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Enhanced Furfural Extraction from Aqueous Media Using Neoteric Hydrophobic Solvents

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Abstract : This research reports a systematic top-down approach for designing neoteric hydrophobic solvents –particularly, deep eutectic solvents (DES) and ionic liquids (IL)– as furfural extractants from aqueous media for the application of sustainable biomass conversion. The first stage of the framework entailed screening 32 neoteric solvents to determine their efficacy against toluene as the application's conventional benchmark for comparison. The selection criteria for the best solvents encompassed not only their efficiency in extracting furfural but also low viscosity and minimal toxicity levels. Additionally, for the DESs, their natural origins, availability, and biodegradability were also taken into account. From the screening pool, two neoteric solvents were selected: thymol:decanoic acid 1:1 (Thy:DecA) and trihexyltetradecyl phosphonium bis(trifluoromethylsulfonyl) imide [$P_{14,6,6,6}$][NTf_2]. These solvents outperformed the toluene benchmark, achieving efficiencies of 94.1% and 97.1% respectively, compared to toluene's 81.2%, while also possessing the desired properties. These solvents were then characterized thoroughly in terms of their physical properties, thermal properties, critical properties, and cross-contamination solubilities. The selected neoteric solvents were then extensively tested under various operating conditions, and an exceptional stable performance was exhibited, maintaining high efficiency across a broad range of temperatures (15–100 °C), pH levels (1–13), and furfural concentrations (0.1–2.0 wt%) with a remarkable equilibrium time of only 2 minutes, and most notably, demonstrated high efficiencies even at low solvent-to-feed ratios. The durability of the neoteric solvents was also validated to be stable over multiple extraction-regeneration cycles, with limited leachability to the aqueous phase (≈0.1%). Moreover, the extraction performance of the solvents was then modeled through machine learning, specifically multiple non-linear regression (MNLR) and artificial neural networks (ANN). The models demonstrated high accuracy, indicated by their low absolute average relative deviations with values of 2.74% and 2.28% for Thy:DecA and [$P_{14,6,6,6}$][NTf_2], respectively, using MNLR, and 0.10% for Thy:DecA and 0.41% for [$P_{14,6,6,6}$][NTf_2] using ANN, highlighting the significantly enhanced predictive accuracy of the ANN. The neoteric solvents presented herein offer noteworthy advantages over traditional organic solvents, including their high efficiency in both extraction and regeneration processes, their stability and minimal leachability, making them particularly suitable for applications involving aqueous media. Moreover, these solvents are more environmentally friendly, incorporating renewable and sustainable components like thymol and decanoic acid. This exceptional efficacy of the newly developed neoteric solvents signifies a significant advancement, providing a green and sustainable alternative for furfural production from biowaste.

Keywords : sustainable biomass conversion, furfural extraction, ionic liquids, deep eutectic solvents
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