# Mechanistic modeling of post-consumption plastic pyrolysis oil purification: Lumping approach for distillation and solvent extraction processes

T.L. Nguyen[1], J. Hogie[1], K. Van Geem[2], S. De Meester[1]

[1]Department of Green Chemistry and Technology, Ghent University, Graaf Karel de Goedelaan 5, B-8500 Kortrijk, Belgium
[2]Laboratory for Chemical Technology, Ghent University, Technologiepark 125, B-9052 Ghent, Belgium
Keywords: plastic waste pyrolysis oils, purification, characterization, pseudo-components.
Presenting author email: thien.nguyenluuminh@ugent.be

Because of its excellent properties such as water resistance, corrosion resistance, and durability, plastic is an irreplaceable material. These properties, however, are also the reason why plastics become easily trapped in the natural environment and cause a slew of environmental issues. Mechanical recycling is frequently regarded as the most efficient method of dealing with plastic waste, but it has limitations when it comes to recycling certain types of plastic. These impediments reduce the quality of post-recycled plastic and prevent it from being reused in some applications, such as food packaging. Pyrolysis of plastic waste followed by steam cracking will assist in converting the plastic waste into a base chemical that can be used as a secondary raw material to produce virgin-graded plastic, thereby closing the loop in plastic production.

However, using waste plastic pyrolysis oils as a feedstock for steam crackers is fraught with difficulties. Waste plastic pyrolysis oil is more complex, heavier, and more contaminated than conventional naphtha feedstock. The presence of many heteroatoms (Cl, N, O, S, metals) in the pyrolysis oil is the primary cause of bottleneck towards steam cracking (Kusenberg et al., 2021). Although good pre-treatment and pyrolysis can reduce large amounts of heteroatoms, post-treatment is still required to upgrade the pyrolysis oil quality up to par with naphtha feedstocks. Hydro-treatment is a technically suitable post-treatment technology. However, given the small scale of waste plastic pyrolysis oils, the cost of hydro-treatment is a barrier to the commercialization of chemical recycling of plastics. This study looks into the purification of plastic waste pyrolysis oils using the combination of distillation and solvent extraction processes.

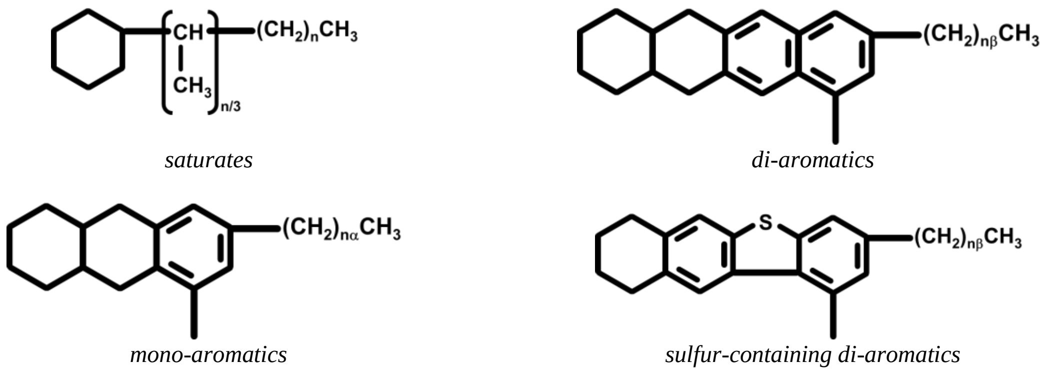


Figure 1: Model-molecules structures for the proposed pseudo-components. Adapted from (Espada et al., 2007)

Despite the post-consumption plastic pyrolysis oils being studied since 1997 (Joo & Guin, 1997), very little research has been done on modeling and simulating the pyrolysis oil behavior in distillation and extraction columns. The complexity of pyrolysis oil has hampered the use of process simulation packages (for example, ASPEN). Similarities can be observed in the petrochemical industry. The complex hydrocarbon mixture is simplified by grouping compounds with similar physicochemical properties into lumps known as pseudo-components. Pseudo-components are generated for crude oil distillation by grouping the boiling point, which is a standard function of almost all commercial process simulation packages. In contrast, pseudo-components complicate solvent extraction simulation. The fluid activity model is often used to determine the component distribution coefficients describing the liquid-liquid extraction process. However, the activity coefficients for the unknown molecular structure of pseudo-components are still unknown. Different approaches to generate pseudo-components for liquid-liquid extraction have been reported, particularly the de-aromatization of lubricating oils using furfural. Saturates, aromatics and polars were used as three pseudo-components in the first approach (van Grieken et al., 2005). The composition of each pseudo-component was determined using various physical properties (average boiling point, specific gravity, liquid density, and refractive index at 343 K and sulfur content). The binary interaction coefficients between saturates, aromatics, polars, and furfural are measured experimentally and fitted using the NRTL model. Another approach (Espada et al., 2007) described lubricant oil by four average model-molecules (Figure 1) characterized by their molecular structure. Based on their molecular structure, the binary interaction coefficients of those pseudo-components were determined using a group contribution method such as UNIFAC. However, no studies have been conducted on developing a systematic lumping approach to simulate plastic waste pyrolysis oils in liquid-liquid extraction and distillation processes.

This presentation focuses on such developments and will propose an approach that can group plastic waste pyrolysis oil into a number of suitable pseudo-components capable of describing both VLE and LLE behavior. This will enable the development of a reliable distillation and extraction model in ASPEN, which can potentially be coupled to determine the best topology design for the pyrolysis purification process. Developing such reliable models is crucial towards the further commercialization of large-scale chemical recycling of plastic waste via pyrolysis.

**References**


Kusenberg, M., Eschenbacher, A., Djokic, M., Zayoud, A., Ragaert, K., De Meester, S., & Van Geem, K. (2021). Opportunities and challenges for the application of post-consumer plastic waste pyrolysis oils as steam cracker feedstocks: To decontaminate or not to decontaminate?. Waste Management, 138, 83-115. https://doi.org/10.1016/j.wasman.2021.11.009

Joo, H., & Guin, J. (1997). Hydrocracking of a Plastics Pyrolysis Gas Oil to Naphtha. Energy & Fuels, 11(3), 586-592. https://doi.org/10.1021/ef960151g

van Grieken, R., Coto, B., Romero, E., & Espada, J. (2005). Prediction of Liquid−Liquid Equilibrium in the System Furfural + Heavy Neutral Distillate Lubricating Oil. *Industrial & Engineering Chemistry Research*, *44*(21), 8106-8112. https://doi.org/10.1021/ie050069l

Espada, J., Coto, B., & Peña, J. (2007). Liquid-liquid equilibrium in the systems furfural+light lubricating oils using UNIFAC. *Fluid Phase Equilibria*, *259*(2), 201-209. https://doi.org/10.1016/j.fluid.2007.06.024