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Design and Simulation of a Radfrac Absorption Unit for Acetic Acid Purification via Ethylene Oxidation Using Aspen Plus

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تصميم ومحاكاة وحدة امتصاص *Radfrac* لتنقية حمض الاسيتيك الناتج من أكسدة الايثيلين *Aspen Plus* باستخدام

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Abstract
This study aims to design RadFrac absorption unit for the purification and separation of acetic acid (CH3COOH) from a stream containing carbon dioxide CO in order to obtain high-purity acetic acid and an inert gas stream consisting of nitrogen and carbon dioxide. Acetic acid is produced via ethylene oxidation, yielding acetic acid, carbon dioxide and water. Under operating conditions of 29 0C and 10 bar, acetic acid was recovered in the bottoms stream at a flow rate of 35.496 kg\hr. All process stages were simulated evaluated, and investigated using Aspen Plus V10.

Keywords: Acetic acid, Aspen plus, RadFrac, Ethylene Oxidation.

الملخص
تهدف هذه الدراسة الي تصميم وحدة امتصاص RadFrac لتنقية وفصل حمض الأسيتيك (CH3COOH) من تيار يحتوي علي ثاني أكسيد الكربون (CO2)، وذلك للحصول على حمض الأسيتيك بدرجة نقاوة عالية وتيار غاز خامل يتكون من النيتروجين وثاني أكسيد الكربون. حيث يتم الحصول على حمض الاسيتيك عن طريق أكسدة الايثيلين، والتي تنتج أيضا ثاني أكسيد الكربون والماء. وعند ظروف تشغيل تبلغ درجة حرارة C290 وضغط bar10، تم الحصول على حمض الأسيتيك بمعدل تدفق kg\hr35.496في تيار القاع. وقد قمنا بمحاكاة وتقيم جميع مراحل العملية ودراستها باستخدام برنامج Aspen plus V10 .

الكلمات المفتاحية: أسبن بلس، حمض الأسيتيك, RadFrac , أكسدة الايثيلين.

Introduction

Acetic acid (CH_3COOH) is an important organic acid that is frequently utilized in both daily life and industry it acts as indispensable precursor in synthesizing food preservatives, medications, polymers, and solvents. Millions of tons are demanded annually worldwide, highlighting its pivotal role in the global chemical economy [1]. In the past, ethanol oxidation and fermentation were the primary methods used to produce acetic acid. However, due to the ongoing advancements in chemical technology, companies now favor more effective processes. commercially, acetic acid is mainly produced from methanol carbonylation and acetaldehyde oxidation, which presents operational and environmental challenges, such as corrosion and waste disposal [2,4]. Therefore, considerable efforts have been made to develop alternative approaches for acid production, among which the direct oxidation of ethylene to acetic acid has shown promise. Ethylene oxidation has become [3] a significant alternative method for producing acetic acid in recent years. This process selectively converts

ethylene into acetic acid by the catalytic reaction of ethylene (C_2H_4) with oxygen. As an example, a process using palladium-based heteropoly acids catalysts for ethylene oxidation to acetic acid was commercialized by Showa Denko in1997[4]. The presence of both palladium and acidic support is a common feature of the catalysts used in the selective oxidation of ethylene to acetic acid [4,5]. Unlike traditional manufacturing pathways, this route offers benefits in terms of raw material accessibility and the potential for process integration into current industrial systems. In order to get an optimum design appropriate for industrial application, Aspen Plus is utilized in the current work to simulate the oxidation process, allowing the investigation of important operating factors including pressure, temperature, and flow rate[6].

Methodology

There are many different methods for producing acetic acid, and one of the methods used is the oxidation of ethylene to produce acetic acid. Ethylene is converted into acetic acid, carbon dioxide and water. Using the Aspen Plus simulation software an absorption unit is designed Refract [7]

1- This is to separate and purify acetic acid from carbon dioxide.

2- Using the NRTL(Non-Random-Two-Liquid) model, which describes the liquid-vapor equilibrium state.

Simulation of a design for separating acetic acid from carbon dioxide

The current CO_2 enters absorption unit from the bottom of the tower and contains acetic acid at a concentration of (0.6K. Mol\hr) carbon dioxide at a concentration of (98.2 K mol\hr) and nitrogen at a contraction of (1.2 K mol\hr) from the top of the tower enters a stream of H_2O containing (150K mol \hr) water. Two currents exit the Radfrac unit, one from the top and one from the bottom, where it contains stream Top-STRE on carbon dioxide and a small amount of acetic acid and the current Strem BTM-STRE contains acetic acid a small amount of carbon dioxide.

Results and discussion

Tables 1 and 2 show the molar and mass flow to REDFRAC. The flow rate of carbon dioxide is (98.2 Kmol/hr entering from the bottom of the Redfrac at a temperature of 93C$^\circ$ and a pressure of 10 bar. As for the water, the flow rate is 150Kmol/hr at room temperature and pressure 10 bar, and it enters from the top. After the separation process, the primary product, acetic acid, is obtained from the bottom of the RedFrac at a flow rate of 0.57 kmol/hr at a temperature of 29C$^\circ$ and a pressure of 10 bar.

Table 1. Mole flows

compound name	Unit	Stream CO_2	Stream H_2O	Stream BTM-STRE	Stream TOP-STRE
WATER	Kmol/hr	0	150	150	8.05517e-35
CH_3COOH	Kmol/hr	0.6	0	0.575615	0.000243853
CO_2	Kmol/hr	98.2	0	18.7756	79.4244
N_2	Kmol/hr	1.2	0	6.74801e-12	1.2
C_2H_4	Kmol/hr	0	0	0	0
MASS FLOWS	Kmol/hr	100	150	169.351215	80.6246439

Table 2 Mass flows

compound name	Unit	Stream CO_2	Stream H_2O	Stream BTM-STRE	Stream TOP-STRE
WATER	Kg/hr	0	26738.965	2557.487	5.853
CH_3COOH	Kg/hr	35.964	0	35.496	6.638e-12
CO_2	Kg/hr	4319.968	0	35.423	3989.999
N_2	Kg/hr	32.897	0	0.004	32.865
C_2H_4	Kg/hr	0.0428365	0	0	0
MOLE FLOWS	Kg/hr	4388.87184	26738.965	2628.41	4028.717

Table 3 Liquid and Vapor phase in unit RadFrac

Table 3.1 Liquid phase

	Unit	Stream CO_2	Stream H_2O	Stream BTM-STRE	Stream TOP-STRE
Molar Enthalpy	Cal/mol	-107234	-68262.2	-70230.4	-90614
Molar Entropy	Cal/mol-k	-51.928	-38.9652	-26.2473	-27.0426
Molar Density	Mol/cc	0.0177287	0.055173	0.035952	0.0300601
Enthalpy Flow	Cal/sec	-18.0153	-157880	-197826	-11826.8
Average MW		58.299	18.0153	22.6812	42.5653

3.2 Vapor phase Table

	Unit	Stream CO_2
Molar Enthalpy	Cal/mol	-92129.4
Molar Entropy	Cal/mol-k	-3.38754
Molar Density	Mol/cc	0.000384079
Enthalpy Flow	Cal/sec	-58439.3
Average MW		43.7761

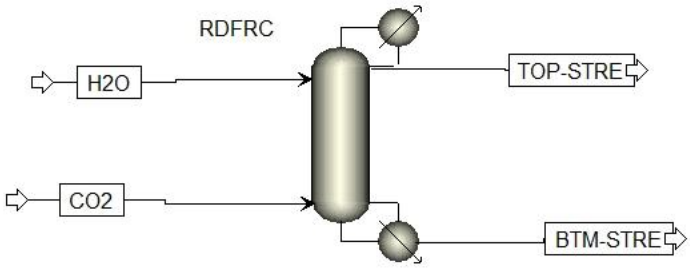

Figure 1: Main flow sheet for the modeling process

Conclusion

The principal objective of this study was to design and investigate a simulation model for acetic acid production via ethylene oxidation using Aspen Plus. Although the entire production encompasses six distinct operating stages, recovering the acetic acid from the carbon dioxide gas stream with high purity was successfully achieved using a rigorous RadFrac absorption unit. The NRTL property method was applied, proving its high capability to handle such non-ideal multi-component mixtures. Based on the simulation results presented in the material balance tables (Table 3.1 and Table 3.2), the designed absorber demonstrated a high separation efficiency, capturing approximately 95.9% of the acetic acid into the bottom liquid stream (BTM-STRE), while reducing the loss in the top vapor stream (TOP-STRE). Furthermore, the thermodynamic properties, including molar enthalpies and phase densities detailed in Table 3.3), confirm the stability and process viability of the simulated absorption process.

Compliance with ethical standards

Disclosure of conflict of interest

The authors declare that they have no conflict of interest.

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