OPTIMAL SOLVENT CYCLE DESIGN IN SUPERCRITICAL FLUID PROCESSES

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Abstract— This work addresses the determination of optimal solvent cycle scheme for supercritical fluid processes. The optimization model, which includes reliable thermodynamic predictions and rigorous process models, has been extended to include potential units that constitute the solvent recovery cycle. Capital cost functions, based on graphical correlations from the literature, have been derived for each unit in the superstructure. A mixed integer nonlinear programming model has been formulated, where the objective function is net profit maximization. Process and solvent cycle design has been performed for the deterpenation of lemon peel oil.

Keywords— Optimal Solvent Cycle, Supercritical Fluid Processes, Optimization.

I. INTRODUCTION

In this paper solvent cycle design in supercritical fluid deterpenation processes is addressed. Citrus peel oils are mainly composed of hydrocarbon terpenes and oxygenated compounds. The last ones, which constitute the valuable aroma fraction, can be obtained from citrus peel oil by extraction with supercritical carbon dioxide (Budich et al., 1999; Espinosa et al., 2000). In previous work, simulation and optimization models have been developed to minimize solvent-to-feed ratio in several supercritical extraction processes, as operating costs mainly depend on this ratio (Diaz et al., 2000). However, to evaluate economic feasibility of supercritical deterpenation against conventional processes, capital and operating costs of process and solvent recovery units must be taken into account and the optimal solvent cycle scheme must be determined.

As high-pressure processes are energy intensive, they must be highly integrated to be economically feasible. Special attention must be devoted to the solvent cycle scheme (Brunner, 2000). There are different alternatives for solvent recycling in supercritical fluid processes. They depend on operating conditions of the main process, the nature of the solvent and the scale of the process unit. The solvent can be driven either by a compressor or by a pump and it can be recycled either in supercritical or in liquid state. In the case of a pump cycle, lower capital costs are associated to pumps as compared to compressors and energy consumption is lower than the compressor process for pressures higher than 300 bar (Brunner, 1984). As a disadvantage, the pump cycle requires several heat exchangers and condensers and additional heat energy at low extraction pressures. The compressor cycle needs only one heat exchanger and it shows low heat energy consumption but it has higher investment costs for the compressor and higher electrical energy consumption compared to the pump cycle for pressures lower than 300 bar. Solvent cycle selection constitutes a significant step in the design problem of supercritical fluid processes.

In this paper, a mixed integer nonlinear model has been formulated to represent both lemon peel oil deterpenation process and its solvent recovery system, embedding potential units that constitute the solvent cycle. The objective is net profit maximization while rendering specified aroma fraction recovery and purity. Rigorous simulation models for process units have been formulated and a Group Contribution Equation of State (GC-EOS, Skjold-Jorgensen, 1984) has been used to provide phase equilibrium and solubility predictions. Pure group and binary interaction parameters have been determined for GC-EOS aldehyde group and a comparison of predictions with experimental data is presented. Investment costs correlations from Ulrich (1984) and Institut Français du Pétrole (1981) have been associated to each process unit.

II. THERMODYNAMIC MODELING

Lemon peel oil is composed of several compounds, but it can be modeled as a mixture of two key components: limonene and citral (Kalra et al., 1987). Limonene is the main hydrocarbon terpene in all peel oils, with concentrations ranging between 30 and 95 % weight. Citral is the most representative oxygenated aroma in lemon peel oil. Figure 1 shows their chemical structures.

![Figure 1. Chemical structures](image-url)