SIMULATION OF DEACIDIFICATION PROCESS BY MOLECULAR DISTILLATION OF DEODORIZER DISTILLATE

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Abstract— **A computer program has been developed to simulate the deacidification of sunflower deodorizer distillate. The developed mathematical model is based on momentum, mass and energy balances. The Langmuir-Knudsen constitutive equation was used in order to represent the kinetics of evaporation and condensation. Physical and transport properties have been evaluated using correlations, which are functions of temperature and composition. The obtained partial differential equation system was solved by means of the Crank-Nicholson technique, and the calculation programs employed were developed and debugged using Matlab 7.1.**

The mathematical model was used to analyze the phenomena that take place during the molecular distillation process, and it also allowed studying the influence of operating variables on the performance of the process. In this investigation, we analyzed the influence of the operating temperature on purity and yield of the components. Trials at three evaporating temperatures (110 ºC, 130 ºC, and 140 ºC) were carried out in a KDL4 (UIC) molecular distillation apparatus to verify the model.

Keywords — **Molecular distillation, simulation, free fatty acids, tocopherols, sterols.**

I. INTRODUCTION

Molecular distillation operation, which is also known as short-path distillation, is a useful separation technique in the purification of compounds which are thermally unstable and have low volatility. Molecular distillation is based on the evaporation of compounds in a mixture. These phenomena take place in two types of distillers: falling film or centrifugal. In the falling film method, one film is in contact with a heated surface and the other film is in contact with a cold surface. The cold surface is near the heated surface, at a distance shorter than the mean free path of the residue gas. The main operating characteristic is the working pressure, and it ranges from 10^{-2} to 10^{-4} KPa. Under these conditions, the volatility of the components increases and the operation temperature decreases, allowing the compounds to separate at lower temperatures. The molecules that leave the evaporation surface suffer virtually no collisions at lower operating pressures. As a result, the molecules take a short path before their condensation; that is, they arrive at the condenser surface in a brief period of time. It is for this reason that very high evaporation velocities are reached. Under these two conditions, short residence time and low temperature, the thermal decomposition of the components is reduced and separation occurs at acceptable velocities (Weissberger, 1951; Perry *et al.*, 1984).

The separation level that is obtained in a molecular distillation process is not only a function of the volatility of the components, but it is also a function of the mass and heat transfers in the liquid phase and its molecular kinetics play an important role in the performance of the operation. When the liquid is evaporated, the vapor-liquid interface becomes cold and, in mixtures, it decreases the composition of the more volatiles components. This leads to the formation of driving forces for the diffusive transfer of mass and heat. All these resistance affect not only the evaporation velocity, but also the product purity (Bose and Palmer, 1984).

Advances in the theoretical modelling of this operation have been reported. Bose and Palmer (1984) showed that the existence of concentration and temperature gradients in the liquid phase decreases the separation efficiency. Bandarkar and Ferron (1991) worked in the mass and heating transference in a liquid film on a centrifugal still. Batistella and Maciel (1996) have shown results of efficiency and performance with two types of distillers. The pressure effect in the molecular distillation process has been analyzed by Cvengros and Lutisan (1995) using both Boltzmann proposals and the Maxwell distribution function for the molecular velocity in the vapor phase. Cvengros *et al.* (1997) used a model to theoretically analyze the operation of molecular distillation for binary mixtures.

Tocopherols and sterols are compounds with important economical value. They decompose at the high temperatures that are required in the conventional distillation operation (Yankah and Jones, 2001; Dunford, 2001). These compounds can be obtained from a by-product of the deodorization stage of the vegetable oil refining process: the ‘deodorizer distillate’. Besides sterols and tocopherols, the distillate generally contains lighter compounds such as free fatty acids, and heavier components such as mono, di and triglycerides, and esters from sterols and pigments (Winters, 1994). This mixture must be treated with separation techniques in order to obtain the purified compounds. The separation of free fatty acids from the remaining components of the mixture is generally the first stage of distillation in the separation and purification process, because the fatty acids are more volatile than the rest of the components. However, the conventional distillation requires high