SAQN Scoping Study End of Project Report

Project Title

On track of NH3: cross-validation of satellite and ground-level measurements

Project Team

Name	**Role (PI / Co-I)**
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Proposed activities (copy from your project proposal)

This project aims to evaluate the goodness of satellite NH_3 concentrations to predict ground-level NH_3 concentrations in the UK. More specifically, the objectives of the project are:

1) To evaluate the monthly and interannual variability of NH_3 concentrations as observed from ground-level measurements and satellite retrievals across the UK
2) To evaluate the geographical distribution of NH_3 concentrations in the UK as observed by ground-level measurements and satellite retrievals
3) To evaluate possible trends of NH_3 concentrations over the last five years as observed from ground-level and satellite measurements, across the UK and across the differentiated areas.

To achieve the objectives of the project, the following tasks are planned:

- ***Task 1***. Evaluation of the inter-annual variability of NH_3 concentrations in the UK. Comparison of the monthly mean concentrations as measured by the ground-level sites (including both monthly integrated and high-time resolve measurement sites) *vs* monthly satellite retrievals from the CrIS instrument. This would evaluate how satellite column data is sensible to ground-level measurements; and if the monthly and inter-annual variability as observed by the two data sets are the same. Linear models, including type-II linear models will be considered in this exercise when comparing satellite data versus individual sites.

- ***Task 2.*** Evaluation of the graphical distribution of NH_3 concentrations in the UK as observed by satellite retrievals and evaluate if such variability is observed by ground-level measurements.

- ***Task 3.*** Evaluation of trends in NH_3 concentrations in the UK, as observed by the two data sets; national and organized by regions, in the last five years (2015-2020). Theil-Sen linear trends (Theil, 1950) will be used in this task. Evaluation if the trends are consistent through the different regions are going to be evaluated by ground-level and satellite measurements.

Please report on the activities completed in the project

Task 1 & 2. The interannual variability as measured by monthly means by both ground-level and satellite data was evaluated. The spatial distribution of concentrations was also analysed.

Ground-level data from the UK EAP network has a total of 85 sites offering a good spatial coverage across the UK territory in all NUTS1 areas (Figure 1). Data was extracted from 2008 onwards. Data was reported from the start and end date for each sampling period (varying from a week to over a month). In order to unify the sampling period, data was re-gridded to the start of the month.

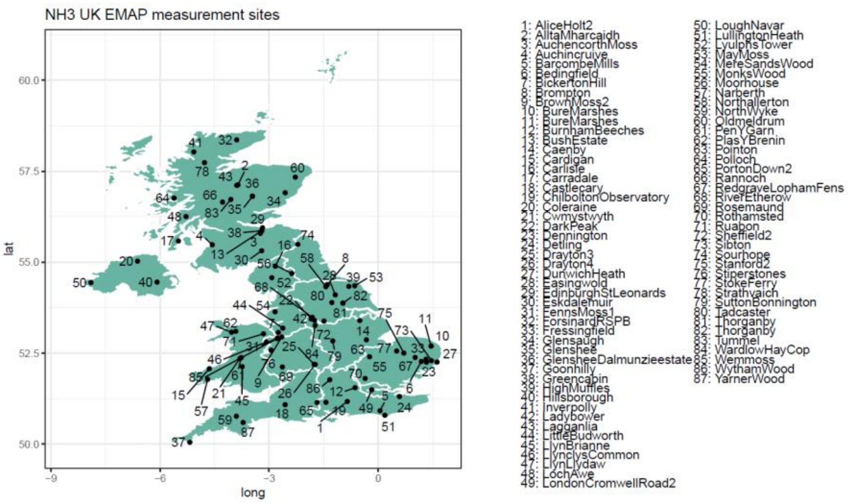

Figure 1. Ground-level sites measuring NH_3 in the UK. Green areas represent the NUTS1 areas in the UK.

A mixed of passive and active samplers were used to measure NH_3 in the network (Figure 2) with some sites with a change of instrument along the time series (e.g. Wem Moss) and others with coexistence of the two (e.g. Chilbolton Observatory). Sites with long-time series measured by both samplers, those were kept independently; sites with a change of instrument and without a clear step-change in concentrations were merged and only one time series analysed (i.e. Auchencorth Moss, Dennington, Dunwich Heath, Fenn Moss 1, Inverpolly, Glensough, Llynclys Common, Wytham Wood, Stanford2 and Llynclys Common).

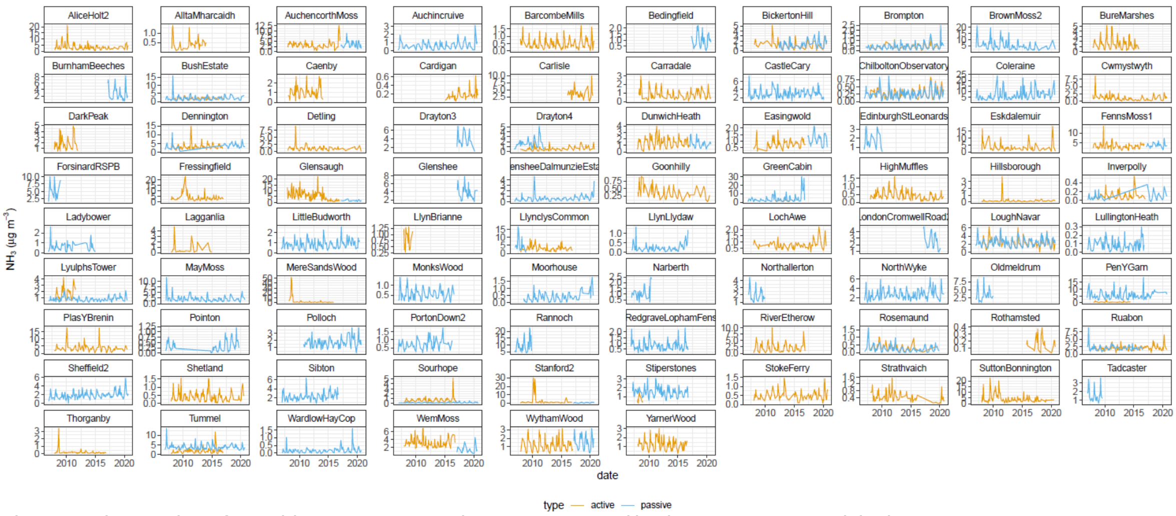

Figure 2. Time series of monthly NH_3 concentrations as measured by the UK EAP network in the UK.

Ground-level data showed a clear seasonal pattern with higher concentrations in spring; and in some areas (North West England, Northern Ireland, Wales and West Midlands) showed a later peak towards the end of the summer (Aug – Sep) (Figure 5).

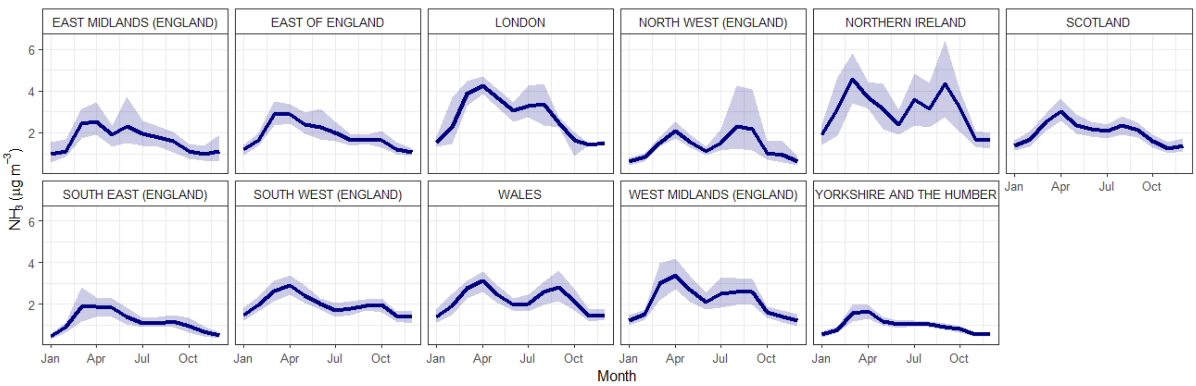

Figure 3. Monthly mean (±95% confidence interval) NH_3 concentrations grouped by NUTS1 area.

High-time resolved NH_3 concentrations are available at three rural locations in the UK: Auchencorth Moss (Scotland) (2006 – 2019); Harwell (South-East England) (2011 – 2015); and Chilbolton Observatory (South-East England) (2016 – 2019). The mean diurnal pattern indicates that the highest concentrations of NH_3 were observed by 8-9 am. After that time, NH3 concentrations levelled off at Auchencorth Moss and Harwell. A second peak was observed around 8 pm at Chilbolton site. The higher concentrations at Chilbolton in comparison to Harwell was studied by (Walker et al., 2019) and was associated with a presence of a farm south-west of the monitoring site. There are some papers in the scientific literature that indicates that the concentrations peak in the early morning may be an instrument artifact by the formation of morning dew around the inlet of the instrument leading to the absorption of NH_3 into the dew, which evaporates a few hours later following the increase of temperature due to the rising sun (Makkonen et al., 2012).As further investigations were needed to verify if the pattern in concentrations were real or an instrument artifact, the high-time resolve data was not further use in the project.

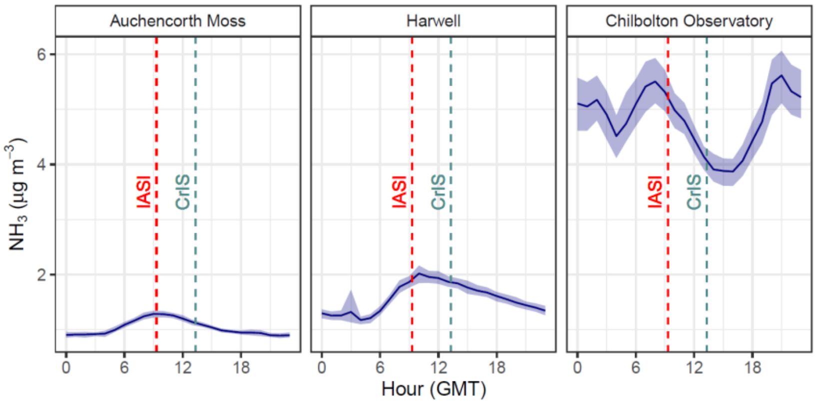

Figure 4. Mean diel plots of NH_3 concentrations measured in the locations in the UK with high-time resolved data. The pass times for both IASI and CrIS are indicated with vertical dashed lines.

Satellite data from RAL Level 3 product gridded at 0.025 degrees resolution was used for both IASI and CrIS instruments measuring column-integrated NH_3 concentrations. The mean concentrations showed a strong seasonal pattern with higher concentrations in spring and summer (Figure 5). Hotspots of NH_3 were observed in Northern Ireland, East England and West Midlands.

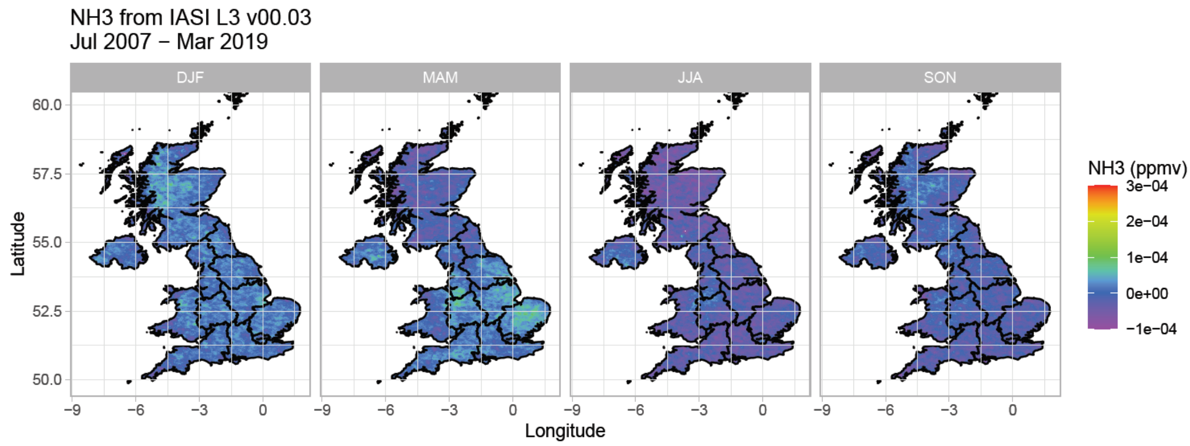

Figure 5. Mean NH_3 column concentrations from IASI RAL product (v00.02) from July 2007 to March 2019. DJF: winter; MAM: spring; JJA: summer; SON: autumn.

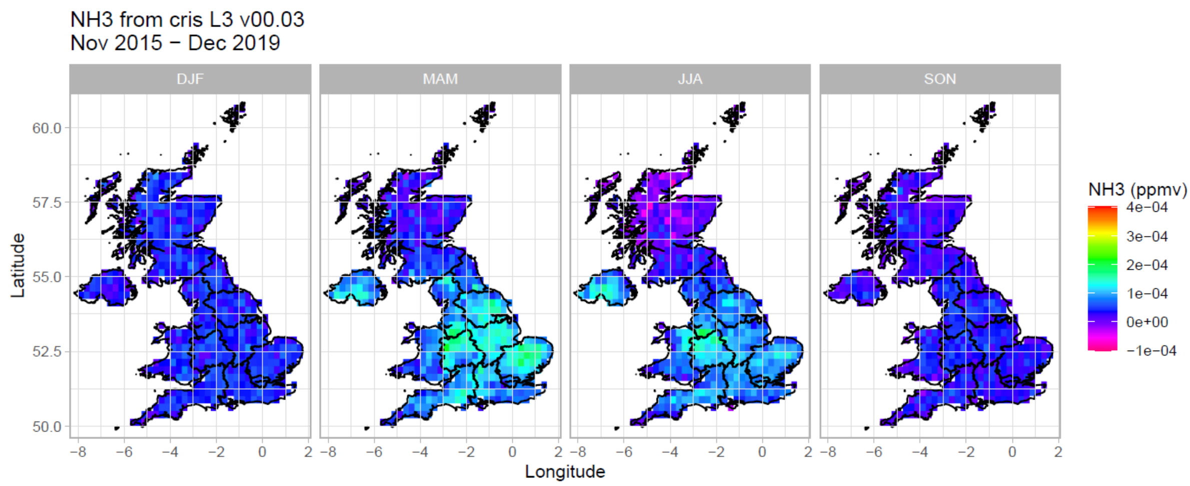

Figure 6. Mean NH_3 column concentrations from CrIS RAL product (v00.03) from November 2015 to December 2019. DJF: winter; MAM: spring; JJA: summer; SON: autumn.

Median concentrations for each of the NUTS area in the UK were calculated. A sensitivity analysis on the satellite data was undertaken based on the cloud cover fraction (grids with large cloud cover were filtered out; levels >0.1, >0.2 & >0.3) and the surface temperature contrast at 1 km (kept the grids with a contrast temperature >5K, 10K & 15K). Grids a surface altitude > 400 m were also removed as satellite data have difficulties to observe the surface in areas with complex topography.

The coefficient of correlation (R) were used to evaluate the goodness of satellite data to capture the temporal variability as observed by the ground-level sites. This was done on NUTS areas and using different filtering criteria (cloud cover; surface air temperature contrast at 1 km; and altitude). R was also evaluated without applying any filtering to satellite data. An example of comparison can be observed in Figure 7. The number of NUTS1 area where satellite data were well capturing the temporal variability was also quantified and used to evaluate the goodness of satellite data to capture the spatial distribution. Results are summarized in Table 1. Overall, there were some NUTS area where the correlation between the ground-level and satellite showed good correlations when filters were applied (max. 0.5470 for IASI Jul 2007 – Mar 2019; and up to 0.6650 for Nov 2015 – Feb 2016). Data from CrIS were quite similar to those from IASI with a maximum correlation of 0.6738 when filtering were applied. CrIS showed significant correlations in 6 of the 12 NUTS areas whereas IASI showed significant correlations in 5 areas for the same period of time.

Table 1. Summary of the comparison between ground-level and satellite data. 'without' filtering indicates that satellite data were extracted including all values. 'with filtering' means that different cloud cover fractions, contrast temperature and grid surface altitude values were considered.

	IASI	**CrIS**
Date coverage	**Jul 2007 – Mar 2019**	**Nov 2015 – Dec 2019***
R time series (significant correlation) without filtering	0.1859 – 0.4128	0.3474 – 0.6278
Range slopes without filtering	-0.043 – 0.0586	0.0351 – 0.1217
R time series (significant correlation) with filtering	0.1698 – 0.5470	0.3242 – 0.6738
Range slopes with filtering	-0.0301 – 0.1357	0.0358 – 0.1419
NUTS areas	8 out of 12	6 out of 12
Date coverage	**Nov 2015 – Mar 2019**	
R time series (significant correlation) without filtering	0.307 – 0.3740	0.3334 – 0.6170
Range slopes without filtering	-0.039 – 0.0500	0.0347 – 0.1213
R time series (significant correlation) with filtering	0.3261 – 0.6650	0.3242 – 0.6738
Range slopes	0.0266 – 0.1100	0.0358 – 0.1419
NUTS areas	5 out of 12	6 out of 12

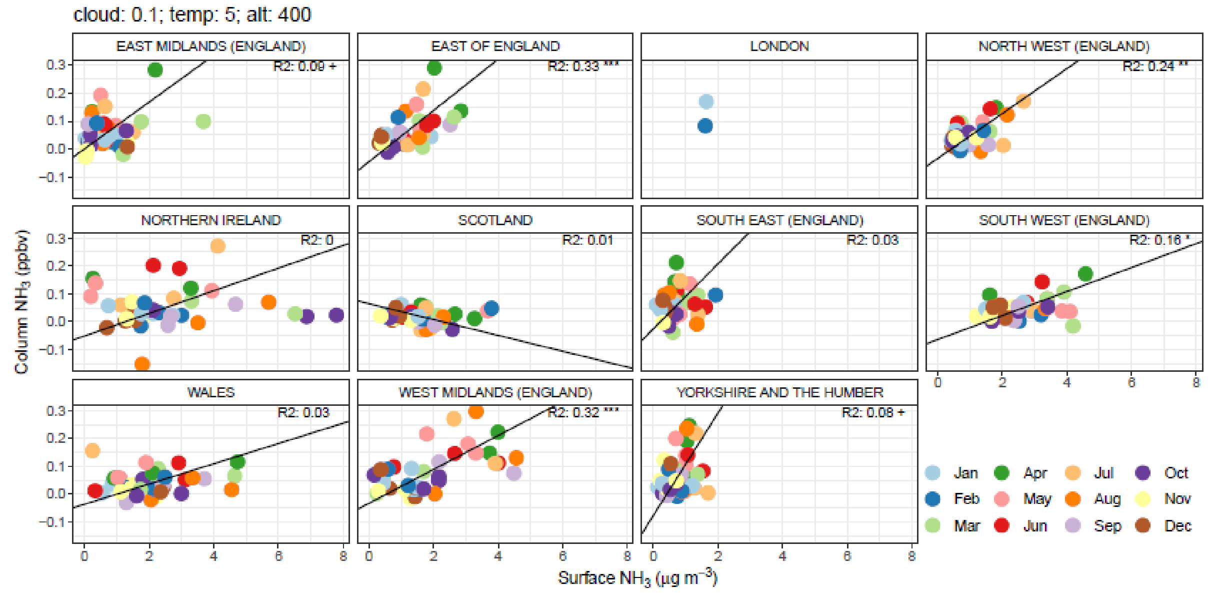

Figure 7. Scatter plot relating column-integrated satellite data from CrIS vs ground-level median concentrations. A filter on the cloud cover of 0.1 was applied; only grids with a surface contrast temperature greater than 5 K were selected and grids with an altitude less of 400 m.

Task 3. Linear-trends for the ground-level sites were calculated using the Theil-Sen method (Sen, 1968; Theil, 1950) available from the R/Openair package (Carslaw & Ropkins, 2011). Trends were calculated for the period 2008 – 19; and 2015 – 19 (period when CrIS measurements were available). Trends were calculated for those time series with more than 75% data capture for the period considered; and deseasonalized (seasonal cycle removed using the loess method). Individual trends were calculated and overall trends were calculated for each of the NUTS1 area using the random-effects model as in Font & Fuller (2016). Results are shown in Figure 8 and Figure 9.

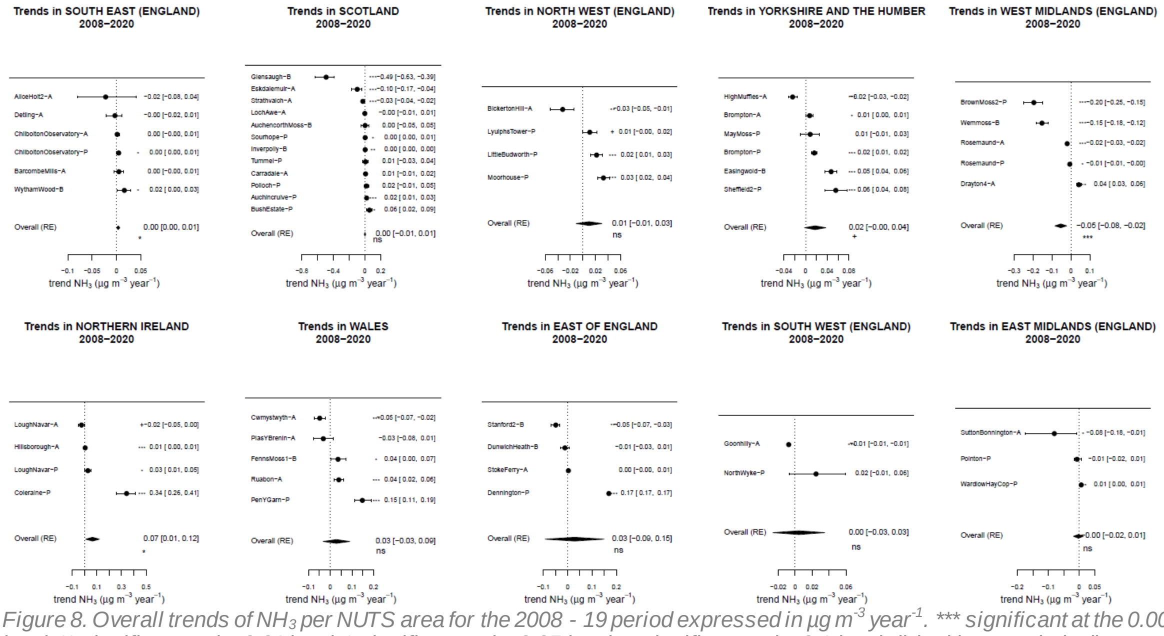

*Figure 8. Overall trends of NH_3 per NUTS area for the 2008 - 19 period expressed in µg m^{-3} $year^{-1}$. *** significant at the 0.001 level; ** significant at the 0.01 level; * significant at the 0.05 level; + significant at the 0.1 level; (blank) not statistically significant. Overall (RE) refers to the overall trend.*

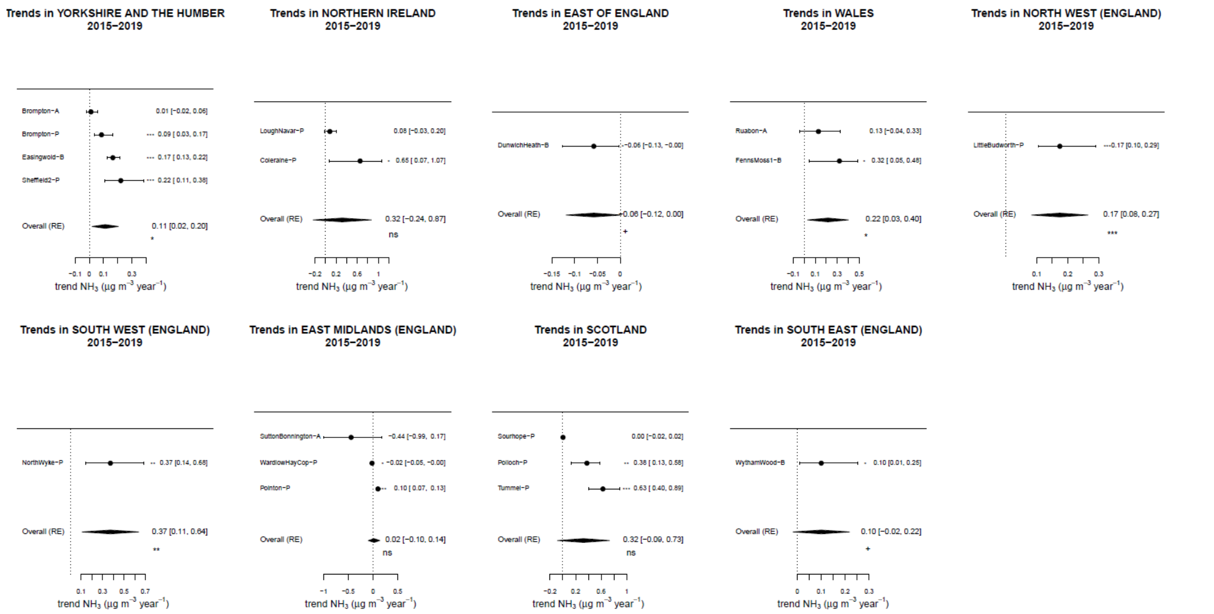

Figure 9. Same as Figure 8 for the 2015-19 period.

Based on the ground-level measurements there is no evidence of downward trends in any of the NUTS1 areas in the UK with the exception of West Midlands for the period 2008-19; and for East of England for 2015-19.

What are the next steps for this research? Will you be applying for further funding? What will you need to continue researching this topic?

- The next steps of the research will involve using the daily satellite soundings: apply adjustments and filtering to daily level 2 (L2) data to generate improved monthly gridded L3 data considering also meteorological conditions.
- RAL aims to improve the retrieval algorithm taking onboard insights from the analysis.
- Apply daily L2 data and compare to individual stations ideally with high-time resolved data (i.e. hourly) for a better comparison.

Please outline the role of STFC in this project

- STFC RAL provided the Level 3 satellite NH_3 data for both IASI (July 2007 to March 2019) and CrIS (November 2015 to December 2019)
- STFC RAL provided the knowledge about satellite data products
- STFC RAL input about the data analysis
- Fortnight two-weekly meetings were scheduled since April (start of the project) to discuss about the progress of the project

Please list a brief list of all outputs and impacts below. These may include papers, articles or blogs, presentations at events or conferences, meetings about future plans for the research. Please include links wherever possible

- A blog entry was published in the SAQN newsletter (4 May 2021) (https://www.saqn.org/2021/05/04/feature-scoping-study-on-track-of-nh3/)
- Fortnight two-weekly meetings were scheduled since April to discuss about the

progress of the project • A final meeting was held with the project mentor (Prof. Roderic Jones) to discuss the results of the project and discuss possible future research directions
Were there any unexpected outcomes as part of the project?
• Positive trends in ground-level NH_3 concentrations were unexpected. Since the publication in 2018 of the Code of Good Agricultural Practice to reduce emissions of NH_3 from agricultural practices, it was expected to observe signs of decreasing trends.
What are your plans to share the outcomes of this research with others? (Give details of any future meetings, conferences, papers or other dissemination planned)
• Part of the results have been reported in the Annual RAL report to Defra
Project Impact: What is the most significant output/impact from this project?
There is a current plan to reduce NH_3 emissions from agricultural activities in the UK. The UK government aims to reduce ammonia emissions by 8% in 2020 and 16% in 2030, compared to 2005 levels. In order to achieve that, the Code of Good Agricultural Practice (COGAP) was published in 2018. From the trend analysis undertaken in this project, there is not a general evidence that the COGAP has an impact on atmospheric NH_3 levels. Ground-level network of sites measuring NH_3 concentrations is limited and does not cover the entire of the UK. The use of new satellite data products can help monitor and evaluate possible trends over time.