INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Extraction of Lower Alcohols using Novel Hydrophobic Deep Eutectic Mixtures: Synthesis, Phase Equilibria Experiments and Process Economics

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SHORT ABSTRACT

Globally, in the present scenario fossil fuel is full filling nearly 80% of the energy demand. Today, world is heading towards alternate fuel in order to decrease the dependency upon the fossil fuel. Presently, there are so many alternate source of energy like biofuel, nuclear, solar, wind, hydropower etc. Butanol, a potential fuel can play strong role as an alternate source of energy in future. Butanol, produced by Acetone-Butanol-Ethanol (ABE) fermentation with proportion of 3:6:1 under anaerobic conditions. The butanol concentration in product stream higher than 20 g/L retards the growth of microbes resulting in a low yield. This necessitated the use of LLE (liquid-liquid Extraction) for the removal of butanol from ABE streams. Thus the extraction of butanol by hydrophobic solvents has been proposed in the present work. Economical level commercial production of Butanol is up to now at R&D stage. Now days, DESs (deep eutectic solvents), which are considered as green solvent, offers an interesting alternative to ILs (Ionic liquids). In the present study, DESs, which are hydrophobic in nature, made via synthesis of DL-menthol (act as a hydrogen bond accepter) and organic acids (act as a hydrogen bond donor) in the different molar ratio. The present study has been divided in to two parts, first experimental and second simulation. Experimental study has been focused to under liquid-liquid extraction of butanol using different solvent like mesitylene, oleyl alcohol, as well as the organic acids based DESs. In order to evaluate the potential of separation mesitylene, oleyl alcohol, and new synthesized solvent DESs have been chosen for the experimental studies. All the organic solvent and DESs are lighter than water used for butanol extraction from aqueous solution. Experimental study carried out for 1-butanol-water-psudosolvent at T=298.15 K and p=1 atm. Distribution coefficient and selectivity have been calculated to understand the best solvent

from the experimental data. Thermodynamically, NRTL and UNIFAC model have been used for the prediction of binary interaction parameters using MATLAB based code. The ternary experimental tie line data were then correlated with the Gibb's free energy models namely NRTL (Non Random Two Liquids) and UNIQUAC (UNIversal QUAsiChemical). NRTL and UNIQUAC models gave deviation less than unity for all systems indicating an excellent fit. The binary interaction parameters by NRTL model were then used for optimization of multistage extractor. As density plays a major role in piping and vessel design, the density of the all the solvents have been measured at 298.15-328.15 K. Density of synthesized DESs measured by the density meter instrument made by Anton Paar, model-DMA 4500M. Simulation point of view process design software, Aspen Plus has been used for economical and efficient separation of extracted stream product obtained from extractor. Also, the UNIFAC and COSMO-SAC have been used to find the missing parameters in the Aspen Plus. Hybrid extraction−distillation system has been used for optimized the separation process. Rigorous optimization calculation has been used to optimize the multistage Extractor and Distillation column, as well as economically-TAC (total annual cost) has been calculated for the predation of the investment needed for the desire separation.