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Chemical pathway analysis of Titan's upper atmosphere: Oxygen species

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Abstract

CO, CO_2, and H_2O are the only oxygen bearing species in Titan's atmosphere which have been clearly detected so far. Their abundances are controlled by the interaction of external and internal sources, photochemistry and condensation. In this contribution, we determine all significant chemical pathways responsible for the production and consumption of CO, CO_2, and H_2O. Furthermore, we investigate the effects of different oxygen sources on the efficiencies of the pathways. In order to achieve this, we apply a unique algorithm, called the Pathway Analysis Program - PAP to the results of a 1D photochemical model of Titan's atmosphere.

1. Introduction

Titan is a moon with an extended, dense, and reducing atmosphere in the Saturnian system. Its atmosphere is mainly composed of N_2 and CH_4. The oxygen bearing species CO, CO_2, and H_2O are only present in small amounts. CO was detected by ground based observations [9], CO_2 by Voyager/IRIS [11], and H_2O with ISO/SWS [2]. The latter measurements have been complimented by the more recent observations with Cassini/CIRS [1] and the Herschel space observatory [10].

The existence of molecules, such as CO, CO_2, and H_2O in Titan's reducing atmosphere is rather unexpected [17]. Several (external) sources have been suggested to deliver oxygen to Titan's atmosphere and to balance the oxygen sink by CO_2 condensation. The most discussed sources, which have been proposed, are the plume activity of Enceladus forming a water torus [3], Saturn's magnetosphere [5], and micrometeoroid ablation [7, 11, 13, 16]. Additionally, it has been suggested that CO might also be of primordial origin [14, 15]. Several photochemical models have been developed to study, among others, Titan's oxygen chemistry [4, 5, 6, 7, 13, 14, 16].

In order to gain more insight about reaction networks in general, it is useful to inspect chemical pathways. Due to the relatively large number of chemical reactions involved, the identification of all dominant pathways is, however, a challenging task and it is quite impossible to construct them manually.

Therefore, we apply an automated algorithm [8] to the output of an updated version of a 1D photochemical model of Titan's upper atmosphere [7, 10] to investigate the production (consumption) of CO, CO_2, and H_2O. Furthermore, we determine the efficiencies of all dominant pathways as functions of altitude and investigate the effect of the different oxygen sources.

2. Method

The identification of chemical pathways in complex reaction networks and the quantification of their efficiency is generally demanding. In this study, we use an automated computer algorithm, the Pathway Analysis Program (PAP, [8]) and apply it to the results of the updated photochemical 1D model of Titan's atmosphere extending from $z = 32\,\mathrm{km}$ to $z = 1432\,\mathrm{km}$ [7, 10] to determine all significant pathways producing (consuming) CO, CO_2, and H_2O. The 1D model provides the necessary quantities for the computation of chemical pathways with PAP, i.e. time-averaged number densities, time-averaged reaction rates, and net changes in number densities due to the chemical reactions included in the model. Rates of individual CO, CO_2, and H_2O production (consumption) pathways are computed for different altitudes by applying the PAP algorithm to each vertical layer of the column model separately as described by [12]. From these results the global contributions of chemical pathways are obtained by integration over atmospheric height. To investigate the effect of different oxygen sources on the pathways, we investigate three cases which reproduce the observed CO, CO_2 and H_2O concentration profiles:

case I OH originating from Enceladus water torus

case II H_2O release by micro-meteoroid ablation

case III OH release by micro-meteoroid ablation

Furthermore, we added in all three cases an $O(^3P)$ source in form of a Chapman layer centered at $z = 1000\,\mathrm{km}$. This Chapman layer represents the oxygen influx originating from Saturn's magnetosphere.

3. Results and Conclusions

Preliminary results suggest, that the net water production $P_{H_2O} - L_{H_2O}$ (P_{H_2O}: total H_2O production by all chemical pathways, L_{H_2O}: total H_2O consumption by all chemical pathways) depends on the altitude where OH is released. Furthermore, different pathways dominate the H_2O production for cases I to III. CO is produced above $z = 600\,\mathrm{km}$ and the CO formation pathways are unaffected whether oxygen is supplied by Enceladus' water torus or micro-meteoroid ablation. H_2O consumption takes place below $z = 700\,\mathrm{km}$ altitude and the corresponding dominant pathways are the same that consume CO and produce CO_2. These are likewise not affected by the location of the OH/H_2O sources.

In this contribution, we will present for the first time the chemical pathways identified by the PAP algorithm, relevant for the production and destruction of CO, CO_2, and H_2O in Titan's atmosphere. The altitude variations of these pathways and the effect of the different oxygen sources are discussed with respect to their efficiency.

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