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The hydrocarbon lakes of Titan: uncertainties on their chemical composition

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Abstract

Between 2004 and 2007 the CASSINI spacecraft discovered dark patches in the polar regions of Titan. These features are interpreted as hydrocarbon lakes and seas with ethane and methane identified as the main compounds. In this context, we have developed a lake-atmosphere equilibrium model allowing the determination of the chemical composition of these liquid areas present on Titan. The model is based on uncertain thermodynamic data of organic species predicted to be present in the lakes. Here we explore the influence of these uncertainties. The errors and uncertainties relevant to thermodynamic data are simulated thanks to a Monte-Carlo method. Global Circulation Models (GCM) are also employed in order to investigate the possibility of chemical asymmetry between the south and the north poles, due to differences in precipitation rates. We find that mole fractions of compounds in the liquid phase have a high sensitivity to thermodynamic data used as inputs. When we combine all considered uncertainties, the ranges of obtained mole fractions are rather large (up to $\sim 8500\%$). No significant difference is found between the composition of lakes located in north and south poles.

1. Introduction

After years of speculations, Cassini RADAR [7] found evidences of hydrocarbon lakes at the surface of Titan. Due to a large atmospheric fraction of CH_4, determining the composition of these lakes is not straightforward. This is why we developed a numerical model, based on a thermodynamic equilibrium between the atmosphere and lakes. The results of our calculations depend on the quality of thermodynamic data used as inputs, the sensitivity of computed mole fractions is tested thanks to a Monte-Carlo method. Beside this, the possibility of a pole to pole asymmetry in chemical composition is questioned.

2. The lake-atmosphere equilibrium model

Our model is based on regular solution theory and thermodynamic equilibrium is assumed between the liquid and the atmosphere. This equilibrium, which is expressed by the equality of chemical potentials, can be written as follows (Eq. 1 of DUB89):

$$Y_k\, P = \Gamma_k\, X_k\, P_{vp,k}, \qquad (1)$$

where P is the total pressure at Titan's surface, Y_k and X_k respectively the mole fractions of the k compound in the atmosphere and in the liquid, and $P_{vp,k}$ its vapor pressure. The activity coefficient Γ_k (dimensionless) of the k compound is given by the regular solution theory [6]. The Γ_k's depend on the temperature, molar volume and enthalpies of vaporization. Species heavier than ethane have their abundancies taken proportionnaly to their mixing ratio into precipitations. Our model is described in detail in [1, 2, 3].

Table 1: Influence of uncertainties of thermodynamic data on Titan's lakes putative species.

	$\overline{X}$ $(P_{\rm vap})$	$\Delta_{P_{\rm vap}}$ (%)	$\sigma^*_{P_{\rm vap}}$ (%)	$\Delta_{\rm All}$ (%)	$\sigma^*_{\rm All}$ (%)
N_2	$4.9 \cdot 10^{-3}$	37	8	8540	282
CH_4	$9.7 \cdot 10^{-2}$	32	9	1370	157
Ar	$4.9 \cdot 10^{-6}$	31	7	1270	104
CO	$4.2 \cdot 10^{-7}$	37	8	5840	223
C_2H_6	$7.6 \cdot 10^{-1}$	3	1	108	10
C_3H_8	$7.4 \cdot 10^{-2}$	3	1	108	10
C_4H_8	$1.4 \cdot 10^{-2}$	3	1	108	10
HCN	$2.2 \cdot 10^{-2}$	16	4	150	52
C_4H_{10}	$1.2 \cdot 10^{-2}$	3	1	108	10
C_2H_2	$1.1 \cdot 10^{-2}$	3	1	108	10
CH_3CN	$9.9 \cdot 10^{-4}$	3	1	109	14
CO_2	$2.9 \cdot 10^{-4}$	3	1	108	10
C_6H_6	$2.3 \cdot 10^{-4}$	3	1	108	10

3. Influence of thermodynamic data on estimated chemical composition

Assuming a maximum uncertainty of $\pm 10\%$ for vapor pressure, molar volumes, enthalpies of vaporization and parameters of interaction l_{ij}'s; the mole fractions X_i's of considered species are computed. The dispersion of results is quantified by $\Delta = (X_{\rm max} - X_{\rm min})/\overline{X}$ ($\overline{X}$: average value) and the relative standard deviation σ^*. Table 1 gathers the average values $\overline{X}$ corresponding to the case for which only vapor pressures are uncertain (quantities labeled "P_{vap}"), $\Delta_{\rm All}$ and $\sigma^*_{\rm All}$ refer to the simulation done with all the data undergoing uncertainties. As one can notice, the abundancies of compounds for which the thermodynamic equilibrium is written (equation 1) are the most affected (i.e. N_2, CH_4, Ar and CO). Others (C_2H_6, ...) have abundancies much less sensitive to not well known data.

4. Influence of location

As on Earth, the precipitation rates on Titan are function of location (and time). We have restricted our study to the geographic dependence of lakes composition and more precisely to a possible south/north asymmetry. We used precipitation rates coming from 2D models of Titan's atmosphere [4]. Using thermodynamic conditions ($T = 90$ K and $P = 1.467$ bar) relevant for Titan's pole we did not find any significant differences between the composition of south and north lakes (i.e. differences of the order of 1%) except for C_3H_8 ($\sim 30\%$), C_4H_{10}, CH_3CN and C_6H_6 (both around $\sim 20\%$).

5. Conclusion

Our work strongly suggests *in vitro* simulation of the Titan's lakes. This would be particularly relevant in the perspective of proposed future missions to Titan like *Titan Saturn System Mission* [5] or *Titan Mare Explorer* [8].

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