1,3-Propanediol (93S15)

Chemists have long sought a glycol for polyester production that did not impart the stiffness of ethylene glycol, yet avoided the flexibility of 1,4-butanediol or 1,6-hexanediol. Shell Chemical has recently announced that it plans to make polytrimethylene terephthalate (PTT), a polyester derived from 1,3-propanediol and terephthalic acid, available in developmental quantities of 12 million pounds per year in second quarter 1996.

The required diol will be produced by a Shell developed process based on hydroformylation of ethylene oxide. This report develops a conceptual process flowsheet for the Shell process and estimates its economics. For comparison, a conceptual process flowsheet and economics are also developed for the hydration of acrolein and hydrogenation of the aldehyde intermediate, as practiced by Degussa, which is considering building a 1,3-propanediol plant in either Antwerp or Mobile, Alabama. A final decision is expected in 1996.

Several companies have been active in developing technology for the manufacture of 1,3- propanediol (1,3-PDO) starting with ethylene oxide (EO) as the main raw material. The ethylene oxide is reacted with synthesis gas (syngas), a mixture of carbon monoxide and hydrogen, which may be obtained by steam reforming of natural gas or partial oxidation of hydrocarbons (usually liquids). Early work in this area was reported by Hoechst Celanese in a series of patents in 1989-1991. Union Carbide has also been granted patents in this field. Shell has done some of the most recent work on 1,3-propanediol production from ethylene oxide and syngas.

Conceptual process flow schemes for both the ethylene oxide and acrolein based routes are presented in this report. Process economics for both routes are also analyzed. Our results indicate that the acrolein-based process has higher raw material costs but lower capital investment requirements as compared to the ethylene oxide-based process.

1-3-propanediol is a clear, colorless, odorless liquid that is miscible with water, alcohols, ethers, and formamide. It reacts with diacids to form polyesters. The polyester with terephthalic acid, polytrimethylene terephthalate (PTT), is reported to have a crystalline melting point of 228%C. Polyurethanes can also be synthesized from 1,3-propanediol. For carpet applications, polyester derived from 1,3-PDO offers the chemical (stain) resistance characteristics of polyethylene terephthalate (PET) and the elastic recovery of nylon. Additional favorable properties of PTT are easy printability and dyeability, good colorfastness against ultraviolet light, low static generation, and low water absorption.