Reanalysis of Cassini Huygens GCMS results- an effort to extract composition of trace gases

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Introduction

In Titan, the two major species N₂ and CH₄ are ionized and/or photolyzed at high altitudes by To quantify the trace gases in Titan's atmosphere using the Gas Chromatograph the sunlight and the energetic particles from Saturn's magnetosphere, resulting in rich Mass Spectrometer (GCMS) onboard the Cassini Huygens probe. We have used a atmospheric chemistry and a wide variety of carbon and nitrogen-bearing atmospheric mass spectra deconvolution code (Gautier et. al. 2019) that runs Monte Carlo compounds.

Huygens GCMS: The mission was conducted on 14 January 2005 for nearly 3.5 hours. GCMS ratios. sampled data from an altitude of 147 km. In our work we focus on the atmospheric segment only and use measured spectra from one of the five ion sources (in the spectrometer) that directly samples from the atmosphere. The process is shown below:

Objective

simulations to vary the peak intensities of some species and measure their mixing

Methodology





Data treatment:

- Pulse pile up correction (*Niemann et.al.2010*)
- Correcting mass-28 saturation using a proxy peak (of mass-29) (Gautier et.al. in prep)
- Background removal

Mass spectra deconvolution code (Gautier et.al.2019):

- A database containing the mass spectra of ten species-N₂, CH₄, C₂H₂, HCN, H₂, C_2H_4 , C_2H_6 , Ar, CO_2 , Ne (taken from Cassini INMS and NIST calibrations).
- Monte Carlo simulations by varying the database by ± 30% (100,000 runs).
- Implementing ionization and transfer cross sections to the code.



Results and discussions

For trace gases in lower atmosphere, GCMS results do not agree with results from CIRS and other microphysical models (figure 2).

 \succ Mixing ratios of HCN, C₂H₆, C₂H₄ is higher.

 \geq CO₂ was present as a background in the ion source. Hence this might be the reason for its

Possible hypotheses:

$ightarrow C_2H_2$ mixing ratio is similar. ▲ Our results (at 145 km) C. Mathe et.al.,2020, flyby T18 (at 150 km 10^{-3} Figure 2: Comparison $\frac{1}{2}$ 10-5 between our results $\sum 10^{-6}$ those calculated and using CIRS results for 10^{-7} flyby T18 10^{-8} C₂H₂ HCN C₂H₄ C₂H₆ CO2

Species

○ Aerosol outgassing –

o Instrument inlet temperature higher than ambient temperature (figure 3) -> possible that some aerosols might have evaporated at the entrance.

 \circ Experimental results show that it is possible for light molecules (like HCN, C₂H₂, C₂H₄) to outgass at this temperature (Morisson et. al. 2016).

○ Recombination inside ion source –

• Possible that fragments inside ion source might have recombined if the pressure inside the ion source changed during descent.

high mixing ratio.

• Do not have information on ion source pressure.

○ No change in the filament current in the first 2000 seconds of the descent (no data on the later part of the mission though) -> recombination might be negligible.

• Deposition of ice on the instrument –

• Possible that at high altitudes (when the instrument did not start working), ice might have gotten stuck at the entrance.



300

instrument

— Instrument inlet temperatu

— Ambient temperature

100 150 200 250 Temperature (K)

ambient and

temperature

| ≽ Fi

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Figure 3: Vertical profile of

• By the time the instrument started to sample, it had evaporated and thus was measured.

Cross contamination between two consecutive peaks –

olf one mass peak has a very high count rate, it is possible that some of it's counts might have been detected at it's previous or next peak.

• Might explain why we see such a high mixing ratio in HCN.

• We see cross talk between m/z 27,28,29 (figure 4). Currently trying to correct for this!

Future work and it's impact	References	Acknowledgement
nd an efficient way to correct for the cross talk between ass peaks- hopefully that will reduce the mixing ratios of ome gases. ook for a way to separate aerosol contribution from the easured data. cudy of these results can be beneficial to the future ragonfly mission which will be landing on the surface for	 Gautier et al. Decomposition of electron ionization mass spectra for space application using a Monte-Carlo approach. Rapid. Com. Mass Spec. 34(8), e8659 (2020) Niemann et al. Composition of Titan's lower atmosphere and simple surface volatiles as measured by the Cassini-Huygens probe gas chromatograph mass spectrometer experiment. JGR 115, E12006, 2010 Mathé et al. Seasonal changes in the middle atmosphere of Titan from Cassini/CIRS observations: Temperature and trace species abundance profiles from 2004 to 2017, Icarus 344 (2020) 113547 Gautier et al. Reevaluation of methane mixing ratio in Titan's lower atmosphere from Huygens/GCMS data (in prep) Morisson et. al. Titan's organic aerosols: Molecular composition and structure of laboratory analogues inferred from pyrolysis gas chromatography mass spectrometry analysis, Icarus 277 (2016) 442–454 	The funding for this research was provided by ANR (ANR "TOMTA" - ANR-20-CE49-0004-01) and PNP. We also thank PLANET- ESLAB for providing us a partial grant for this conference.