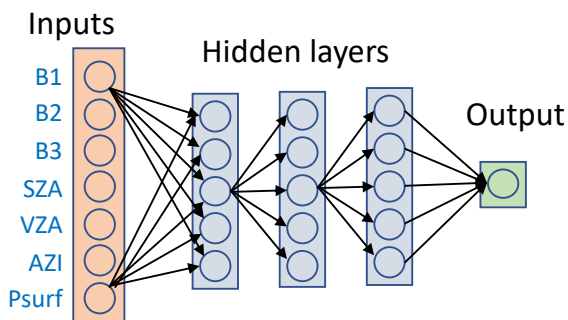
Figure 1: Graphical representation of the NN used in this paper. The outputs from all neurons feed in all neurons of the next layer. There is a variable number of hidden layers. Similarly, there is a choice on the number of neurons in each layer. Not all inputs are used for the various versions of the NN that are described in this paper.

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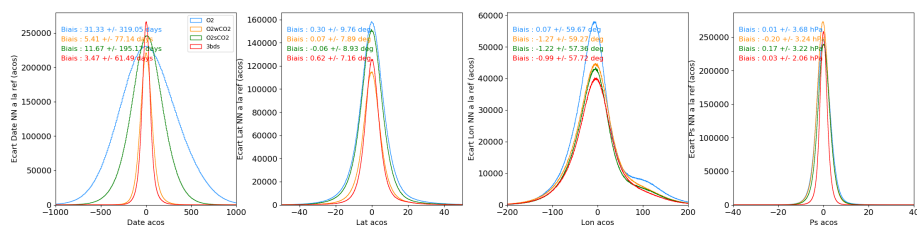
Figure 2: Analysis of the ability of the NN to estimate the date, location (latitude, longitude) and surface pressure from the input spectra and observation geometry. The graphs show the histograms of the differences between the NN estimate and the true value. Several versions of the NN were analyzed using either all three bands (red), only the wCO2 and O2 bands (orange), sCO2 and O2 (green) and only the O2 band (blue).

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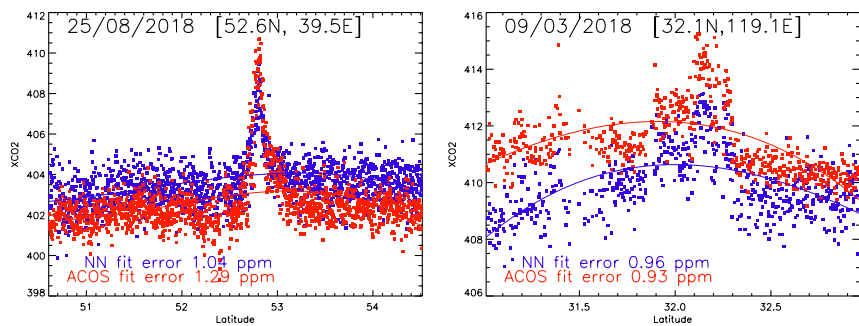
Figure 3: Two examples of XCO2 plumes that are captured by the ACOS bias-corrected XCO2 estimates. These were not shown by the first version of the NN algorithm (an example shown in Figure A1), but are well captured by the second version that does not use the wCO2 band (shown here). The NN estimates are in blue whereas the ACOS estimates are in red. The lines are simple polynomial fits on the XCO2 estimates and

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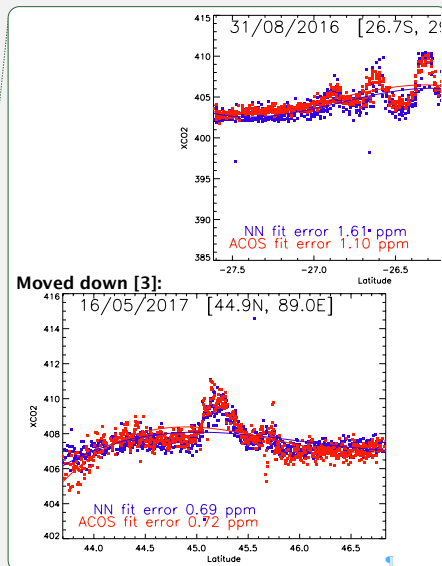
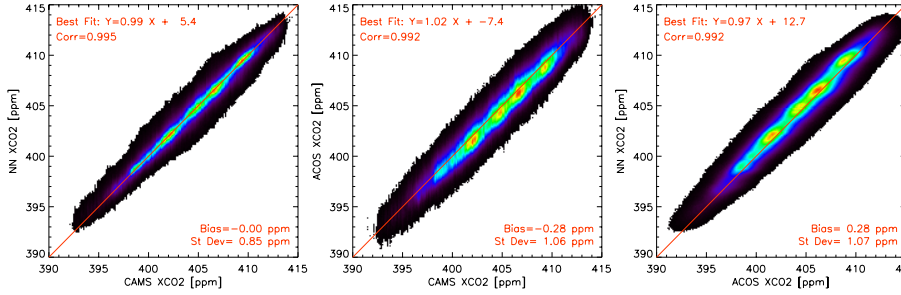

do not aim at capturing the plume signature. These cases were identified and discussed in Reuter et al (2019)

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Figure 4: Inter-comparison of XCO2 estimated from CAMS, ACOS, and the NN. The density histogram is based on nadir observations from February 2015 do December 2019. A similar figure for the glint cases is shown in the supplementary figure A3.

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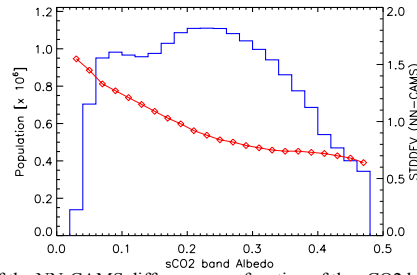
Figure 5: Standard deviation of the NN-CAMS difference as a function of the sCO2 band albedo (red, right scale). The computation is made over 0.02 bins, the population of which is shown by the blue line (left scale).

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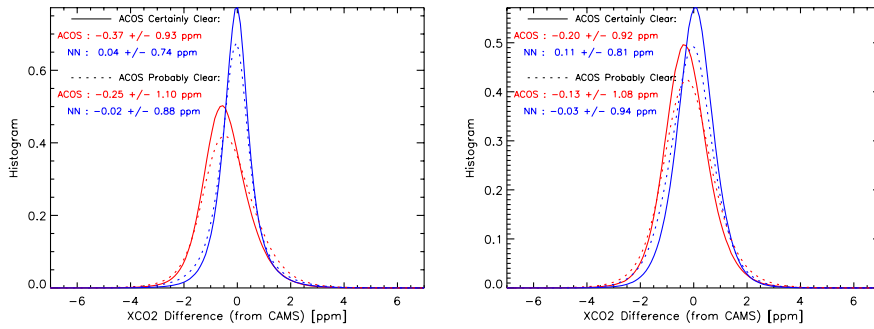
Figure 6: Histogram of the differences between either one of the two satellite datasets and the CAMS model. We distinguish cases when the flag *cloud_flag_idp* is "certainly clear" and "probably clear". The left figure is for the nadir dataset, whereas the right figure is for the glint.

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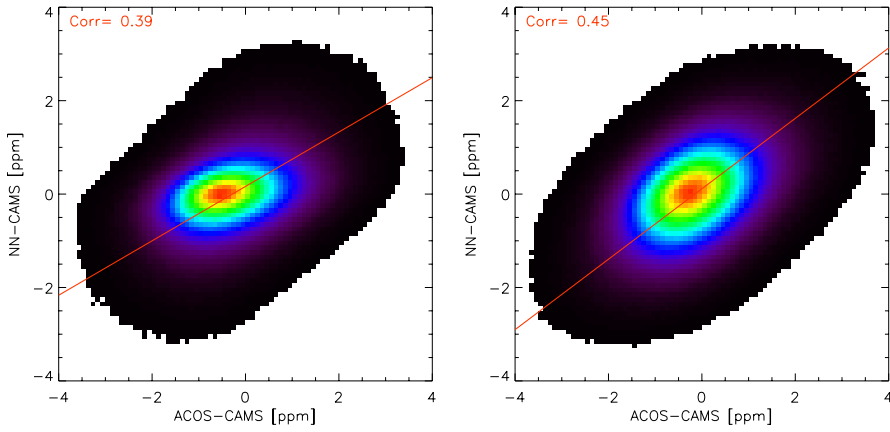
Figure 7: Density histogram of the innovation, i.e. the difference between the satellite product and the model estimates. differences between either one of the two satellite datasets and the CAMS model. The red line shows the result of a linear fit through the datapoints aiming at a minimization of the distance to the best line. The left figure is for the nadir dataset, whereas the right figure is for the glint.
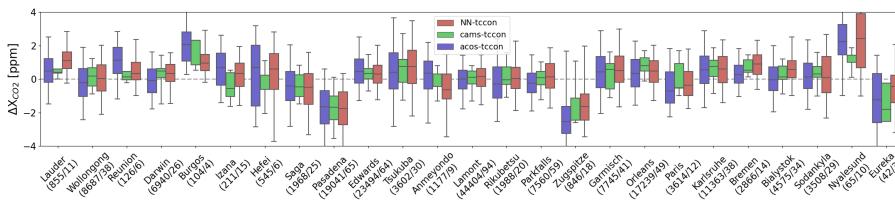
Figure 8: Statistics of the differences between the NN retrieval (red), the CAMS model (green) or the bias-corrected ACOS retrievals (blue) and the TCCON retrievals. The boxes indicate the 25-75% percentiles and the median is shown by the horizontal line within the box. The whiskers indicate the 5-95% percentiles. Stations are ordered by increasing latitudes. The numbers below the station name indicate the number of individual observations and coincidence days used for the statistics. The references of the various TCCON observations are provided in table 1. Figure A4 provide similar results for the Glint case

Table 1: TCCON stations used in this paper (Figures 8 and A4). The data have been obtained from the tccondata.org web site on Feb 4th, 2021.

Stations	[lat ; lon]	Alt [m]	Reference	Nadir CAMS / ACOS / NN			Glint CAMS / ACOS / NN		
				North/Nobs	Biases	Std Dev	North/Nobs	Biases	Std Dev
Lauder	[-45.04 ; 169.68]	370	Sherlock et al. 2017	11 855	0.4 0.5 1.1	0.2 1.2 1.0	53 5508	0.4 0.5 0.8	0.3 1.2 1.2
Wollongong	[-34.41 ; 150.88]	30	Griffith et al. 2017b	38 8687	0.1 -0.2 0.2	0.7 1.3 1.3	23 4059	-0.6 -0.9 -0.7	1.2 1.3 1.3
Réunion Island	[-20.90 ; 55.49]	90	De Mazière et al. 2017	6 126	0.2 1.0 0.6	0.3 1.4 1.2	6 123	-0.8 -0.5 -1.2	0.6 1.4 1.7
Darwin	[-12.43 ; 130.89]	30	Griffith et al. 2017a	26 6940	0.4 -0.1 0.4	0.7 1.1 1.0	28 7432	0.4 -0.2 0.4	0.6 1.2 1.1
Burgos	[18.53 ; 120.65]	35	Morino et al, 2018	4 104	1.3 2.0 1.5	0.7 1.3 1.0	9 789	0.3 0.6 0.2	0.4 1.3 1.1
Izana	[28.3 ; -16.48]	2300	Blumenstock et al. 2017	15 211	-0.5 0.6 0.6	0.8 1.3 1.1	6 183	-0.1 1.0 0.5	0.6 1.4 0.9
Hefei	[31.90 ; 118.67]	30	Liu et al. 2018	6 545	-0.2 0.3 0.3	1.0 2.1 2.0	9 1581	0.3 -0.5 -0.1	1.1 1.5 1.3
Saga	[33.24 ; 130.29]	10	Shiomi et al. 2017	25 1968	-0.4 -0.4 -0.3	0.8 1.5 1.6	33 2934	-0.3 -0.5 -0.8	0.6 1.4 1.4
Pasadena	[34.14 ; -118.13]	240	Wennberg et al. 2017b	65 19041	-1.8 -1.7 -1.6	1.1 1.5 1.5	51 13589	-1.6 -1.2 -1.5	1.1 1.3 1.4
Edwards	[34.96 ; -117.88]	700	Iraci et al. 2017	64 23494	0.3 0.5 0.5	0.6 1.2 1.0	70 25890	0.3 0.6 0.1	0.7 1.3 1.1
Tsukuba	[36.05 ; 140.12]	30	Morino et al. 2017a	30 3602	0.6 0.5 0.9	1.1 1.9 1.7	24 1535	-0.1 -0.1 -0.2	0.9 1.5 1.4
Anmeyondo	[36.54 ; 126.33]	30	Goo et al. 2014	9 1177	-0.2 0.1 -0.6	0.7 1.4 1.5	1 396	0.2 -0.2 -0.3	0.2 1.1 0.5
Lamont	[36.6 ; -97.49]	320	Wennberg et al. 2017c	94 44404	-0.0 -0.1 0.3	0.9 1.0 1.0	96 41423	0.1 -0.0 0.0	0.6 1.0 1.0
Rikubetsu	[43.46 ; 1473.77]	390	Morino et al. 2017b	20 1988	0.1 -0.2 0.2	0.9 1.6 1.3	17 2192	0.5 0.3 0.3	0.5 1.3 1.7
Park Falls	[45.94 ; -90.27]	440	Wennberg et al. 2017a	59 7560	-0.0 -0.2 0.3	0.8 1.0 1.2	45 5150	-0.3 -0.3 -0.4	1.0 1.2 1.2
Zugspitze	[47.42 ; 11.06]	2960	Sussmann and Rettinger 2017b	18 846	-2.0 -2.3 -1.4	1.1 1.8 1.6	9 1404	-1.0 -0.2 -0.2	1.4 1.6 1.5
Garmisch	[47.48 ; 11.06]	740	Sussmann and Rettinger 2017a	41 7745	0.3 0.4 0.8	0.9 1.5 1.5	38 7248	0.3 0.7 0.2	0.9 1.4 1.3
Orléans	[47.97 ; 2.11]	130	Warneke et al. 2017	49 17239	0.8 0.3 0.6	0.5 1.2 1.1	34 10418	0.8 0.6 0.5	0.7 1.0 1.0
Paris	[48.85 ; 2.36]	60	Te et al. 2017	12 3614	-0.0 -0.5 -0.0	0.9 1.3 1.2	14 3421	-0.6 -0.4 -0.9	1.6 1.7 1.6
Karlsruhe	[49.1 ; 8.44]	110	Hase et al. 2017	38 11363	0.6 0.6 0.8	0.7 1.4 1.3	45 8883	0.4 0.6 0.1	0.6 1.2 1.1
Bremen	[53.10 ; 8.85]	7	Notholt et al. 2017	14 2866	0.7 0.3 0.9	0.4 0.9 1.1	9 1415	1.1 0.9 0.6	1.0 1.2 1.0
Bialystok	[53.23 ; 23.02]	180	Deutscher et al. 2017	34 4575	0.3 -0.0 0.8	0.7 1.3 1.1	31 8326	0.4 0.2 0.4	0.3 1.0 1.1
Sodankylä	[67.37 ; 26.63]	190	Kivi et al. 2017	29 3508	0.4 0.2 0.3	0.8 1.3 1.5	21 4698	0.8 0.8 0.3	1.2 1.3 1.7
Ny-Ålesund	[78.9 ; 11.9]	20	Notholt et al. 2019	10 65	1.2 2.1 2.2	0.6 2.5 2.3	7 18	1.0 3.1 1.4	0.7 2.9 1.5
Eureka	[80.05 ; -86.42]	600	Strong et al. 2017	3 42	-1.4 -1.3 -0.5	1.0 2.0 1.9	9 429	0.6 -0.1 -0.8	1.5 2.6 1.7

Appendix

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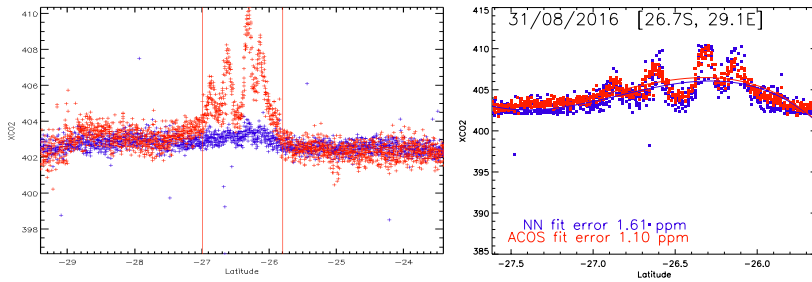
Figure A1: XCO2 estimated by the ACOS algorithm (Red) and the NN approach (Blue) as a function of latitude using its initial version as published in David et al. (2021) (left) and the new

850 version presented in this paper (right). The ACOS product showed a number of XCO2 enhancements that are not shown by the NN estimates. The plumes are observed downwind of large coal power plants, which make these features trustworthy. The date is August 31st, 2016.

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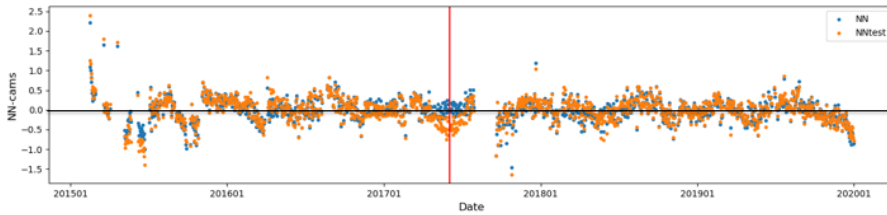
Figure A2: Mean difference, at daily scale, between the NN XCO2 estimate and the CAMS model. The blue dots show the results for the nominal training. The orange dots show the results when the training was made with a dataset biased by 1 ppm but only the observations of June 2017, the center of which is indicated by the red vertical line.

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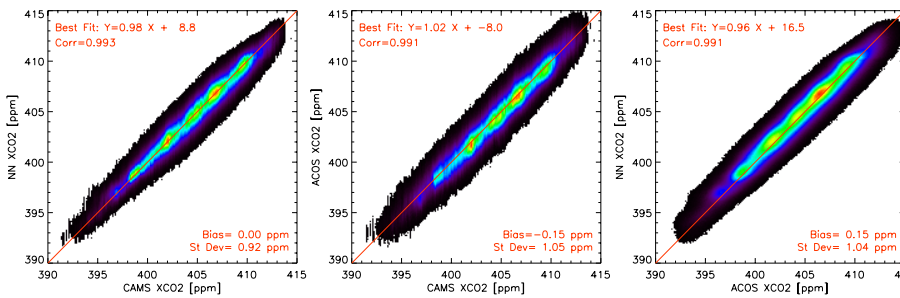


Figure A3: Same as Figure 4, but for the glint observations.

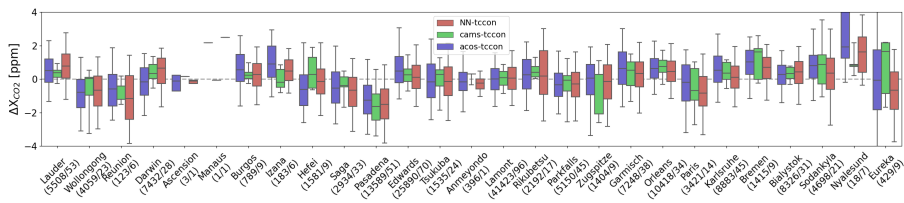
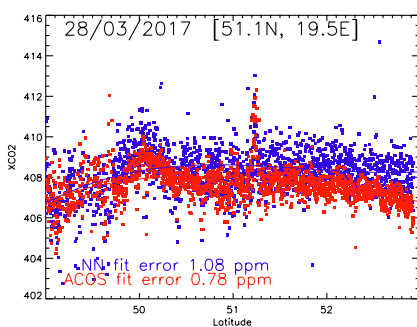
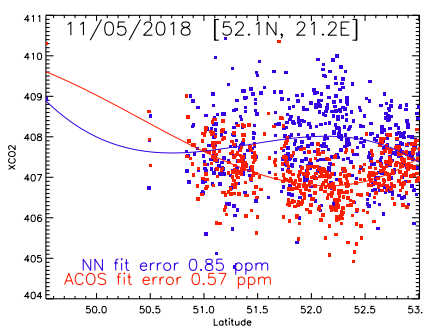
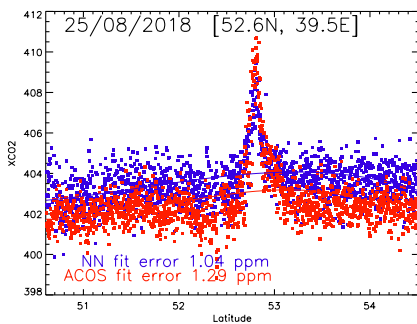
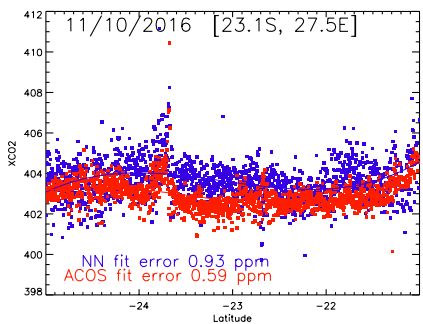
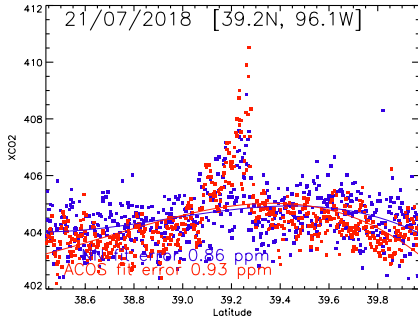
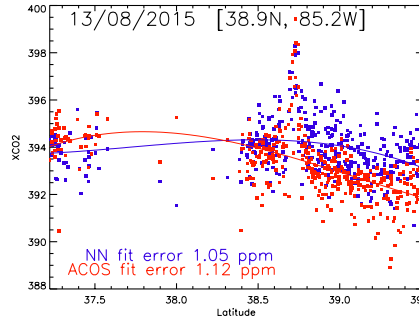



Figure A4: Same as Figure 8, but for the glint observations.

Kozienice (2018/05/11)   Belchatow (2017/03/28)

Matimba (2016/10/11)   Lipetsk (2018/08/25)

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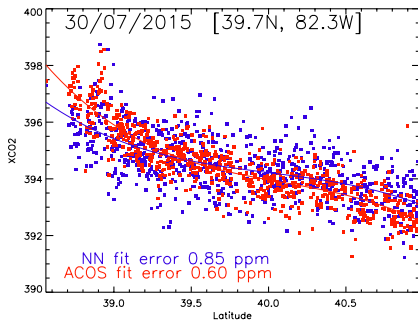
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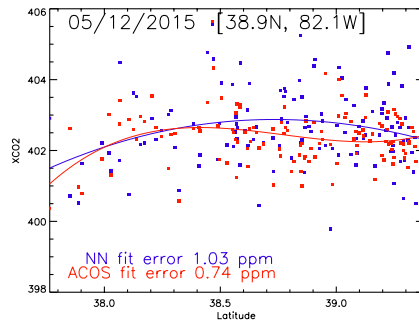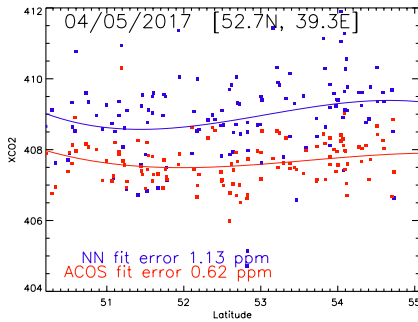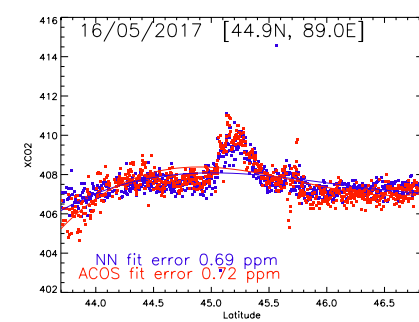
Lipetsk (2017/05/04)   HuoShaoshan (2017/05/16)

Figure A5 Exemples of anthropogenic CO2 plumes as seen by the OCO2 instrument processed with the ACOS algorithm (red) and the Neural Network described in this paper (blue). The cases have been identified and described in Reuter et al. 2019 and Nassar et al, 2021.

Moved (insertion) [3]