THERMODYNAMIC-BASED SOLVENT SELECTION FOR THE SEPARATION OF LIGNIN-DERIVED MOLECULES

Amir Jalalinejad, Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology, Germany
amir.jalalinejad@kit.edu
Jaber Yousefi Seyf, Department of Chemical Engineering, Hamedan University of Technology, P.O. Box: 65155-579, Iran
Axel Funke, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany
Nicolaus Dahmen, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

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The separation of valuable monomers from a liquid phase mixture of depolymerized lignin and lignin fast pyrolysis is of particular importance. For separating the desired lignin monomers, there are several techniques such as liquid-liquid extraction using different solvents, countercurrent chromatography (CCC), and centrifugal partition chromatography (CPC). Despite these experimental methods being applicable, lignin monomers are mostly complex aromatic and polar compounds with similar structures. From the experimental point of view, finding the proper solvent is expensive, time-consuming, and difficult for individual separation. Therefore, it is vital to apply thermodynamic models to screen the pool of solvents. Although many studies have been carried out to develop effective thermodynamic models to be used in bio-oil-related procedures, there are some challenges to achieving reliable results for novel molecules with no experimental data. In this study, we predict suitable solvents by the NIST-UNIFAC activity coefficient model for the separation of lignin-derived molecules from Barta's, Liu's, Luterbacher's, and Stahl's products. We used this predictive model to find suitable solvents for isothermal mutual solubility, temperature-dependent mutual solubility, liquid-liquid phase equilibria of phenolic compounds, the partition coefficient of 29 lignin-derived molecules, and the phase equilibria of quaternary conventional solvents systems (Arizona, HEMWat, HIMWat, HMMWat, TEMWat, TIMWat, and TMMWat in the counter-current chromatography (CCC)). Finally, based on the solvent selection criteria for CCC, the results for Barta's, and Liu's products are promising so that, some binary, ternary, and quaternary solvent systems were found to meet the separation criteria. The obtained results by the NIST-UNIFAC model were in quantitative and qualitative agreement with the experimental data.
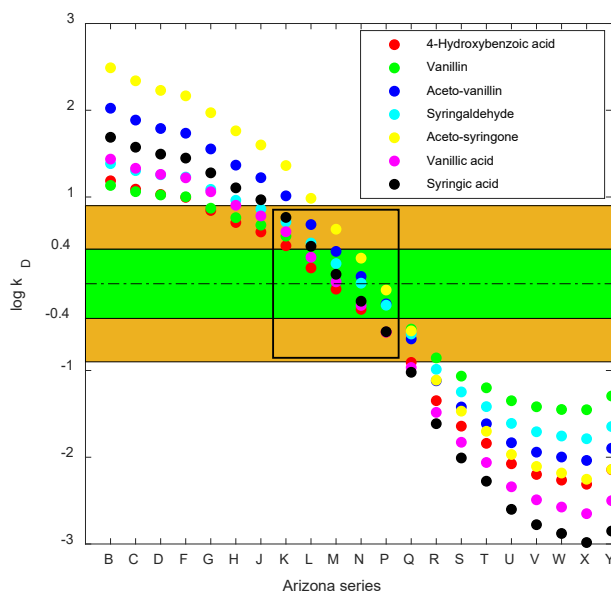
Figure 1 – The predicted partition coefficient of the lignin depolymerization monomers (4-hydroxybenzoic acid, vanillin, acetovanillone, syringaldehyde, acetosyringone, vanillic acid, and syringic acid) by Arizona series and the NIST-UNIFAC model