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PHYSICS

# PROCESSING OF SUGARCANE CELLULOSE EMPLOYING ATMOSPHERIC-PRESSURE PLASMAS

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*Figure1. Illustration of an atmospheric-pressure plasma jet of Ar/H2 generated by a radio-frequency wave at 50W. In this case, the microplasma jet glow length is about 15.0 mm, considering a gas flux of 700 sccm*

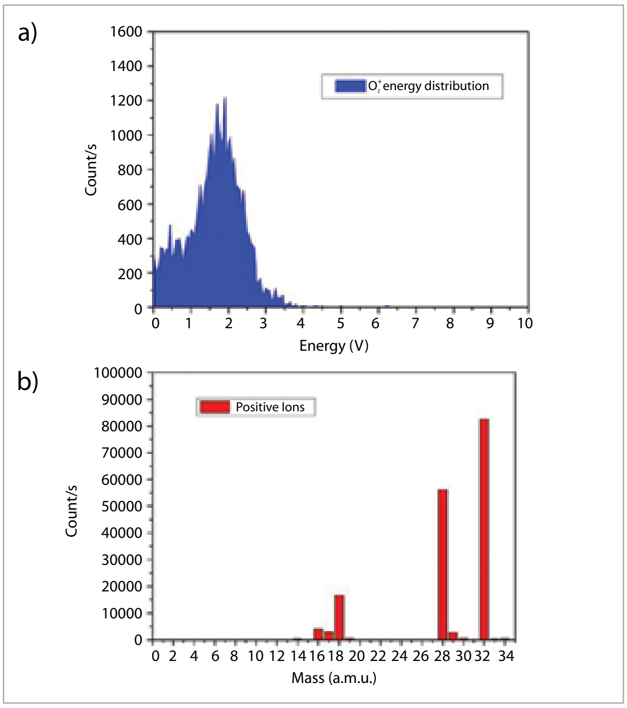

*Figure 2. Specimens yielded by He DBD plasma at atmospheric pressure: (a) Energy distribution for $O_2^+$; (b) Mass concentration of positive ions inside the discharge*

In this project we propose the implementation of a new method for selective treatment of lignocellulosic material based on atmospheric-pressure plasmas (*Figure 1*), which may become an important step towards the industrial production of second generation ethanol from sugarcane. The experiments in laboratory scale and the development of the equipment to produce the plasmas will be carried out at Brazilian Bioethanol Science and Technology Laboratory (CTBE). The experiment will be scaled-up in order to be implemented in the Pilot Plant, which is now under construction at CTBE.

From the theoretical point of view, the interaction of the plasma electrons with lignocellulosic material should be better understood. A study on this complex matter will be carried out in three different parts: (1) low-energy electron scattering from α-glucose and β-glucose monomers and dimmers. We expect these results to elucidate the differences in resonant processes responsible for the breakage of the respective (α1→4) and (β1→4) linkages. This study will be carried out at CTBE and the resonance energies should provide invaluable information for optimizing the plasma-based pretreatment of lignocellulosic raw materials. (2) Once the resonance states are identified, we plan to study dissociation mechanisms by electron impact with the help of nuclear dynamics simulations, at Federal University of ABC. (3) Lignocellulosic material contains a large amount of water. We also propose to investigate micro- and macrosolvation effects through some standard approaches coded in quantum chemistry computational packages. This study will be done at University of São Paulo.

## SUMMARY OF RESULTS TO DATE AND PERSPECTIVES

By applying the so-called atmospheric-pressure plasma (APP), low gas and power consumption could be achieved as well as a non-expensive operation [1]. The APP allows creating a convenient environment of chemical specimens, such as ozone and singlet oxygen, which have an important role in the deconstruction of a biomass lignocellulosic matrix, particularly degrading lignin with good efficiency [2, 3, 4, 5]. In this sense, it is necessary to apply diagnostic tools in order to investigate the chemical composition and physical properties of these plasmas. By using Optical Emission Spectroscopy, we are able to determine, for example, the electron density and the temperature of the plasmas [6,7]. Moreover, through Mass Spectrometry Analyzes (MSA), the concentration and energy of neutral specimens as well as of negative and positive ions in the APP can be determined. So far, we have applied MSA to study a helium APP created by a Dielectric Barrier Discharge (DBD). This DBD is going to treat the sugarcane bagasse in a reactor. Some chemical radicals existing in this kind of APP are shown in *Figure 2*.

The first theoretical results are related to the study of elastic collisions of low-energy electrons with the $CH_2O$-$H_2O$ complex [8]. Previous studies reported a shape resonance for $CH_2O$ at around 1 eV. In the presence of water, the resonance appears at lower energies due to mutual polarization between the two molecules. This indicates that the presence of water may favor dissociation by electron impact.

Another interesting theoretical study is the low-energy electron collision with $\alpha$-D-glucose and $\beta$-D-glucose monomers [9]. Our results show a strong isomeric effect for electron impact energies below 15 eV. The integral cross sections for both monomers present shape resonances located at different positions. As a consequence, low-energy electrons may dissociate these two monomers at different energies, suggesting a specific bond-selective behavior. The next step is to study electron scattering by the D-glucopyranose dimmers, in order to investigate possible influence of electron capture in the rupture of the $(\alpha 1 \rightarrow 4)$ and $(\beta 1 \rightarrow 4)$ linkages.

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