Steady State Simulation of Production of Ethyl Acetate using Ethanol and Acetic Acid

Rahul Selvakumar[1], Rodney Craig Cutinho[1] R Shivakumar[2]

[1]Department of Chemical Engineering, BMS College of Engineering, Bengaluru 560019

[2]Assistant Professor, Department of Chemical Engineering, BMS College of Engineering, Bengaluru 560019

Mail ID: [1] rahulselvakumar98@gmail.com rodneycutinho@gmail.com

[2] shivakumarr.che@bmsce.ac.in

INTRODUCTION

Ethyl acetate is normally produced by esterification of ethanol and acetic acid. A rigorous distillation column, combining the reaction and separation into a single stage, is proposed.

The costs of a chemical process are often dominated by the costs for the separation and purification of the products. Between the different separation techniques, distillation is one of the most important and commonly used in all chemical and petrochemical industries. Ethyl acetate is one of the most widely used fatty acid ester and is a quick-drying solvent with excellent solubility. As an excellent industrial solvent it finds an application as an important component of extractants used for antibiotics concentration and purification and an intermediate in the manufacture of various drugs.

ABSTRACT

This simulation was conducted to optimize the process of production of Ethyl Acetate by the Fischer esterification reaction between acetic acid and ethanol with the aid of the software 'DWSIM'. The two reactants were mixed in a mixer 1 and the output was sent to mixer 2 where the feedback was added. This was then sent to CSTR followed by a distillation column. The products were collected and a feedback provided.

INTRODUCTION

Ethyl acetate has been largely employed as a solvent in paints, coatings, inks and adhesives. It can be used as an ideal substitute for aromatic compounds for the purpose of improving working environment because aromatic compounds cause serious damage to human beings and the production of ethyl acetate in industries is mainly classified into three categories. First, the classical Fischer esterification process of ethanol with acetic acid. This process includes the usage of acid catalysts such as sulfuric acid and p-toluene sulfonic acid. Second, by Tishchenko reaction of acetaldehyde. This makes use of aluminium triethoxide as a catalyst. Third process is the one which has just been recently commercialized, is

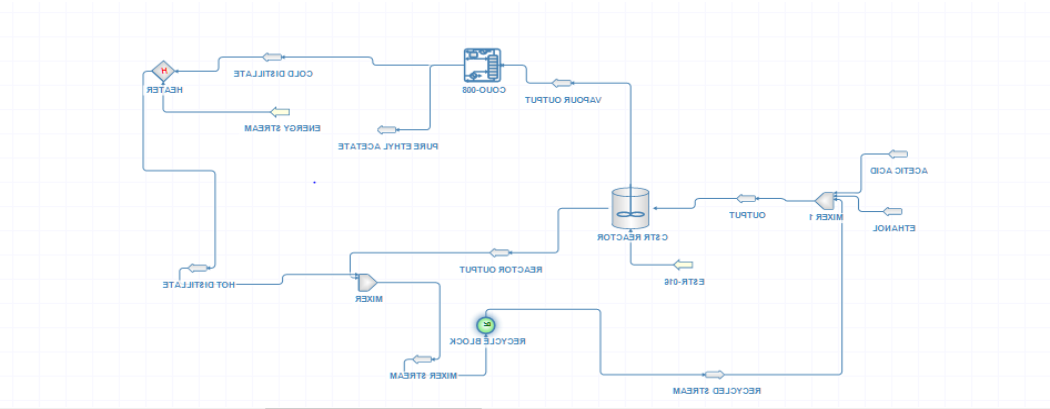
addition of acetic acid to ethylene using clay and heteropoly acid as the catalyst of the reaction. Fischer esterification process of producing ethyl acetate is an equilibrium reaction occurring between acetic acid and ethanol. In using this process for the production of ethyl acetate, one of the key issues that should be addressed is low reaction conversion. As a result of this low conversion, heavy capital investments and high energy costs are inevitable in this process, especially, based on the experience especially, based on the experience. The equilibrium reactor has two products streams both of which were distilled. The streams gave the following results.

The output vapour steam had 95% Ethyl Acetate and

Ethanol 3.8% with minute quantities of water and acetic acid

The residue containing ethanol, acetic acid and water was recycled.

FLOWSHEET



RESULT TABLE

MASTER TABLE					
Object	VAPOUR OUTPUT	RECYCLED STREAM	REACTOR OUTPUT	PURE ETHYL ACETATE	OUTPUT
Temperature	77	-25.7897	77	-46.0998	25
Pressure	1	0.001	1	0.001	1
Molar Flow	165.904	130.162	34.0974	69.84	200
Vapor Phase Molar Fraction	1	0.904407	2.62408E-06	1	0
Molar Fraction (Liquid Phase 1) / Ethanol	4.37924E-08	2.48484E-10	1.48089E-08	1.029E-07	0.5
Molar Fraction (Liquid Phase 1) / Acetic acid	3.23377E-07	2.24497E-08	1.5671E-07	3.44666E-07	0.5
Molar Fraction (Liquid Phase 1) / Water	0.654869	0.999758	0.956821	5.72919E-20	0
Molar Fraction (Liquid Phase 1) / Ethyl acetate	0.345131	0.0002424	0.0431793	1	0

MIXER STREAM	HOT DISTILLATE	ETHANOL	COLD DISTILLATE	ACETIC ACID	
-25.7897	100	25	-71.3407	25	C
0.001	0.001	1	0.001	1	bar
130.162	96.0645	100	96.0645	100	kmol/h
0.904407	1	0	0	0	
2.48484E-10	2.59834E-14	1	2.50943E-13	0	
2.24497E-08	4.12346E-23	0	5.37905E-23	1	
0.999758	0.997178	0	0.701361	0	
0.0002424	0.00282201	0	0.298639	0	

Master Property Table for the Simulation process.