Assessing the future IRS-MTG NH_3 observations

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Introduction

Ammonia (NH_3), primarily emitted by agriculture[1], is a key atmospheric pollutant linked to public health[2] and climate change[3]. While satellite data have assessed **NH_3 variability** globally[4], regionally[5], and locally[6], understanding its diurnal changes and relationship with temperature remains limited, impacting accurate modeling of NH_3 emissions and associated pollution events.

IASI[7] (Infrared Atmospheric Sounding Interferometer) instruments (**Fig 1**) aboard Metop-A,B and C satellites, launched in 2006, 2012 and 2018 respectively, retrieve NH_3 total columns within the 800-1200 cm^{-1} spectral range. The upcoming **IRS[8]** (InfraRed Sounder) on the MTG (Meteosat Third Generation) satellite[9], scheduled for late 2025, will offer high-resolution observations in space and time, promising insights into the role of NH_3 and temperature during pollution episodes. In this study we assess the future satellite **measurement uncertainties** and explore its contribution to the observation of atmospheric NH_3.

	IASI	IRS
Spatial resolution (nadir)	Circle of 12 km diameter	4 km X 4 km
Temporal resolution	Twice a day 9:30 AM - 9:30 PM	Every 30 minutes (Europe)
Spectral resolution	0.5 cm^{-1}	0.754 cm^{-1}
Spectral bands	645cm^{-1} – 2760cm^{-1}	700cm^{-1} - 1210cm^{-1} and 1600cm^{-1} -2175cm^{-1}

Figure 1: Technical comparison between IASI and IRS

Method

This study explores the potential of the IRS-MTG mission in capturing NH_3 variability over the Brittany region in France. To assess IRS NH_3 measurement capabilities, synthetic IRS spectra are computed using the **4A/OP[10]** radiative transfer model and a realistic atmosphere simulated by the **CHIMERE model[11]** (**Fig 2**) with a temporal resolution of 1 hour and a spatial resolution of 4 km x 4 km for July 2016.

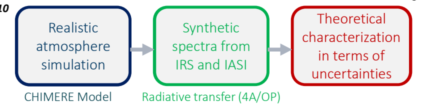

Figure 2: Methodology applied to assess the potential of IASI/IRS to measure NH_3

Fig 3 illustrating the **absolute Thermal Contrast** (TC) on the 19th of July 2016 at 1 AM shows lower TC near urban areas, such as Paris (TC 2 times lower). In this study, TC is defined as the difference between the surface temperature (T_{surf}) and the temperature at 600 meters above ground level (**Equation 1**).

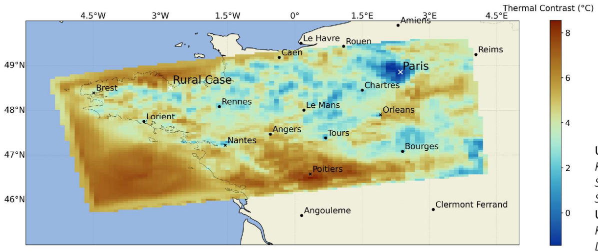

Figure 3: Monthly average of absolute thermal contrast (°C) simulated by CHIMERE for the 19/07/2016 at 1AM

Measurement uncertainties are determined using **Equation 2[12]**, utilizing the NH_3 Jacobian (**Equation 3**) and the Instrumental Noise Covariance Matrices for IASI and IRS (given by Eumetsat).

$$TC = Tsurf - T_{600m} \quad (1)$$

$$\sigma^2_{instrument} = S = (K^T S_\varepsilon^{-1} K)^{-1} \quad (2)$$

$$K = (L(X + dX) - L(X))/dX \quad (3)$$

Units Equation 2 :
K :NH_3 Jacobian ($W/(m^2.sr.cm^{-1})/(molecules/cm^2)$)
Sε :Full Instrumental Noise Covariance Matrix($W/(m^2.sr.cm^{-1})$)²
S :Measurement Uncertainty Matrix ($molecules/cm^2$)²
Units Equation 3 :
K :NH_3 Jacobian ($W/(m^2.sr.cm^{-1})/(molecules/cm^2)$)
L(X) :Radiance spectra ($W/(m^2.sr.cm^{-1})$)
X :NH_3 total column ($molecules/cm^2$)
dX :0.01% increment of the total column (~10^{12} $molecules/cm^2$)

Results

1. Computing IRS and IASI measurements uncertainties

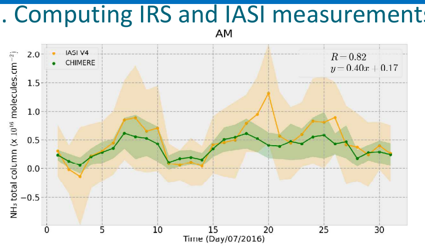

Figure 4: Timeseries of daily NH_3 total column derived from IASI and CHIMERE simulation in July 2016

1.1 Can CHIMERE simulate a real atmosphere ?

The monthly NH_3 total column measured by IASI and simulated by CHIMERE coincident with the morning overpasses in July 2016 are 0.46 ± 0.06 10^{16} and 0.37 ± 0.03 10^{16} molec/cm², respectively (**Fig 4**). The main difference between both datasets is the NH_3 enhancement observed by IASI on the 20th of July 2016, which is almost 4 times higher than the CHIMERE simulation.

The **strong correlation** (R=0.82) between IASI observations and the CHIMERE model suggests that CHIMERE represents a realistic atmosphere.

1.2 Distribution of measurement uncertainties

Fig 5 displays measurement uncertainty over the CHIMERE domain for the 19th of July 2016 at 1 AM. The measurement uncertainty variability is very high (9.4 10^{15} molec/cm² corresponding to 1.17 times the mean total column of NH_3) with the minimum at 3.2 10^{14} molec/cm² and the maximum at 4.6 10^{17} molec/cm². These high measurement uncertainties are correlated to areas with a thermal contrast close to 0 (**Fig 3**).

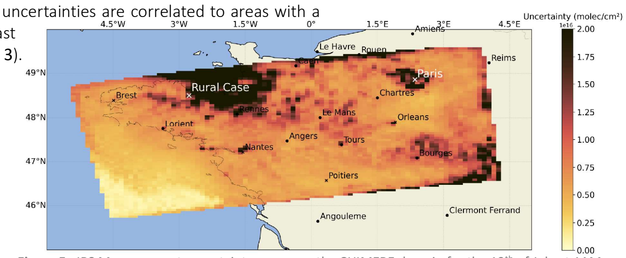

Figure 5 : IRS Measurement uncertainty map over the CHIMERE domain for the 19th of July at 1AM

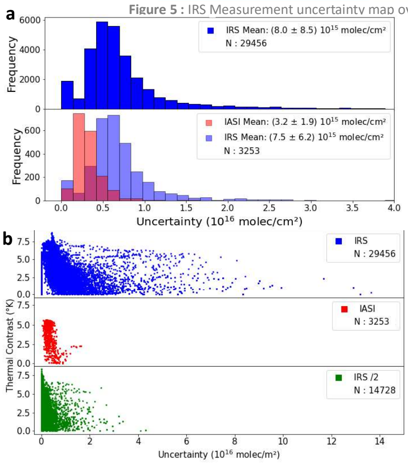

Figure 6: (**a**) Measurement uncertainty distribution for IRS (top), IASI and IRS at the overpass time of IASI (bottom). (**b**) Thermal Contrast as a function of measurement uncertainties of IRS (blue), IRS averaged by pairs of observations (green), and IASI (red).

The average of the IRS measurement uncertainties (**Fig 6.a**; 7.5 10^{16} molec/cm²) is **twice higher** than IASI one (3.2 10^{16} molec/cm²) but with a variability **3 times higher** than IASI. This larger variability of IRS measurement uncertainty might be due to the higher number of observations (factor of 10) with respect to IASI.

Measurement uncertainties depend on thermal contrast with higher measurement uncertainties associated with lower thermal contrast (**Fig 6.b**). Considering the entire IRS dataset (top panel), the averaged IRS measurement uncertainty is 2.5 times larger than the IASI one (middle panel). However, considering IRS data averaged every 2 hours (bottom panel), the IRS measurement uncertainty decreases by a factor of 2.3 and is similar than IASI measurement uncertainty (3.5 10^{16} molec/cm² for IRS against 3.2 10^{16} molec/cm² for IASI). This means that analyzing IRS data every 2 hours is sufficient to achieve a similar measurement uncertainty than IASI.

2. Difference between urban and rural sites

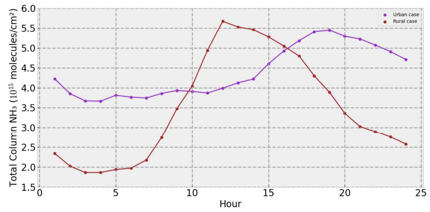

Figure 7: Diurnal variability of NH_3 total column derived from the CHIMERE simulation in July 2016 for urban (purple) and rural (red) case studies

2.1 NH_3 diurnal variability

The mean NH_3 total column simulated by CHIMERE in July 2016 is higher at the rural than at the urban sites with 4.39 ± 2.61 10^{15} molec/cm² compared to 3.50 ± 3.21 10^{15} molec/cm².

The **diurnal variability** of NH_3 for the rural case is **4.73 times higher** than for the urban case (**Fig 7**), suggesting the local influence of NH_3 source at the rural site.

2.2 Diurnal variability of measurements uncertainty

Daily, the **thermal contrast** begins to increase at 6 AM at the urban site, whereas it starts to increase at 8 AM at the rural site (**Fig 8**). The NH_3 total column of the first day of July 2016 (Fig 8 purple big dots) is the **lowest of the month** (2.70 ± 0.88 10^{15} molec/cm²) and the NH_3 Jacobian is one the highest for the month. When the **NH_3 total column is low, the measurement uncertainty is highly linked to the thermal contrast.**

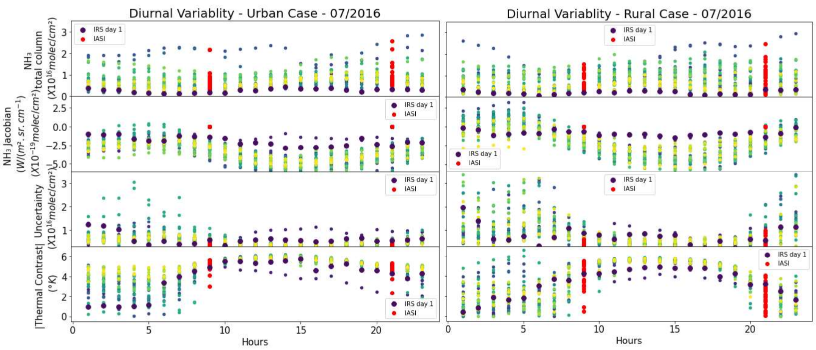

Figure 8: Diurnal Variability calculated at the urban (**a**) and rural (**b**) cases. From top to bottom panels: NH_3 total column, NH_3 Jacobian, measurements uncertainty, and the absolute thermal contrast. Colors indicate days of the month for hourly IRS observations, and red dots correspond to IASI observations.

Conclusion

A realistic atmosphere simulation from the CHIMERE model was used to simulate atmospheric conditions at the pixel size of IRS, generating synthetic spectra for 40 case studies using the 4A/OP radiative transfer algorithm. Comparing NH_3 uncertainties over Brittany in July 2016, IASI showed lower uncertainties than IRS, but IRS exhibited higher variability. Averaging IRS observations every 2 hours reduced uncertainties below those of IASI, suggesting this interval provides better NH_3 concentration estimates. Analysis of rural and urban cases revealed significant variability in TC and uncertainties, especially when NH_3 total column are low. This study demonstrates the ability of the future IRS satellite to study NH_3 variability and how this variability changes as a function of the area. By averaging IRS data by pairs to minimize its uncertainty, it will be possible to use IRS data to improve our understanding of NH_3's relationship with temperature.

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