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The Effect of Temperature on the Production of Nitrobenzene

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Abstract. Nitrobenzene is a compound derived from benzene and quite fundamental in the petrochemical industry. One of which is in the manufacture of aniline. Aniline has an important role as dyes, synthetic rubber materials, rocket fuels and pharmaceuticals. Nitrobenzene can be synthesized by the nitration reaction of benzene. The purpose of the research is to design synthesis process of nitrobenzene by using Aspen Hysys simulator. The effect of changes in operating condition on nitrobenzene will be investigated. The benefits of the research are to obtain the optimum operating temperature for nitrobenzene production so that the use of utility can be minimized.

1. Introduction

Nitration reaction is important because it is the most general process for the preparation of aromatic nitro compounds. This reaction plays a role in the development of theoretical organic chemistry. It is of interest because of its characteristics as an electrophilic substitution [1]. Nitration of aromatics is a large scale industrial process with global production of about 4-5 million tons of commercially valuable chemicals (nitrobenzene, nitrotoluene, 2,4-dinitrotoluene) per year [2].

Nitrobenzene has been produced commercially since 1856 when Simpson, Maule and Nicholson started operation in England [3]. It was first synthesized in 1834 from benzene and fuming nitric acid. Since then the nitration of aromatic hydrocarbons has been the subject of numerous investigations, however, only a few investigators have determined data which are useful for engineering applications [4].

Nitrobenzene is produced by reacting benzene with a mixture of nitric acid and sulphuric acid at a temperature not exceeding 50° C, to avoid getting more than one nitro group [5]. The mixture is held at this temperature for about half an hour. The sulphuric acid is acting as a catalyst. Yellow oilly nitrobenzene is formed. The reaction is as follows:

$$C_6H_6 + HNO3 \rightarrow C_6H_5NO_2 + H_2O \tag{1}$$

(2)

or

The electrophile is the nitronium ion or the nitryl cation, which is formed by reaction between nitric acid and sulphuric acid:

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