A pragmatic approach for analysis of complex pyrolysis oils

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The liquid fraction of pyrolysis products contains a wide variety of carbon chains, so adequately identifying a sufficient portion of the sample requires significant effort and run time when using techniques such as gas chromatography (GC). One technique which can be used to classify the liquid, by analysing the bond structures in the whole sample, is proton-nuclear magnetic resonance (H-NMR). This technique allows an analysis to be done on the sample without having to rely on separation due to boiling point, which is the case for GCs.

NMR relies on the electro-magnetic properties of the electron clouds around the atoms in the hydrocarbon chains. A H-NMR utilises the hydrogen attached to a carbon and provides insight into what type of bonds are present in the liquid, such as methyl (CH3), methylene (CH2), double bonds, or aromatic structures[1][2]. These bonds can be used to describe liquid in sufficient detail, by quantifying the bonds, not the compounds, removing the uncertainty of identification.

In this work, a comparison between the H-NMR and GC-VUV of the liquid fraction from pyrolysis of different plastic rich wastes is presented. GC-VUV has been shown by Mandviwala et al. to provide good identification of compounds, thus providing a reference point to find the least viable information needed from the H-NMR to characterise a sample[3].

[1] Ö. M. Doğan and İ. Kayacan, “Pyrolysis of Low and High Density Polyethylene. Part II: Analysis of Liquid Products Using FTIR and NMR Spectroscopy,” *Energy Sources Part Recovery Util. Environ. Eff.*, vol. 30, no. 5, pp. 392–400, Jan. 2008, doi: 10.1080/15567030701457152.

[2] S. Mondal, K. Chattopadhayay, R. Kumar, J. Christopher, and G. S. Kapur, “A Rapid 1H NMR-Based Estimation of PONA for Light and Narrow Cut Naphtha Samples of Refinery Streams toward BS-VI Gasoline,” *Energy Fuels*, vol. 35, no. 9, pp. 7883–7892, May 2021, doi: 10.1021/acs.energyfuels.1c00413.

[3] C. Mandviwala *et al.*, “Method development and evaluation of product gas mixture from a semi-industrial scale fluidized bed steam cracker with GC-VUV,” *Fuel Process. Technol.*, vol. 253, 2024, doi: 10.1016/j.fuproc.2023.108030.