

Comprehensive study on interactions of cold atmospheric plasmas and Oil

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In recent years, the interactions of cold atmospheric plasma (CAP) and liquids have attracted an increasing attention, which have shown great advantages in plasma medicine. In this study, a room temperature plasma jet produced by Ar + O₂ gas discharge was used to treat vegetable oil (taking perilla seed oil as an example) to produce plenty of new reactive groups, with the formation of Plasma Activated Oil (PAO). Experimental measurements by means of infrared spectroscopy, gas chromatography and nuclear magnetic resonance spectroscopy were applied to diagnose the compositions and functional groups in PAPS. A significant decrease of unsaturated fatty acids accompanied by the decrease of saturated fatty acids was observed, embodied in the dissociation of double C = C bonds, the breaking of sp³ C-H bonds, and the formation of O – H, C – O bonds, which correspond to the production of peroxides and carboxylic acids. To further understand the mechanisms of the plasma treatment, the reactive molecular dynamic simulation was performed to explore the interactions of reactive oxygen species (ROS), such as O, OH and O₃ and five fatty acids in oil with the ReaxFF field. In addition to the dissociation of double C = C bonds, other important reactions were also revealed in the simulation, such as the H abstraction from fatty acids, resulting in the formation of aldehyde groups, alcohol groups and

small molecule carboxylic acids, which is consistent with the experimental results. Moreover, the dose effects of ROS on the oxidation processes were also examined by changing the treatment time in the experiment and the number of ROS in the simulation box. This study unveils the formation and breaking of the key chemical bonds and the production of new reactive groups, which enables us to deeply understand the interaction mechanism of plasma and oil.

References

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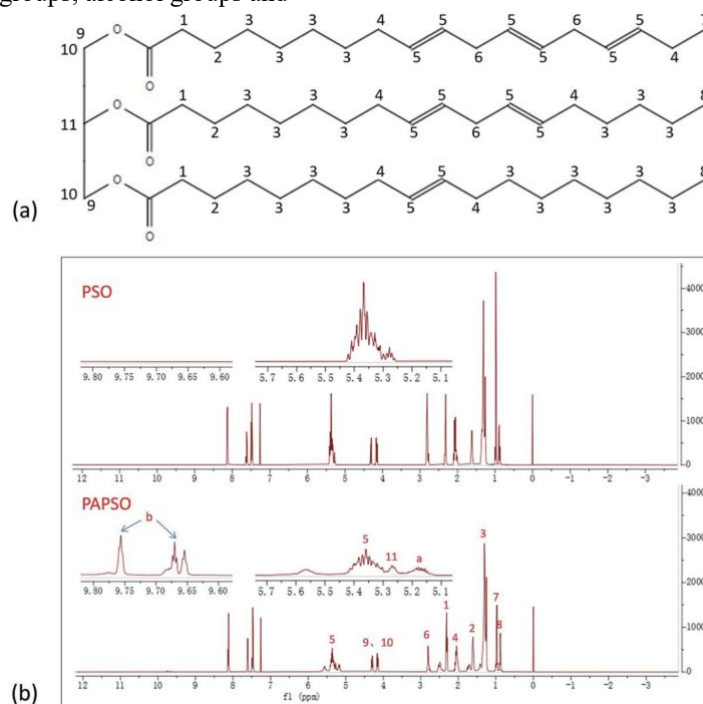


Figure. 1: The ¹H NMR spectra of PSO and PAPS with the correspondence between the H atoms. (a) The structure of a representative triglyceride molecule in PSO. (b) The ¹H NMR spectra of PSO and PAPS.