**UKESM Evaluation Progress Report (March 2017)**

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## 1. Introduction

The United Kingdom Earth System Model (UKSEM) is currently under development with multiple component models (e.g. NEMO – ocean model) all running simultaneously passing information between them (Met Office, 2013). The development of UKESM is a collaboration between the UK Met Office, NERC research centres and UK academic institutions running between 2016 and 2021. As a member of the National Centre for Earth Observation (NCEO), my role (50%) is to evaluate UKESM output of atmospheric composition from prescribed runs using satellite data. However, the UKESM runs are not due for completion until the autumn of 2017. Therefore, codes/datasets have been developed/collected to evaluate the atmosphere only component of UKESM in the interim.

## 2. Model

UKESM uses the Met Office Unified Model (UM) for its representation of the atmosphere. This version of the model can include atmospheric chemistry and aerosols using the United Kingdom Chemistry and Aerosols (UKCA) subroutines covering the troposphere and stratosphere. The model version used here has an ID of UM10.6.1-GA7.1+Strat/Trop, which we label *UM-Chem* for short. The details of UKCA and GLOMAP (aerosol model) are described by O'Connor et al., (2014) and Mann el al., (2010), respectively. UM-Chem is coupled so meteorology and chemistry interact at each model time step. A description of the model dynamical core is provided by Davies et al., (2005) and Walters et al., (2011).

UM-Chem was run by Mohit Dalvi, Met Office, on MONSooN (Met Office and NERC joint supercomputer system) with job ID u-aj841 and output monthly mean tracer files between 1990 and 2008. Unfortunately, for the most accurate model-satellite comparisons, high temporal model output is required (6 hourly or more frequent) to allow the satellite averaging kernels (AKs) to be applied. The AKs describe the satellite's vertical sensitivity to retrieving trace gases and need to be applied to model fields to allow for like-for-like comparisons. However, since the model output is monthly, it is not possible to undertake these robust comparisons. Initial work involved simple monthly comparisons, but future runs (done by Richard Pope) will output full 3D tracer fields at 6-hourly intervals.

## 3. Satellite Data

Satellite data used so far to evaluate UM-Chem include tropospheric column nitrogen dioxide ($NO_2$), sub-column (0-6 km) ozone ($O_3$), total column formaldehyde (HCHO) and upper troposphere – lower stratosphere (UTLS) peroxyacetyl nitrate (PAN). These products include averaging kernels and error statistics which will be used to more robustly assess UM-Chem with higher temporal resolution output in the future.

Ozone Monitoring Instrument (OMI) tropospheric column $NO_2$ data comes from the Tropospheric Emission Monitoring Internet Service (TEMIS) and is known as the DOMINO product (Boersma et al., 2011). OMI is on-board NASA's EOS-Aura satellite and has an overpass time of approximately 13.30

LT. It has a nadir viewing spectrum of 270-500 nm and has a central swath pixel size of 16-23 km. The data has been screened for geometric cloud fraction of under 0.2, good data flags and the OMI row anomaly using the algorithm of Braak (2010).

OMI sub-column $O_3$ data is provided by NCEO colleagues at the Rutherford Appleton Laboratory (RAL) and is based on an optimal estimation algorithm (Rodgers, 1976) utilised by Miles et al. (2015a). The OMI retrievals are quality controlled prior to use (described by Miles et al., (2015b) for GOME-2 data), with data being removed where geometric cloud fraction is greater than 0.2 and the solar zenith angle is greater than 80◦.

OMI total column HCHO data is taken from TEMIS as monthly mean files. Unfortunately, this product does not include AKs or error statistics as it is a Level 3 product. However, we are currently downloading TEMIS Level 2 (swath) data with these metrics, which will be used for future comparisons. We have also requested OMI glyoxal data.

PAN data has been provided by the Karlsruhe Institute for Technology (KIT) from the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), which was on-board ESA's ENVISAT. ENVISAT was in orbit between 2002 and 2012 and had an overpass time of 10.00 LT. All data quality flags were applied and data interpolated to 150 hPa (similar to Pope et al., (2016)) for comparison to UM-Chem. In the future, we will also use MIPAS PAN data provided by David Moore (University of Leicester, NCEO).

## 4. Comparisons

As the model monthly tracer fields cannot be co-located with the overpass and location of each satellite retrieval, there will be sampling errors in these comparisons. Also, as the AKs have not been applied to the model tracers, there will be smoothing errors not accounted for in comparisons. The monthly mean tracers for UM-Chem and the satellite data are merged into winter (December-January-February; DJF) and summer (June-July-August; JJA) composites. Where there is missing satellite data in the seasonal composites, the model is not sampled. The errors statistics represent random and systematic errors, but ignore smoothing errors which are taken care of with the AKs.

### 4.1. Nitrogen Dioxide ($NO_2$)

Figures 1a and c show UM-Chem and OMI tropospheric column $NO_2$ for DJF. There are model hotspots of over 15 x$10^{15}$ molecules/cm$^2$ over Eastern United States (US), Europe and China. There is clear biomass burning $NO_2$ over central Africa of approximately 10 x$10^{15}$ molecules/cm$^2$. Background model and satellite tropospheric column $NO_2$ typically ranges between 0-2 x$10^{15}$ molecules/cm$^2$. OMI observes a larger cluster of peak (>15 x$10^{15}$ molecules/cm$^2$) $NO_2$ over China, but concentrations are lower over the US and Europe (5-10 x$10^{15}$ molecules/cm$^2$). Figure 1e represents the UM-Chem – OMI tropospheric column $NO_2$ mean bias. The green polygonned regions highlight significant differences where the |mean bias| > satellite error. There are wide spread significant biases of 5-10 x$10^{15}$ molecules/cm$^2$ across the US and Europe. Over China, there is a significant dipole of over/under +/- 5 x$10^{15}$ molecules/cm$^2$. Similar biases are seen over Europe in the TOMCAT chemistry transport model in DJF (Monks et al., 2016). There is also some similarities over the Eastern US. Therefore, this could highlight links between the emissions used in the model runs (i.e. similar emissions) and uncertainties in them.

Figures 1b and d show model and satellite JJA column $NO_2$. In the northern hemisphere (NH) the concentrations are much lower (4-10 x$10^{15}$ molecules/cm$^2$) in the industrialised locations peaking over the UK. In the southern hemisphere (SH), biomass burning regions show enhanced

concentrations of 3-7 x$10^{15}$ molecules/$cm^2$. The main significant biases (Figure 1f) are over the Eastern US (2-3 x$10^{15}$ molecules/cm2) and South America (-3 to -2 x$10^{15}$ molecules/$cm^2$), which are much smaller than DJF. Hence, the comparisons agree more in summer than winter.

### 4.2. Ozone ($O_3$)

In winter, UM-Chem (Figure 2a) and OMI (Figure 2c) sub-column $O_3$ are similar with concentrations of 3-15 Dobson Units (DU) over the Southern Ocean. There is enhanced $O_3$ columns of 15-20 DU over the South Atlantic linked to African biomass burning activity. In the northern mid-latitudes, OMI $O_3$ reaches between 10-25 DU peaking over Eastern Russia. In UM-Chem, peak $O_3$ in the region is 20 DU over the oceans. In the Pacific, there is an anomalous feature in the OMI data (Figure 2c & d). We believe this to be related to the satellite orbit and missing quality control flags not applied to the OMI data. In summer, UM-Chem (Figure 2b) and OMI (Figure 2d) again have similar features with peak $O_3$ across the NH of over 20 DU. This is most noticeable over the Mediterranean (28-30 DU). There is also enhanced outflow of $O_3$ out of the biomass burning regions in Africa (20-25 DU). Minimum $O_3$ is over the tropical ocean with concentrations between 10-15 DU. In both seasons there is reasonable agreement with few significant biases. The northern (southern) high latitudes have significant biases of -5 to -1 DU in JJA (DJF). In JJA, there is significant biases of 5-10 DU over the Middle East and in DJF, there are significant biases over the tropical Atlantic and Pacific (3-7 DU). Central Africa also highlights significant biases of 8-10 DU. In DJF this suggests the model overestimates outflow of $O_3$ from indirect continental sources (i.e. biomass burning).

### 4.3. Formaldehyde (HCHO)

For HCHO, the model has higher continental and lower ocean concentrations than OMI in both seasons. Typically, OMI has ocean concentrations of 5-8 x$10^{15}$ molecules/$cm^2$ (Figures 3c & d), while the model has concentrations of 0-6 x$10^{15}$ molecules/$cm^2$ (Figures 3a & b). Peak HCHO is 20-25 x$10^{15}$ molecules/$cm^2$ over the Amazon, Africa (DJF) and US (JJA), while OMI is 15-17 x$10^{15}$ molecules/$cm^2$. In Figure 3e, the land/sea HCHO biases are clear with differences of 5-10/-3 to -1 x$10^{15}$ molecules/$cm^2$. In the northern high latitudes, the biases is near uniform of -3 to -2 x$10^{15}$ molecules/$cm^2$ and in the Southern Ocean. In JJA (Figure 3f), UM-Chem ocean differences are less with near zero biases, apart from the coastline near large land sources (0-2 x$10^{15}$ molecules/$cm^2$). In the northern high latitudes and Southern Ocean, the biases remain at -3 to -2 x$10^{15}$ molecules/$cm^2$, but are not as far ranging. The large positive biases over land potentially suggest that direct and/or precursor (e.g. isoprene) emissions are too large and/or the lifetime is too short (i.e. insufficient transport of HCHO over the ocean). As there are no error statistics, however, it is difficult to assess how important these differences are.

### 4.4. Peroxyacetyl Nitrate (PAN)

MIPAS PAN at 150 hPa peaks over Southern Africa, 150-200 pptv, in DJF (Figure 4c). The background concentrations range between 50-80 pptv. In JJA (Figure 4d), there are still signals over Southern Africa of 150-200 pptv, but peak PAN (200-250 pptv) is over the Middle East and India. This is related to the Asian summer-time anticyclone in the UTLS. Rapid vertical convection uplifts PAN into the UTLS where it is accumulated (high pressure regime). The anticyclone can influence UTLS composition between the Middle East and China, where there is peak PAN concentrations. In UM-Chem, the PAN concentrations are much higher in the source regions. In DJF (Figure 4a), PAN is over 300 pptv in the Amazon and Southern Africa, while only 100-200 pptv in MIPAS. In JJA (Figure 4b), model PAN is over 300 pptv over the Asian summer-time anticyclone region. Larger concentrations are also over Central America (220-230 pptv). Looking at the mean biases, UM-Chem significantly

overestimates PAN in DJF (Figure 4e) by over 100 pptv throughout the southern tropical region. In the high latitudes, there are negative biases of -30 to 0.0 pptv, of which few are significant. In JJA (Figure 4f), positive biases peak over 100 pptv over Central America and Asian summer-time anticyclone. However, these biases are within the satellite uncertainty range. There are non-significant biases in the mid-high latitudes of -50 to 0.0 pptv. Some of the UM-Chem – MIPAS PAN biases are seen in the study by Pope et al., (2016). TOMCAT overestimates MIPAS PAN at 150 hPa by 50-80 pptv over Central America/the Amazon and South East Asia in DJF. Since, there are UM-Chem positive biases in DJF PAN and HCHO over Central America and the Amazon, it potentially suggests problems with emissions in the region. Any biases in volatile organic compounds (VOCs) will likely translate into PAN as it will aid the formation of the peroxyacetyl radical and then PAN in the presents of $NO_2$. UM-Chem, like TOMCAT, underestimates PAN in the high latitudes (i.e. lower stratosphere).

## 5. Summary

As the first set of UKESM runs are not scheduled until the autumn of 2017, we have undertaken initial comparisons against satellite observations of atmospheric composition using the Met Office atmospheric component model which includes tropospheric-stratospheric chemistry. This model version is known as UM10.6.1-GA7.1+Strat/Trop, which we have labelled *UM-Chem*. These runs were completed by Mohit Dalvi, from the UK Met Office, on the high performance computer, MONSooN. Unfortunately, though covering the satellite era, the mode runs where primarily for climate-composition studies and have monthly output. Therefore, the model cannot be co-located with satellite retrieval overpasses and locations. The averaging kernels, a measure of instrument sensitivity to retrieving trace gases in the vertical, cannot be applied either, resulting in sampling and smoothing (satellite profile shape) errors. Nevertheless, initial comparisons have been completed for tropospheric column $NO_2$, sub-column $O_3$, total column HCHO and PAN at 150 hPa.

In JJA, UM-Chem had good agreement with OMI tropospheric column $NO_2$ with few significant biases of +/-2 $x10^{15}$ molecules/$cm^2$ over the US and Amazon. In DJF, model performance decreases with large significant biases of over 5 $x10^{15}$ molecules/$cm^2$ over Europe and the US. Comparisons with OMI sub-column $O_3$ show latitudinal biases in both seasons with overestimation and underestimation in the tropics and mid-high latitudes respectively. These biases are significant in the DJF Southern Ocean and JJA northern high latitudes of -5 to -2 DU. In regions of tropical $O_3$ outflow from precursor gas source regions (e.g. Central Africa) there are significant positive biases of 3-5 DU. There were no error metrics in the OMI HCHO product, but UM-Chem overestimates HCHO in the continental tropical regions, in both seasons, of 0-10 $x10^{15}$ molecules/$cm^2$. This is most noticeable over Amazonia. In the mid-high latitudes, there is a model underestimation of -5 to 0.0 $x10^{15}$ molecules/$cm^2$. Model PAN, at 150 hPa, significantly overestimates MIPAS throughout the southern tropics by over 100 pptv in DJF. This is most noticeable over the Amazon, which correlates with the HCHO biases potentially highlighting the links between model overestimation of VOCs and PAN once the peroxyacetyl radical has reacted with $NO_2$. There are few significant biases in JJA.

For the next steps of the project (i.e. April 2017 – March 2018), we have taken a copy of the UM10.6.1-GA7.1+Strat/Trop job on MONSooN and plan to rerun it for multiple years outputting tracer fields at a higher temporal resolution (i.e. at least 6 hourly). This will allow for co-location with satellite swath data and the application of the AKs resulting more robust comparisons. We also plan to look at several other species such as MOPITT carbon monoxide (CO) and OMI glyoxal (OCHCHO). Finally, we plan to see if the model can reproduce relationships between satellite trace gas observations and global circulation patterns (e.g. North Atlantic Oscillation (NAO) and El Nino and Southern Oscillation (ENSO)).

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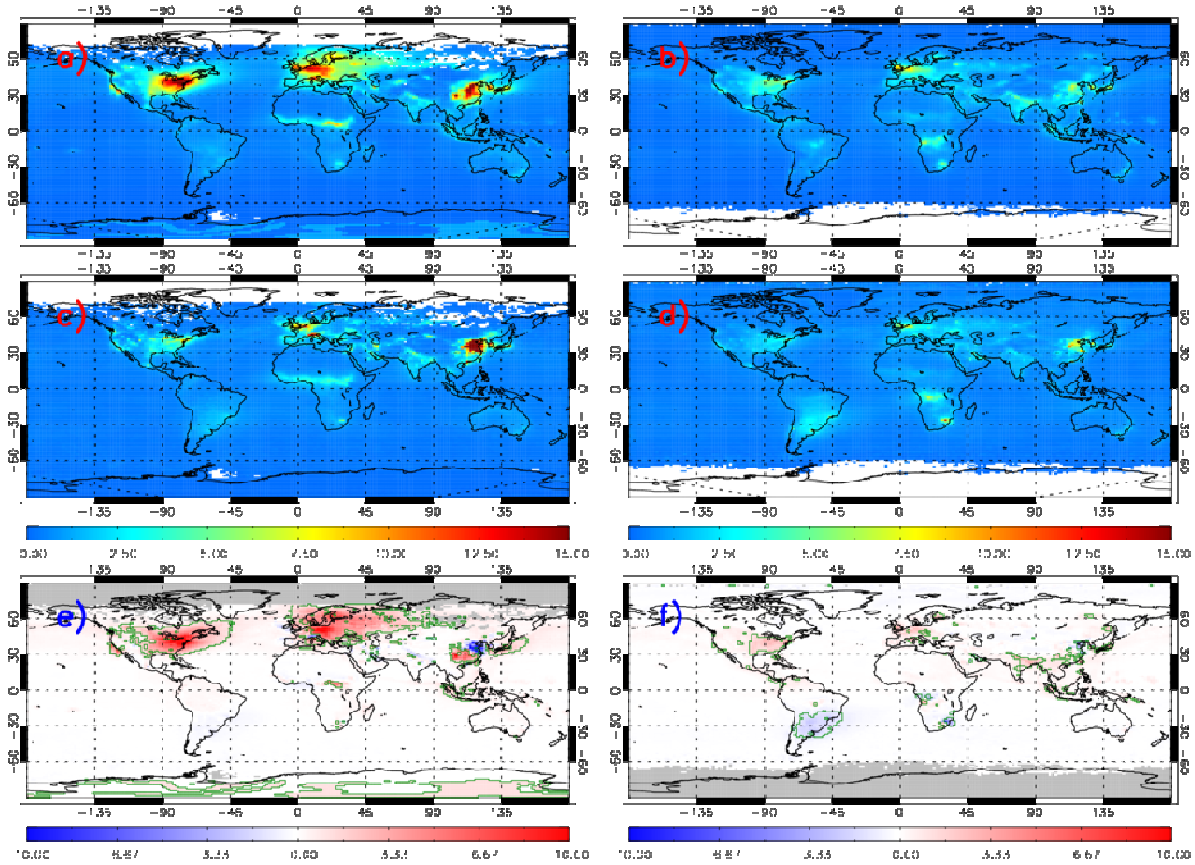


**Figure 1**: Tropospheric column $NO_2$ ($10^{15}$ molecules/$cm^2$) in 2008 for a) UKESM December-January-February (DJF), b) UKESM June-July-August (JJA), c) OMI DJF, d) OMI JJA, e) UKESM-OMI DJF and f) UKESM-OMI JJA. Green polygonned regions show significant differences (|mean bias| > satellite error).

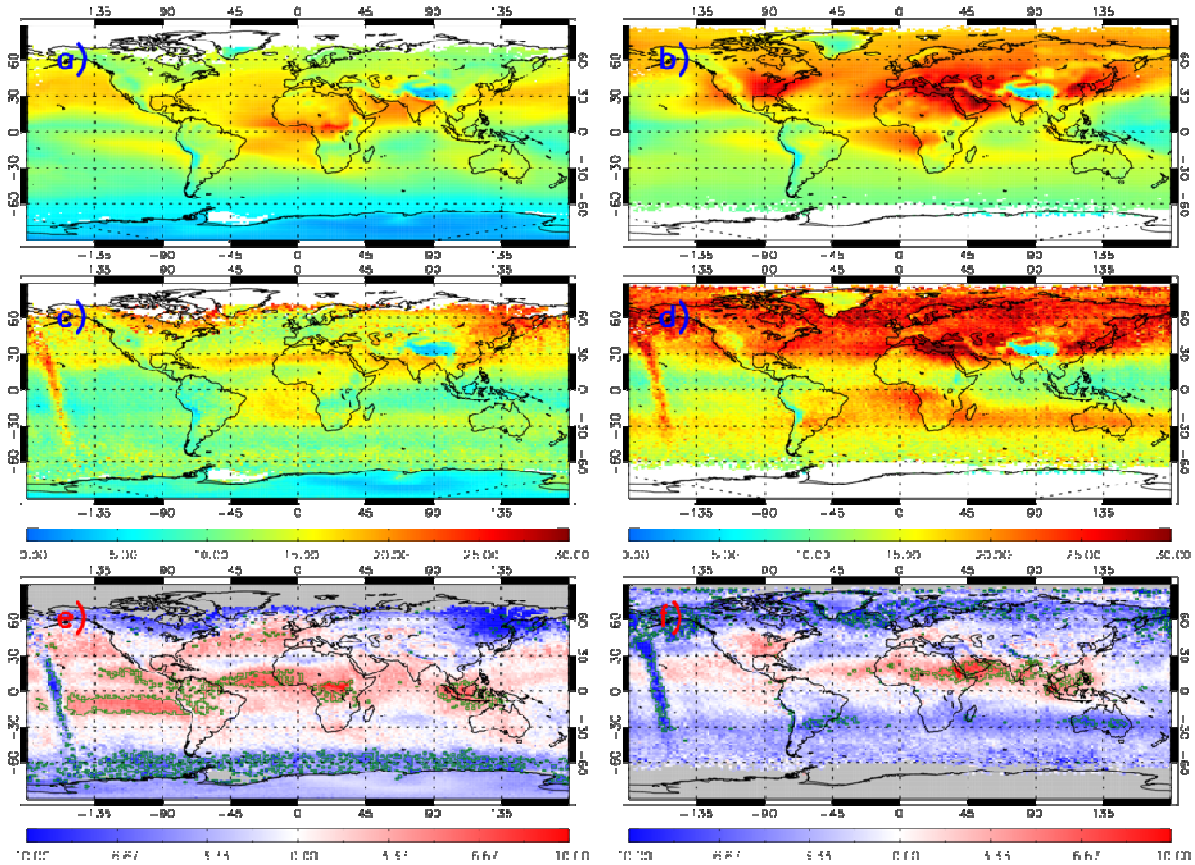


**Figure 2**: Sub-column (0-6 km) $O_3$ (Dobson Units; DU) in 2008 for a) UKESM December-January-February (DJF), b) UKESM June-July-August (JJA), c) OMI DJF, d) OMI JJA, e) UKESM-OMI DJF and f) UKESM-OMI JJA. Green polygonned regions show significant differences (|mean bias| > satellite error).

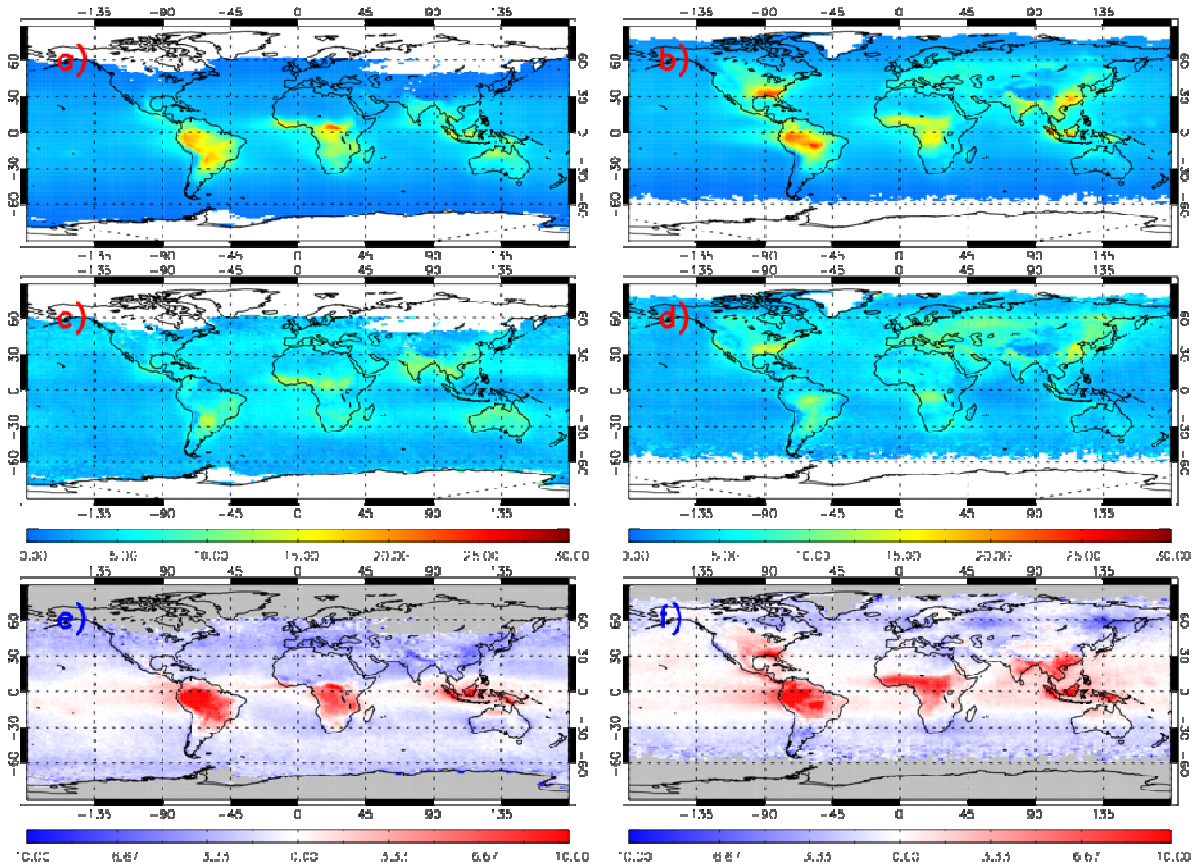


**Figure 3**: Total column HCHO ($10^{15}$ molecules/cm$^2$) in 2008 for a) UKESM December-January-February (DJF), b) UKESM June-July-August (JJA), c) OMI DJF, d) OMI JJA, e) UKESM-OMI DJF and f) UKESM-OMI JJA. Green polygonned regions show significant differences (|mean bias| > satellite error).

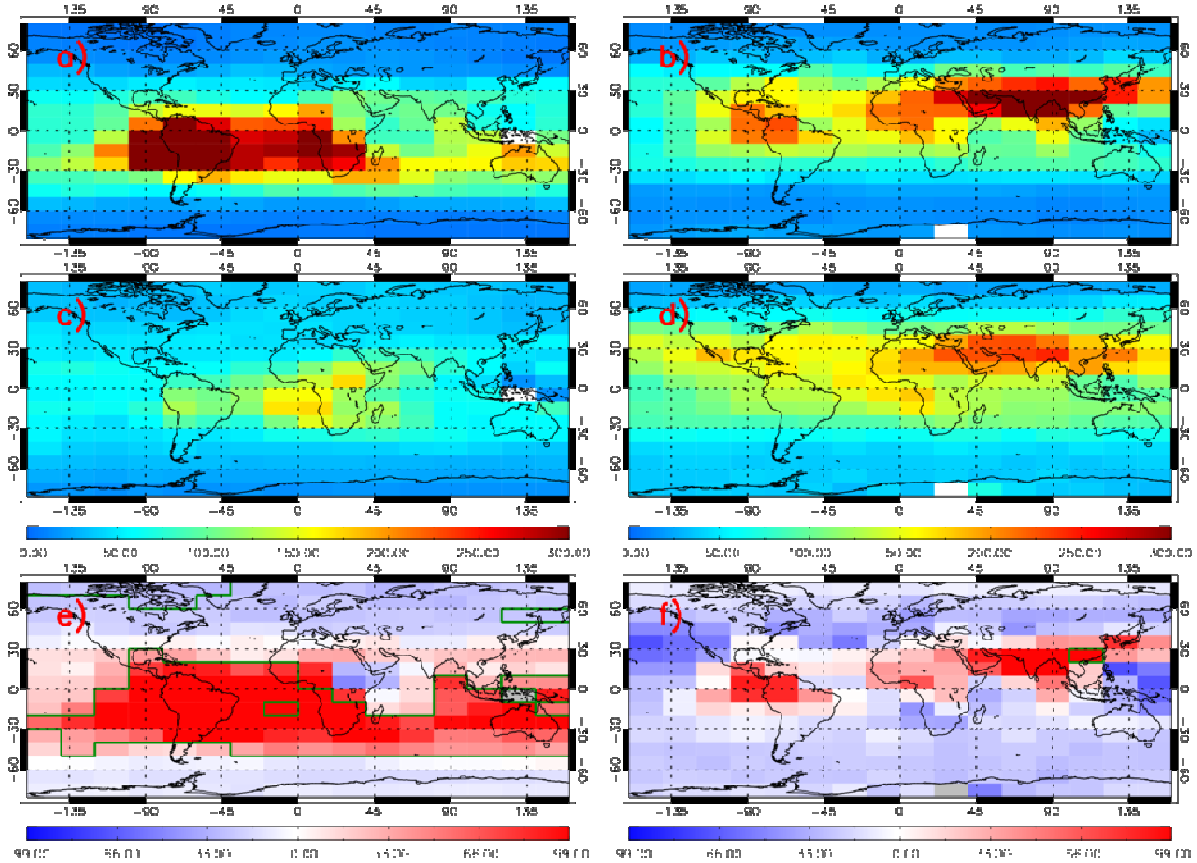


**Figure 4**: PAN at 150 hPa (ppbv) in 2008 for a) UKESM December-January-February (DJF), b) UKESM June-July-August (JJA), c) OMI DJF, d) OMI JJA, e) UKESM-OMI DJF and f) UKESM-OMI JJA. Green polygonned regions show significant differences (|mean bias| > satellite error).