Methane isotopologue parameter assessment of multiple spectral databases using TCCON

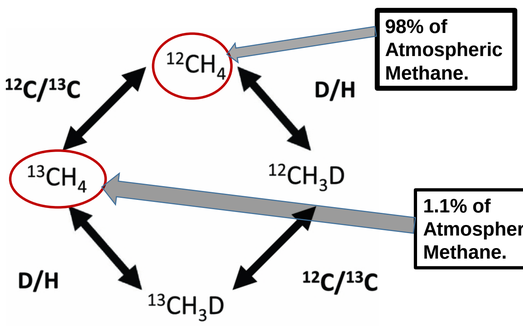
Edward Malina[1], Ben Veihelmann[1], Dietrich G. Feist[2,3] and Isamu Morino[4]
[1]Earth and Mission Science Division – ESTEC/European Space Agency (ESA) – the Netherlands
[2]DLR - Institute of Atmospheric Physics – Germany, [3]Max Planck Institute for Biogeochemistry – Germany
[4]National Institute for Environmental Studies – Japan

SUMMARY

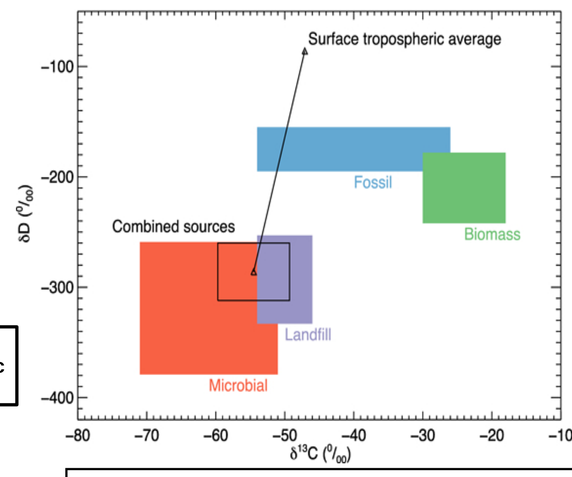
In this study, we perform **retrievals** of the two **main methane isotopologues $^{12}CH_4$ and $^{13}CH_4$** using the Total Carbon Column Observing Network (**TCCON**). With the aim of assessing the **biases** associated with methane retrieval in the future **Copernicus Sentinel 5** spectral regions. To assess the biases we use the TCCON **GGG2014** retrieval environment, and four separate spectroscopy databases, the **JPL/TCCON** spectroscopy database; the **HITRAN2016** database; the **GEISA2015** database; and the **ESA SEOM-IAS** database. We find significant variability in the retrievals of methane isotopologues, both in terms of the band and database. The SEOM-IAS database, with the addition on **non-Voigt** elements tends to show better spectral fits, and agrees closely with the current standard TCCON retrievals.

METHANE ISOTOPOLOGUES

ISOTOPOLOGUES
Chemical species of **molecule** that contains at least one **isotope** in its structure.



Courtesy of Nixon et al (2012).



Atmospheric Methane and its composition. Rigby et al (2012).

METHANE SOURCES:
The ability to **distinguish** between the **isotopologues** of methane, allows an observer to determine the source of the **methane** emissions. (Etiope 2009).

$$\delta^{13}C = \left(\frac{\left(\frac{13C}{12C}\right) sample}{\left(\frac{13C}{12C}\right) standard} - 1 \right) \times 1000$$

$\delta^{13}C$:
Global tropospheric averages of **-45‰,** abiogenic sources **-20‰,** and biogenic sources **-60‰.**

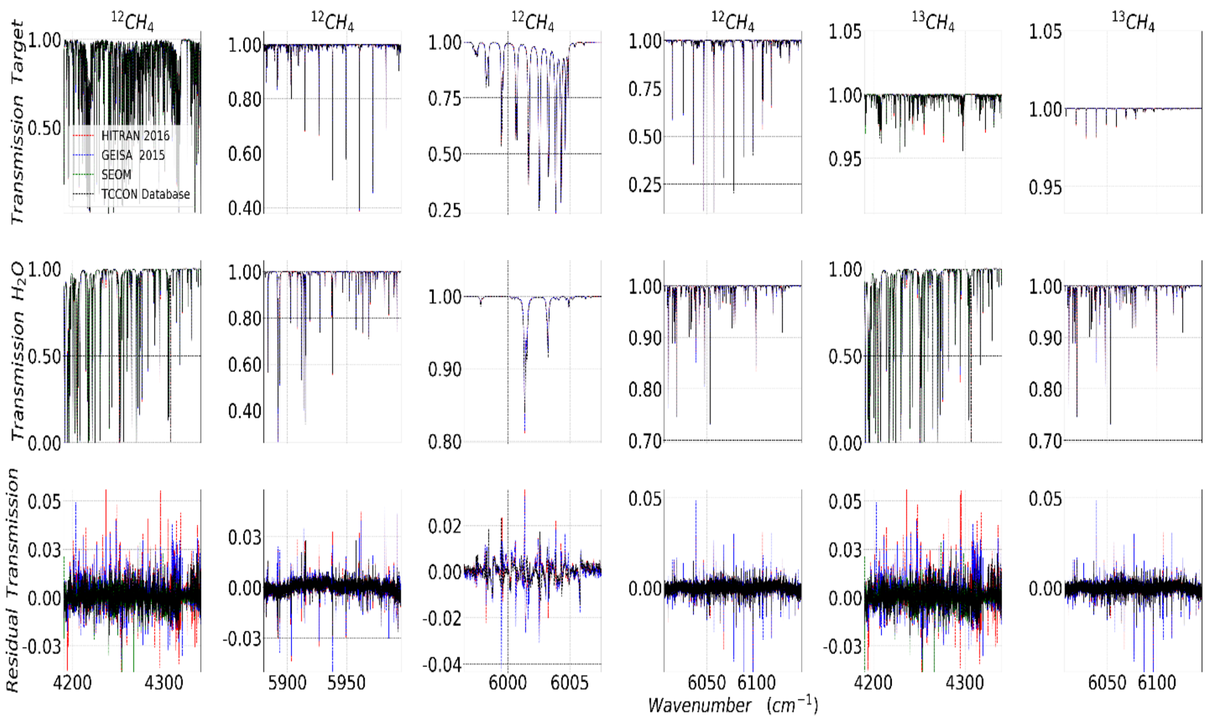
SPECTRAL WINDOWS

Window	Range (cm^{-1})	Target species	Source
1	4190-4340	$^{12}CH_4$	Sentinel 5 baseline
2	5880-5996	$^{12}CH_4$	TCCON Standard
3	5996.45-6007.55	$^{12}CH_4$	TCCON Standard
4	6007-6145	$^{12}CH_4$	TCCON Standard
5	4190-4340	$^{13}CH_4$	Sentinel 5 baseline
6	6007-6145	$^{13}CH_4$	TCCON Standard

TCCON retrieval windows for $^{12}CH_4$, with addition of Sentinel 5 band.

Wide windows only for $^{13}CH_4$.

EXAMPLE TRANSMISSION SPECTRA AND RESIDUAL TRANSMISSION



SPECTROSCOPY (ASSUMED LINESHAPES)

- **JPL/TCCON** (Black – Voigt)
- **HITRAN2016** (Red – Voigt)
- **GEISA2015** (Blue – Voigt)
- **SEOM-IAS** (Green – Non-Voigt)

Retrieval statistics indicate that SEOM-IAS shows the lowest residual error.

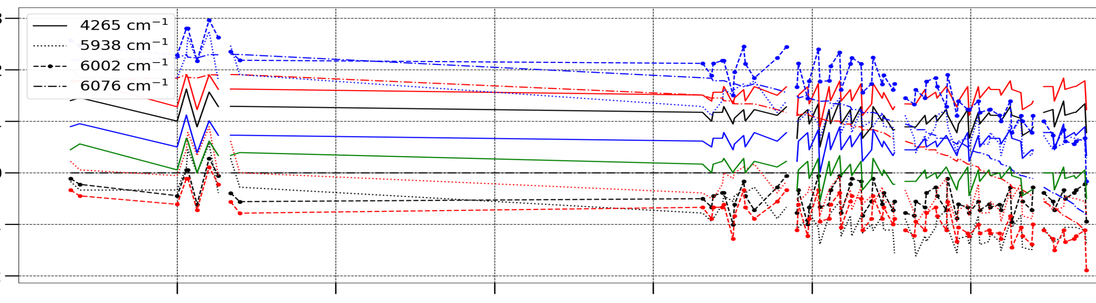
Windows 5 & 6 focused on $^{13}CH_4$ show same fit values as windows 1 and 4.

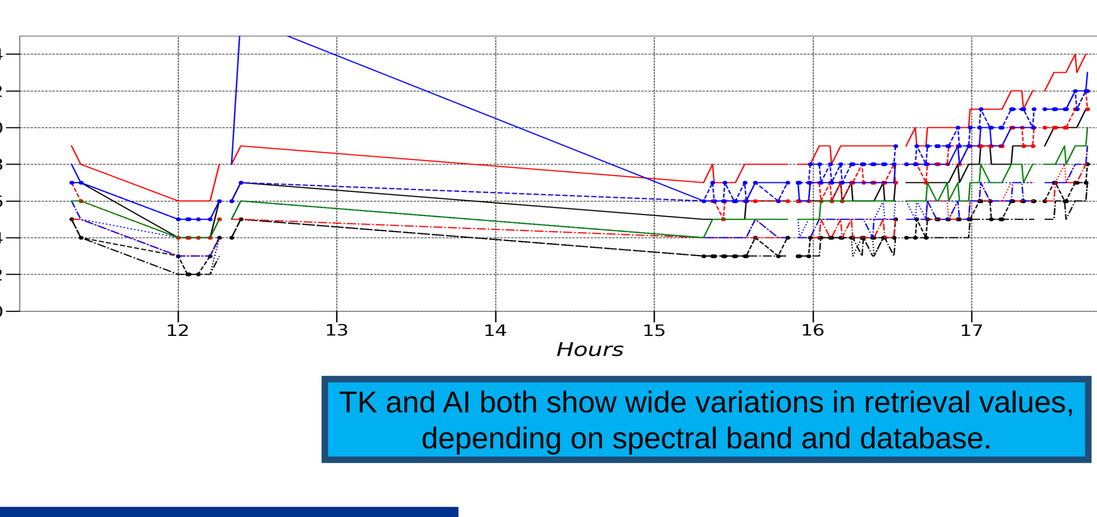
	Window 1	Window 2	Window 3	Window 4
RMSE	TCCON: 4.438×10^{-3}	TCCON: 3.076×10^{-3}	TCCON: 3.846×10^{-3}	TCCON: 2.680×10^{-3}
	HITRAN: 6.803×10^{-3}	HITRAN: 3.747×10^{-3}	HITRAN: 5.302×10^{-3}	HITRAN: 3.578×10^{-3}
	GEISA: 5.678×10^{-3}	GEISA: 3.910×10^{-3}	GEISA: 6.010×10^{-3}	GEISA: 3.722×10^{-3}
	SEOM: 4.268×10^{-3}	SEOM: nan	SEOM: nan	SEOM: nan

EXAMPLE $^{12}CH_4$ RETRIEVAL TIMELINES

TSUKUBA (TK) (01/04/2016)

- **Variable seasons**, hot wet summers, dry cold winters
- High population density region, **anthropogenic** sources.





"rel. difference" refers to differences from band 4 of TCCON/JPL database

ASCENSION ISLAND (AI) (01/10/2016)

- Near the equator, **constant** year round conditions.
- Low populations density, **natural** sources.

TK and AI both show wide variations in retrieval values, depending on spectral band and database.

DAY AVERAGED $\delta^{13}C$ VALUES

$\delta^{13}C$	TCCON Bands 1 & 5	TCCON Bands 4 & 6	HITRAN Bands 1 & 5	HITRAN Bands 4 & 6	GEISA Bands 1 & 5	GEISA Bands 4 & 6	SEOM Bands 1 & 5
TK 01/04/2016	-116‰	-1.52‰	-59.1‰	-33.1‰	-358‰	-193‰	-109‰
TK 07/07/2016	-173‰	74.5‰	-159‰	296‰	-518‰	-202‰	-143‰
AI 23/08/2016	-108‰	-92.4‰	-104‰	-8.47‰	-384‰	-297‰	-95.0‰
AI 01/10/2016	-115‰	43.6‰	-46.7‰	160‰	-419‰	-134‰	-84.2‰

Calculated from the $\delta^{13}C$ equation and retrievals from TCCON spectral windows.

CONCLUSIONS

- SEOM-IAS database **has improved spectral fit performance**, Also shows least variation in $\delta^{13}C$.
- Climate and site do not impact the indicated differences.
- Large **variations** in $\delta^{13}C$ calculation depending on **bands and spectral database**.

8. REFERENCES

HITRAN2016: https://hitran.org/
GEISA2015: http://cds-espri.ipsl.upmc.fr/GEISA/geisa_raie_2015.php
SEOM-IAS: https://www.wdc.dlr.de/seom-ias/
GGG2014: https://tccon-wiki.caltech.edu/