LIQUID-LIQUID EQUILIBRIA AND MICROCHANNEL EXTRACTION STUDIES FOR SEPARATION OF AROMATICS FROM HYDROCARBON MIXTURES

by

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Submitted in fulfillment of the requirements of the degree of Doctor of Philosophy to the

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Dedicated to My Parents

& My Wife
CERTIFICATE

This is to certify that the thesis entitled “LIQUID-LIQUID-EQUILIBRIA AND MICROCHANNEL EXTRACTION STUDIES FOR SEPARATION OF AROMATICS FROM HYDROCARBON MIXTURES”, being submitted by Mr. U. K. Arun Kumar to the Indian Institute of Technology Delhi, for the award of the degree of Doctor of Philosophy, is a record of bonafide research work carried out by him under my guidance and supervision.

The results contained in this thesis have not been submitted in part or full to any other university or institute for the award of any degree or diploma.

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ABSTRACT

Aromatics separation from petroleum mixtures such as naphtha reformate, lube oils is industrially important and is done by liquid-liquid extraction. In recent years there has been an interest in the use of more environment friendly solvents than those in present industrial use like sulfolane, NMP. Further, from process intensification point of view, microchannel extraction has also been the subject of investigations. In this work therefore two solvents of the ‘green’ category – furfural and (Propylene Carbonate + Tetraethylene glycol) mixture -- have been studied for aromatics separation. Extraction in microchannels was also examined.

Major contribution of the present work is the Liquid-Liquid Equilibrium (LLE) study of the above systems of interest. New and detailed LLE data were obtained experimentally for ternary, quaternary, quinary and eight-component mixtures of alkanes + aromatics + solvent (furfural). LLE data for a ten-component synthetic naphtha with PC + TTEG as solvent was also obtained. For the furfural systems results show that overall selectivity of furfural for aromatics ranges between 2.8 to 14.5. Though these selectivity values are not as high as those reported for sulfolane, they are high enough for furfural’s use to be considered especially as the distribution coefficients are high - 0.54 to 0.81. Likewise PC + TTEG selectivities were found to be between 6.5 to 17.5 along with a high distribution coefficient 0.24 to 0.51. Thus the use of this mixture as solvent also appears feasible. In addition to experimental data, modeling of LLE was also done using NRTL and UNIFAC activity coefficient models. Very good correlation/prediction of data (rmsd < 3 % in all cases) was obtained.

In the second part micro-/milli- channel extraction studies were made to the extent of determining the efficiencies of aromatic extraction in these devices. Extraction efficiencies
ranging from 46.3 % to 97.3 %, depending upon the combination of the flow velocity, residence time and channel diameter. The 90 % or more efficiency cases indicate that mass transfer rates may not be that much of an issue. Effect of single parameter on extraction efficiency was also isolated from the various combinations. Efficiency increased from 68 to 83 % as flow velocity increased from 0.11 to 0.96 cm/s while residence time and channel diameter remained fixed at ~ 0.78 minute and 2 mm respectively. Likewise efficiency was seen to increase with residence time but decrease with diameter while the other two parameters were held constant. Quite high (> 85 %) extraction efficiencies in many of the cases indicate further investigation of the process to be of interest.
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