A Thermodynamic Study of Parameters that Affect the Nitration of Glycerol with Nitric Acid

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Abstract: Biodiesel production from vegetable oil will produce glycerol as by-product about 10% of the biodiesel production. The amount of glycerol that was produced needed alternative way to handling immediately so as to not become the waste that polluted environment. One of the solutions was to process glycerol to polyglycidyl nitrate (PGN). PGN is synthesized from glycerol by three-step reactions i.e. nitration of glycerol, cyclization of 13- dinitroglycerine and polymerization of glycosyl nitrate. Optimum condition of nitration of glycerol with nitric acid has not been known. Thermodynamic feasibility should be done before run experiments in the laboratory. The aim of this study was to determine the parameters those affect nitration of glycerol and nitric acid and chose the operation condition. Many parameters were simulated to verify its possibility to experiment under conditions which would get the highest conversion of 1, 3-dinitroglycerine and which was the ideal condition to get it. The parameters that need to be studied to obtain the highest conversion of 1, 3-dinitroglycerine were mol ratio of nitric acid/glycerol, reaction temperature, mol ratio of glycerol/dichloromethane and pressure. The highest conversion was obtained in the range of mol ratio of nitric acid /glycerol between 2/1 - 5/1, reaction temperature of 5-250 C and pressure of 1 atm. The parameters that need to be studied further to obtain the highest conversion of 1.3 DNG are mol ratio of nitric acid/glycerol and reaction temperature.

Keywords: Nitration, glycerol, thermodynamic, optimum condition

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