Validation of COSMO-SAC Thermodynamic model for estimation of activity coefficients For plastic additives and monomers

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1. Introduction

Polyesters represent a cornerstone of modern society, finding application in various everyday products, including clothing fibers and beverage packaging. Chemical recycling, particularly the depolymerization of PET plastic waste which could be achieved through methods like glycolysis presents a sustainable solution for managing plastic waste. However, the efficient separation and purification of components during chemical recycling processes pose significant challenges. This study explores the utilization of thermodynamic models, specifically the COSMO-SAC (Conductor-like Screening Model for Real Solvents with Segment Activity Coefficients) framework, in addressing these challenges by predicting activity coefficients of diverse molecular species in solution (Eckert and Klamt, 2002). COSMO-SAC enables the screening and design of purification methods such as solvent extraction, distillation, and crystallization processes (Malik *et al.*, 2023). Unlike traditional models, COSMO-SAC requires only molecular volume and sigma profile data, derived from quantum chemistry principles, making it a cost-effective and efficient tool for predicting phase behavior in multi-component systems. This abstract underscores the importance of thermodynamic modeling in advancing the efficacy of chemical recycling processes, contributing to a more sustainable future.

2. Thermodynamic Framework and modeling

$$\ln \gamma_i = \frac{A_i}{a_{eff}} \sum_{\sigma_m} p_i(\sigma_m)[ln\Gamma_S(\sigma_m) - ln\Gamma_i(\sigma_m)] + \ln\gamma_i^{SG}$$

The COSMO-SAC model relies on the surface charge density profile (σ) and molecular volume (V_i) to, calculate the segment activity coefficient for different components, energy exchange between segments, hydrogen bonding contributions to energy exchange, and the Staverman-Guggenheim model for combinatorial contributions to the activity coefficient.

For each additive, a series of conformers is generated based on the number of rotatable bonds, utilizing RDKit software. Subsequently, these conformer structures undergo optimization using Gaussian16 software, employing suitable methods and basis sets (Phan *et al.*, 2021). The resulting optimized structures are the input for the surface charge density calculations, which are then integrated into ASPEN Plus through an averaging algorithm (Ferro *et al.*, 2012). The overview of the process is depicted in Figure 1.

3. Materials and Methods

17 additives and 3 monomers were selected based on the diversity of physiochemical properties and structure to evaluate the limitation of COSMO-SAC model applicability. Since all the additives involved in this study are solids at room temperature, the DSC analysis is carried out on all the additives to measure the heat of fusion and the melting point to be used in solubility estimation (Loschen and Klamt, 2016).

To measure the experimental max solubility the additives are added to solvents (Water and Ethylene Glycol) in excess at different fixed temperatures and stirred for 24 hr. The undissolved portion will be separated by a heated centrifuge system and then a sample of the solution will be analyzed by PYRO-GC-MS, ICP-OES, or UV-Vis Spectroscopy.

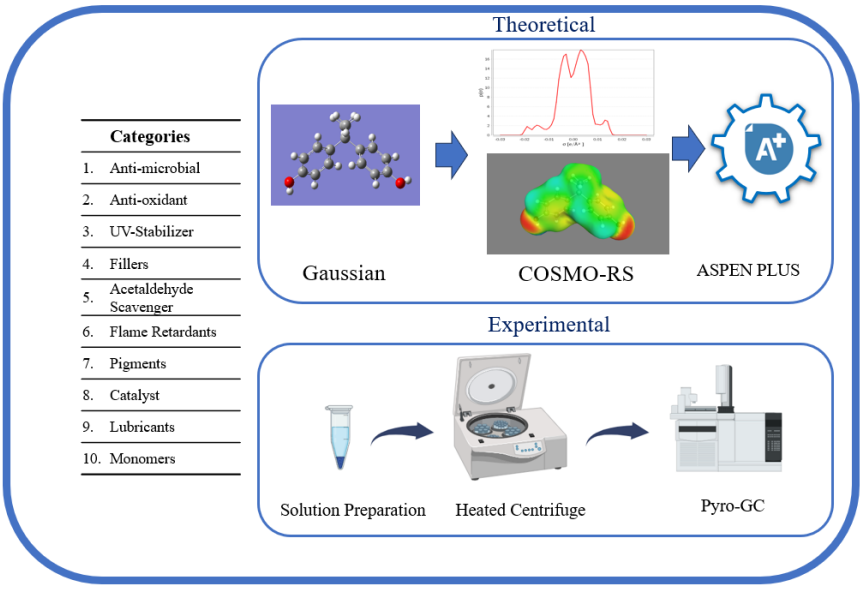

Figure 1: Overview of this study and included material

4. Results

The results of this study will be presented in the form of SLE (T-x) data points and there will be a comparison between theoretical and experimental data.

5. Conclusion

In conclusion, the development of an accurate predictive model holds promise for recycling engineers faced with the task of selecting optimal chemical recycling routes across diverse solvent mediums. This model also enables efficient process design by facilitating comparisons of solubility for specific contaminants or target monomers and significantly enhances the efficacy and sustainability of recycling efforts, paving the way for a more resource-efficient and environmentally conscious future.

6. References

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