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Impact of Spectroscopy on CH_4 Total Column Retrievals from Sentinel-5P/TROPOMI in the Short-Wave Infrared

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Introduction

- Methane (CH_4) strongly affects the global climate
- Short-Wave IR spectra to infer molecular concentrations
- Accurate modeling of molecular absorption mandatory

BIRRA — Beer InfraRed Retrieval Algorithm

Nonlinear least squares (NLS): $\min_x \|\boldsymbol{y} - \boldsymbol{F}(\boldsymbol{x})\|^2$

$$\boldsymbol{F}(\boldsymbol{x}) \;=\; r(\nu)/\pi\ \cos\theta\ I_{\text{sun}}(\nu)\ \exp\left[-\sum_m \alpha_m \tau_m(\nu)\right] \otimes \mathcal{S}(\nu,\gamma,\ldots) + b$$

τ_m molec optical depth; $\mathcal{S}$ ISRF; θ SZA; b baseline

$$\boldsymbol{x} \in (\boldsymbol{r}, \boldsymbol{b}, \boldsymbol{\alpha}, \gamma, \delta, \ldots).$$

- BIRRA infers information from absorption features [2, 3]
- State vector $\boldsymbol{x}$ contains geophysical parameters
- Py4CAtS line-by-line forward model based on GARLIC [6]
- BIRRA was originally developed for SCIAMACHY nadir CO and CH_4

SEOM–IAS — Improved Atmospheric Spectroscopy

- Spectroscopic database for TROPOMI around 2.3 μm [1]
- New line positions, intensities, broadening parameters
- Additional ‘beyond Voigt‘ line parameters
- Speed-dependent Rautian profile + line-mixing (SDRM)

gas	data	# lines	$S\,[\mathrm{cm^{-1}/molec\,cm^2}]$	$\gamma_{\mathrm{air}}^{(0)}\,[\mathrm{cm^{-1}}]$	n	$\gamma_{\mathrm{air}}^{(2)}\,[\mathrm{cm^{-1}}]$	$\nu_{\mathrm{vc}}\,[\mathrm{cm^{-1}}]$
CH_4	SEOM	6205	$6.7 \cdot 10^{-27} - 5.5 \cdot 10^{-21}$	0.019 – 0.182	0.19 – 1.82	0.008405(610)	0.00911(65)
	H16	8375	$1.0 \cdot 10^{-29} - 5.5 \cdot 10^{-21}$	0.034 – 0.077	0.67 – 0.77		
	G15	7213	$9.5 \cdot 10^{-28} - 5.4 \cdot 10^{-21}$	0.034 – 0.077	0.46 – 0.97		
H_2O	SEOM	1177	$1.4 \cdot 10^{-30} - 2.2 \cdot 10^{-23}$	0.004 – 0.141	0.31 – 1.02	0.007197(35)	0.01083(12)
	H16	1197	$1.0 \cdot 10^{-32} - 2.2 \cdot 10^{-23}$	0.004 – 0.109	0.32 – 0.73		
	G15	1101	$8.4 \cdot 10^{-30} - 2.2 \cdot 10^{-23}$	0.004 – 0.096	0.32 – 0.69		
CO	SEOM	110	$1.0 \cdot 10^{-31} - 3.5 \cdot 10^{-21}$	0.042 – 0.081	0.67 – 0.79	0.00607(10)	0.0047(10)
	H16	110	$1.0 \cdot 10^{-31} - 3.5 \cdot 10^{-21}$	0.042 – 0.081	0.67 – 0.79		
	G15	160	$1.1 \cdot 10^{-36} - 3.6 \cdot 10^{-21}$	0.040 – 0.079	0.69		

Table: Spectroscopic line data for the 2311–2352 nm interval. The last two columns show the mean of the ’beyond Voigt’ air-broadening speed-dependence and Dicke narrowing parameters. The number of non-zero values is indicated in the parentheses [4].

Level 1→2 Processing

Input data required for the retrieval

- S5P radiance and irradiance data
- BDPM and ISRF’s
- **Spectroscopic line data**: SEOM–IAS, HITRAN, GEISA
- Atmospheric data on p, T and specific humidity
- A priori information on molecular concentration profiles
- Terrain elevation from the ETOPO global relief model
- Cloud-mask from VIIRS aboard Suomi-NPP
- ...

Impact on CH_4 Spectrum

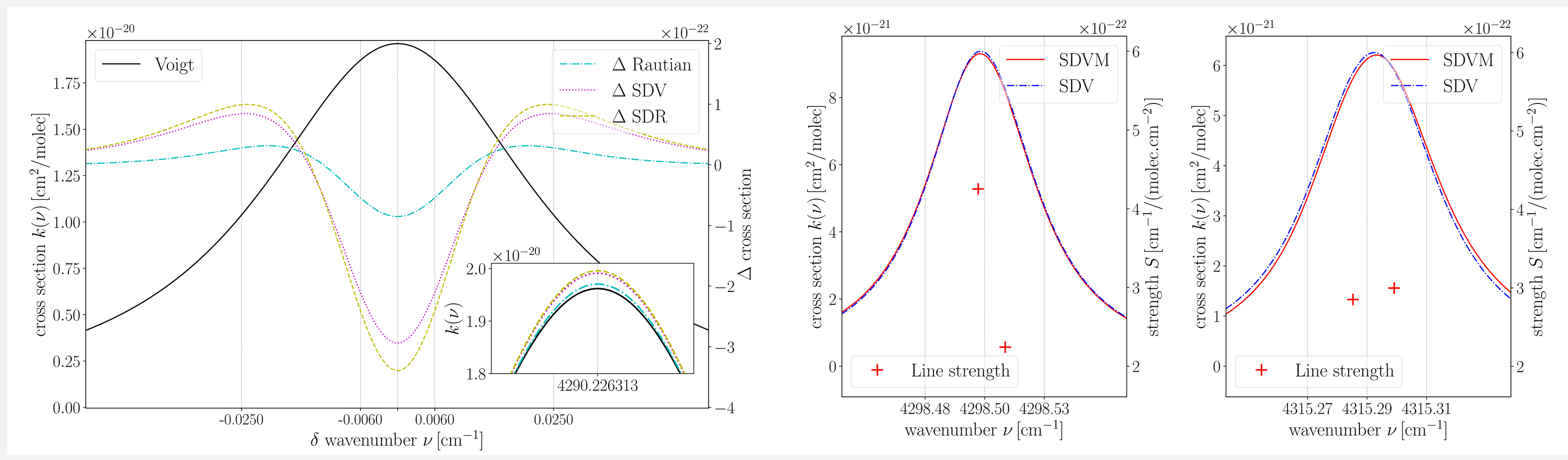

Fig. 1: (Left) CH_4 absorption cross sections for various line profiles at 330 hPa and 243 K computed with SEOM—IAS line data. (Center&Right) The effect of line-mixing on molecular cross sections. Note the dependence on relative line strengths of neighboring lines [5].

Impact on CH_4 Retrieval

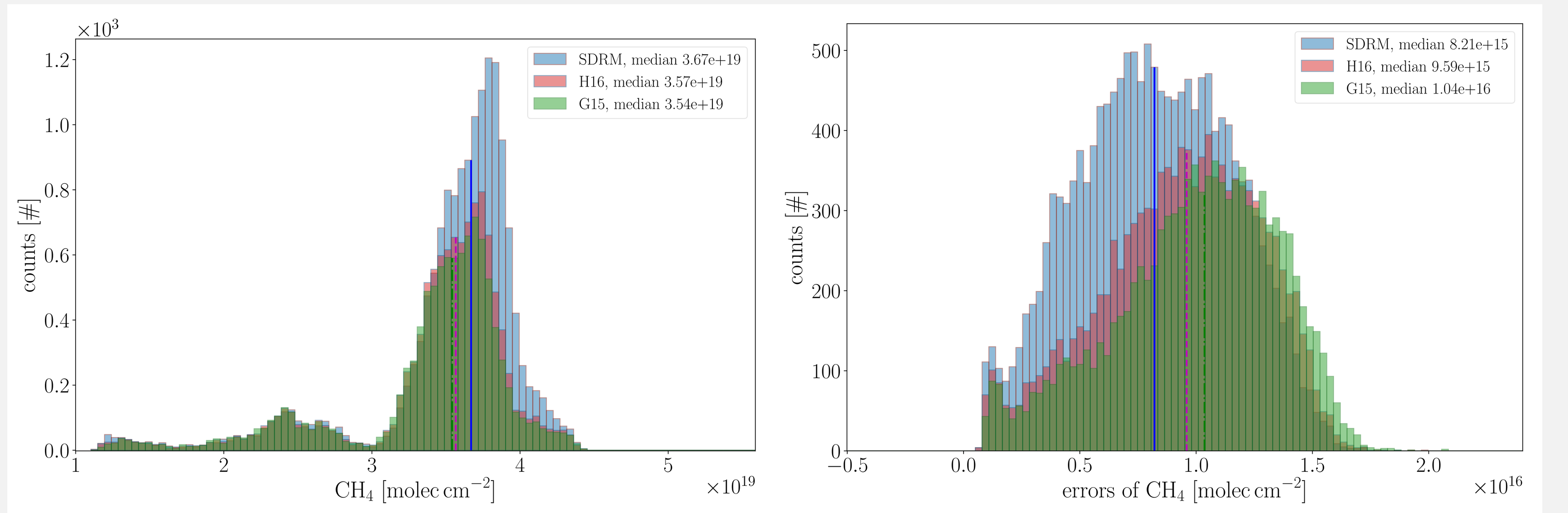

Fig. 2: CH_4 columns (left) over Amazonia in orbit 9553 along with errors (right) for different spectroscopic line lists and models [4].

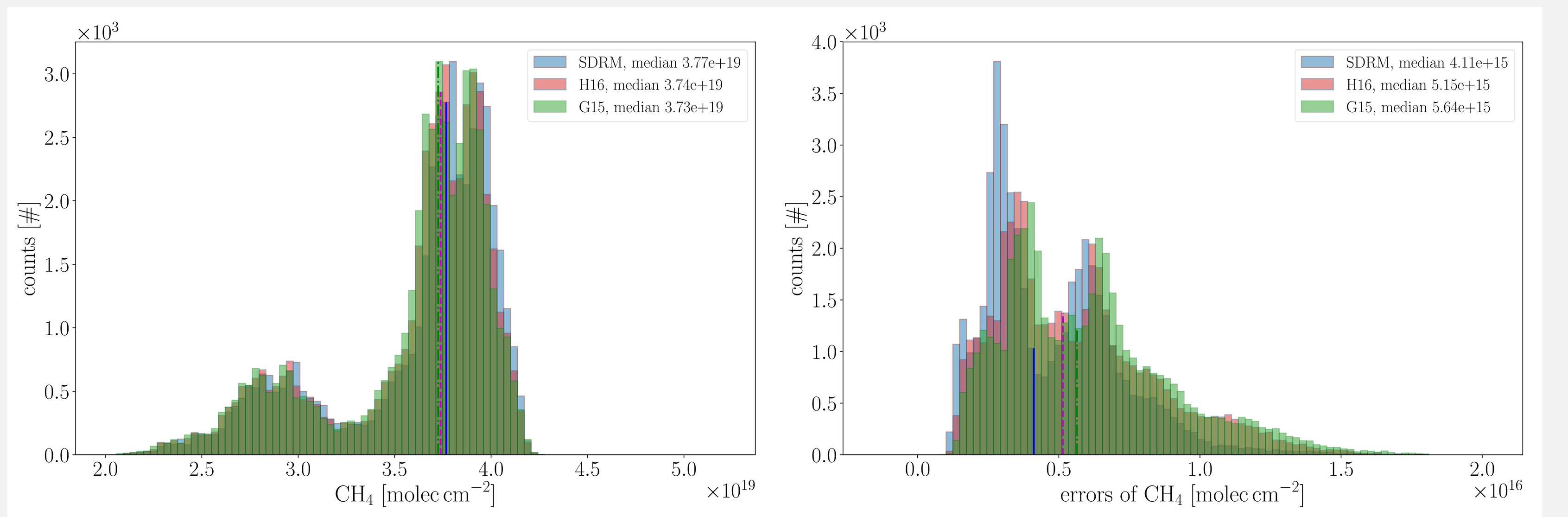

Fig. 3: CH_4 retrieved in orbit 7861 over the Sahara region [4].

Beyond SEOM–IAS/SDRM

	median		mean		variance	
	HTM	SDRM	HTM	SDRM	HTM	SDRM
α_{CH_4}	1.0475	1.0485	1.0467	1.0478	0.0157	0.0158
α_{H_2O}	1.3450	1.3555	1.3929	1.3945	0.4495	0.4487
α_{CO}	0.9566	0.9572	0.9338	0.9344	0.0463	0.0461

Table: Retrieved scaling factors for the Hartmann-Tran (HTM) and SDRM line profiles from TROPOMI measurements in orbit 2923. The partial correlation parameter was manually set in the HTM profile [5].

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