PREPARATION OF OLEOCHEMICAL POLYOLS DERIVED FROM SOYBEAN OIL

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Abstract— **The hydroxylation of epoxidized soybean oil was performed in a well-mixed agitated reactor under isothermal operation. Two agents for hydroxylation were evaluated using a homogeneous catalyst. The tests were positive and the best results are achieved with molar relations of alcohol to epoxide of 4:1 for ethanol (T=70°C) and 6:1 for ethylene glycol (T=80°C), using sulfuric acid (2 % p/p) as a catalyst. The hydroxyl numbers of the oleochemical polyols obtained are 120 and 331 mg KOH/g, with theoretical functionalities of 2 and 6 for ethanol and ethylene glycol soy-based polyols, respectively.**

Keywords— **Soybean epoxide, oleochemical polyester polyols, hydroxylation with ethylene glycol.**

I. INTRODUCTION

In the last decades there has been a growing concern about the industry dependence on petroleum and its derivates. The stability of that market is under analysis, taking into account the price of crude oil (around 18¢/lb), more than a 150% increase from 1985 to 2007 (Zhang *et al.,* 2007). New green technologies have to be developed assuring the use of renewable resources as an alternative to petrochemical products. The epoxidation of oils is a well known technique used in the production of binders, coatings, adhesives and sealants. It is also possible to hydroxylate the epoxidized oil resulting in a polyol structure, a process that has been recently introduced for use in polyurethane foams, reducing the environmental impact (Paster *et al.,* 2003).

In this context, bio-polyols can be obtained from agricultural products like vegetable oils, wood, carbohydrates (cellulose and starch) and lignine (Latere *et al.,* 2005). Oleochemical polyols are a great alternative for the polyurethane industry in applications where hydrofobicity, hardness, flexibility, and mechanical and chemical resistance are needed: foams, coatings and floorings (Höfer *et al.,* 1997). Although most triglycerides contain unsaturations, few oils naturally contain other groups. Therefore, it is necessary to perform the hydroxylation of double bounds through one of four main approaches (Guo and Petrović, 2005; Latere *et al.,* 2005): a) epoxidation followed by the ring-opening, almost secondary hydroxyl groups are generated; b) Hydroformylation and reduction of aldehydes oils; c) Transesterification with different polyols; d) Microbial or enzymatic conversion. It is always desirable to obtain the highest conversion in the preparation of polyols because of the requirements for polyurethane rigid foams (hydroxyl numbers above 300 mg KOH/g) (Guo and Petrović, 2005; Vilar, 2004); for that reason most investigations are focused to increase hydroxyl numbers to improve functionality values. The average molecular weight of oleochemical polyols obtained by this way is between 250 and 2500; due to the low viscosity and good compatibility with methyl-di(phenyl isocyanate) (MDI), these polyols are particularly useful to produce PU rigid foams (Hill, 2000). The value has increased more than twice since the price of soybean crude oil is 28 ¢/lb (Zhang *et al.,* 2007) while epoxidized soybean oil is about 48 – 1 US$/lb (Paster *et al.,* 2003) with a growing market of ~70 000 ton/year (Rangarajan *et al.,* 1995). The aggregate value of PU foams is even higher, reaching prices up to 3 US$ (Paster *et al.,* 2003; Burridge, 2003).

About the conditions of hydroxylation, Petrović *et al.* (2003) patented the alcoholysis of epoxidized oils using fluoboric acid as a catalyst (48%, < 2%p/p) with different hydroxylated molecules like water, monoalcohols (methanol, ethanol, propanol and butanol) and their mixtures, using molar excess to avoid polymerization and products of higher viscosities. They obtained yields of 85-95% and hydroxyl numbers (OH numbers) of 110-213 mg KOH at 25-50°C, using molar relations between 1:1 and 10:1 of a mixture of alcohols (methanol and isopropyl alcohol with water) to epoxide group.

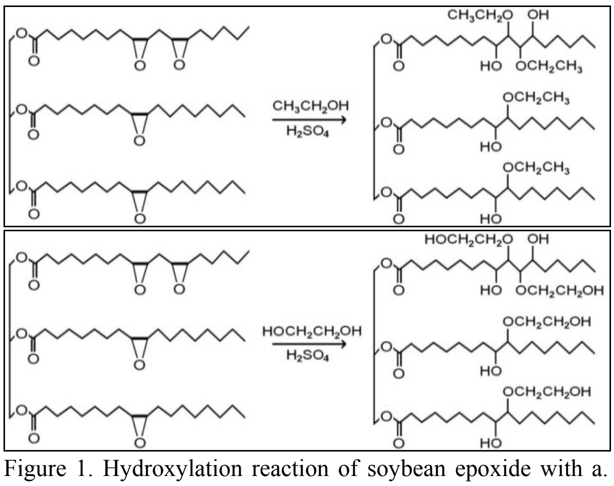

Figure 1. Hydroxylation reaction of soybean epoxide with a. Ethanol, b. Ethylene glycol.