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Reanalysis of trace species in Titan's lower atmosphere from Huygens GCMS

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Introduction

In Titan, the two major gases nitrogen (N_2) and methane (CH_4) are ionized and/or photolyzed at high altitudes by the sunlight and the energetic particles from Saturn's magnetosphere, resulting in a rich atmospheric chemistry comprising of a wide variety of carbon and nitrogen-bearing compounds (see for example Vuitton et al. 2019). These molecules combine to form heavier and more complex molecules until they become heavy enough that they are unable to retain their gaseous phase. These molecules then turn into aerosols and travel down into the atmosphere where they aggregate with other aerosols to form bigger particles, finally forming a haze layer at approximately 500 km. The simple gaseous species also travel deep into the atmosphere until they reach the tropopause, where most of them condense (Wilson and Atreya 2004).

The Cassini Huygens mission which was launched in 1997, reached the Cronian system in mid-2004. The Huygens probe detached itself from the orbiter in December 2004 and entered Titan's atmosphere on 14 January 2005. With the objective of studying the lower atmosphere, the science instruments started operating from an altitude of 150 km and took measurements for three hours-2.5 hrs in the atmosphere and an hour on the ground (Niemann et al 2010). In the present work, we focus on studying the vertical profiles of trace species in the lower atmosphere using the measurements by the GCMS on the probe, to obtain a better insight into the atmospheric processes taking place there.

Methodology

The GCMS stage 2 files were used for this work. It has been corrected for detector dead time and saturation (Niemann et al. 2010). The background was also removed from the data. Finally, upon closer inspection, we find that there has been cross-contamination between mass peaks 26-29 because of mass-28 (from N_2). This was corrected by fitting lognormal curves for each unit mass peak on the fractional mass scans (least count: 0.125 amu) that were taken during the probe descent.

The corrected mass spectra were then used as an input to a mass spectra deconvolution code developed by Gautier et al. 2020. A database of fractionation patterns of 10 species (from NIST and Cassini-INMS calibrations) was created. Our code runs 100,000 Monte Carlo simulations in which the peak intensities of each species's fragmentation pattern are varied by a certain percentage ($\pm 30\%$ in our case). Using a least square linear equations solver, we compute the mole fractions of each species for each simulation at every altitude. The best simulations for each species are chosen when their solutions do not lie near the predefined boundary limits. The solutions of these best simulations are then averaged to get the mole fractions at each altitude.

Results and discussions

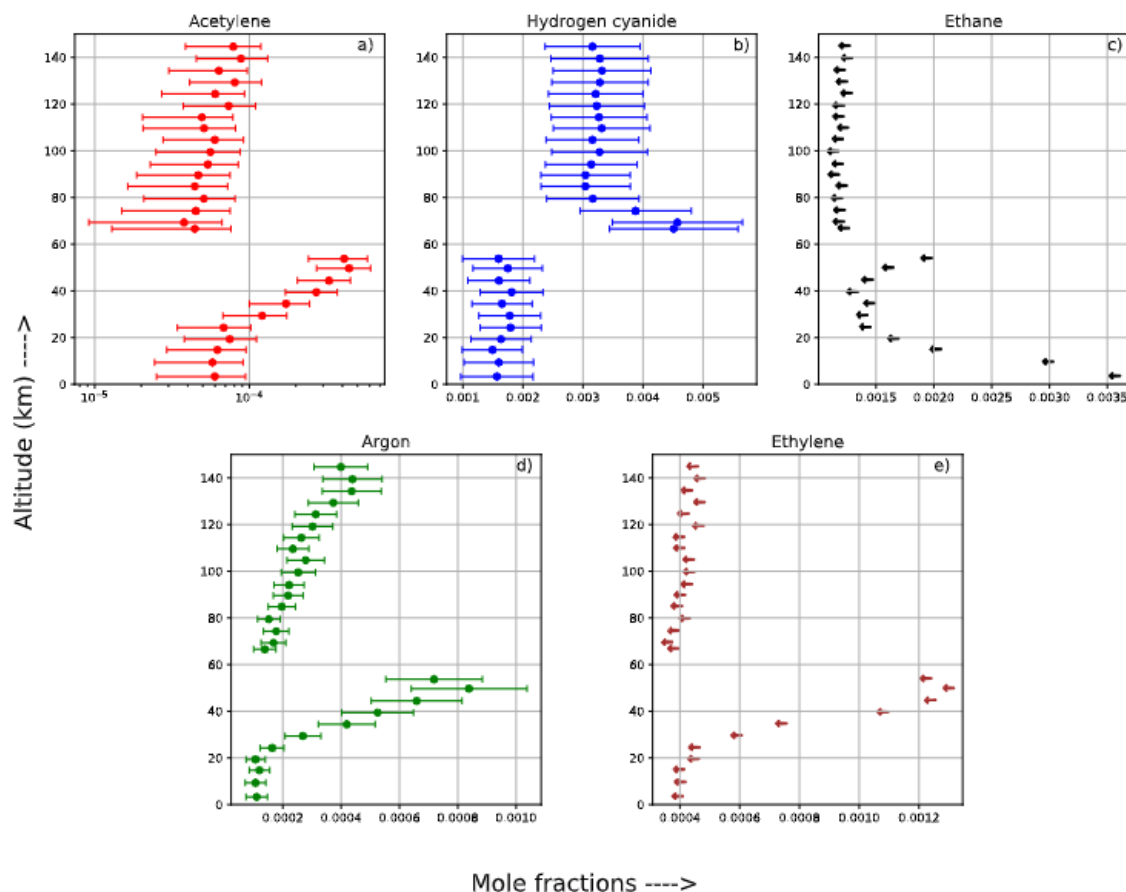


Figure 1: Vertical profile of mole fractions of five trace species- a) acetylene, b) hydrogen cyanide, c) ethane, d) argon, and e) ethylene in their gaseous phase (plotted with their standard deviations) with a resolution of 5 km.

The vertical profiles of five trace species are shown in Figure 1. Ethane and ethylene have been plotted with their upper limits. Upon comparing these results with the computed mole fractions from

CIRS (Mathe et al 2020) and the Titan PCM, it is evident that the mole fractions calculated in this work are higher than what was expected. Most trace gases condense near tropopause, so there should have been a decrease in mole fractions after that, which is not the case here. Hence we present here three hypotheses to interpret the results.

The first hypothesis claims that there might have been significant recombination inside the ion source which could have led to false detection in the spectra. A sudden change in any physical parameters inside the ion source could imply the significance of this phenomenon. However, the lack of available information makes it difficult for us to support this claim which is why we believe that maybe this process was negligible during the descent. The next hypothesis says that frost formed on the surface of the probe while it was passing the condensation region. This could have accumulated at the entrance of the probe which then evaporated by the time the instrument was operational. If any significant layer of frost deposited on Huygens, it would have induced a plateau in the temperature profile measured by the HASI, which was clearly not the case. Thus we cannot explain our results with the existence of frost, and can firmly exclude this hypothesis. Our final hypothesis states that aerosols could be evaporated at certain places inside the probe due to the high temperature inside the instrument compared to the outside. Hence the dataset would contain a mixture of evaporated aerosols and gaseous species which could explain the high mole fractions. The probability of the occurrence of this hypothesis is the strongest among the three.

To summarise, GCMS did not measure just atmospheric gases but could have also measured some aerosols and condensed particles that were trapped in the instrument. Laboratory experiments on Titan tholins are currently being done at low temperatures to investigate this possibility.

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