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Simulation of prebiotic atmospheres by atmospheric pressure glow discharge generated in nitrogen-methane gas mixture

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We studied chemical reactions in N_2 + CH_4 mixture initiated by DC glow discharge. This experiment was designed to mimic prebiotic atmospheres. The content of CH_4 was set to 2%, the total pressure was set to 101 kPa and the gas temperature to 300 K. The composition of products from these reactions was studied by GC-MS and FTIR. A kinetic model for reactions in this mixture was developed. The influence of CO_2 admixture to N_2 + CH_4 was also investigated experimentally and theoretically. It was assumed in the model that 2% of nitrogen was dissociated to nitrogen atoms in the ground state, the CH_4 was fully dissociated into 90% of CH_3 and 10% of CH_2. This was taken as initial conditions for the calculations and the kinetic equations were solved numerically for time from 0 to 10 s.

1. Introduction

The gliding arc configuration of atmospheric pressure discharge has been shown to be a good mimic of processes in the prebiotic atmospheres [1]. The present work is focused on comparison of experimental data and data from kinetic model for chemical reactions in N_2+CH_4 gas mixtures and admixture of the carbon dioxide (CO_2) from 1% to 3 %. The neutral products generated in the discharge were identified and quantified by the means of the Fourier-Transform-Infra-Red spectroscopy (FTIR) and by Gas Chromatography Mass Spectroscopy (GC-MS).

2. Experimental set-up

The experimental set-up was in detail described in our previous studies [1]. An atmospheric pressure DC glow discharge was created between two stainless steel electrodes separated by a 2 mm gap. The discharge was operated at an applied voltage of 350 V and discharge current in range from 15 to 40 mA in pure nitrogen with 1–5 % of CH_4 (both gases having quoted purity of 99.995 %) with admixture of 1 and 3 % of CO_2 at the total flow rate of 50 sccm. The flow rates of all gases through the reactor were regulated using mass flow controllers..

3. Kinetic model

The kinetic model uses mainly the set of chemical reactions and their rate coefficients from Loison et al [2]. In our model 189 different particle types and 986 chemical reactions were taken into account. Also reactions with oxygen and oxygen containing species were involved in the model, although the calculations were performed firstly without any oxygen. The different initial conditions resulted in small changes in the product concentrations, however, the main discrepancies between the model and experimental results were not solved.

4. Results

The comparison of results from experiment and model is shown in Tab.1. The HCN concentration was calculated from the model in agreement with experimental data. The NH_3 concentration predicted by model is about three orders lower than in experiment. This can be caused by surface reactions which are not include in the model.

When from 1 to 3% of CO_2 was added to N_2 + CH_4 mixture, then only CO was detected additionally in the experiment and the production of HCN was increased. No other oxygen containing compounds were detected, however the model predicted creation of formaldehyde.

Tab. 1 Comparison of results from experiment and model.

	experiment (ppm)	model (ppm)
HCN	2000	1600
NH_3	1500	0.2
C_2H_6	n/a	400
C_2H_2	n/a	31

5. References

[1]L. Torokova, J. Watson, F. Krcma, V. Mazankova, N. J. Mason, G. Horvath, S. Matejcik. Contrib. Plasm. Phys., **55** (2015) 470.

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