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Using Aspen Plus Program to Design and Enable the Cracking of Acetone and the Manufacture of Highly Pure Acetic Anhydride

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Abstract:
In order to convert acetone into acetic anhydride, a system that can break down acetone and decompose it into chitin and methane under specific operating conditions of temperature and pressure is required. The produced chitin must then react with acetic acid to produce acetic anhydride.
This system consists of a plug-flow reactor (PFR), where the acetone is first broken down into chitin and methane at 762 °C and 1.8 atm, and a column of RadFrac (RECTIF), which separates the chitin from the methane and the leftover acetone. The chitin and acetic acid reaction, which results in the generation of acetic anhydride, is then continued by adding a continuously stirred tank reactor. The design is then assessed using the program V9 Aspen Plus.

Keywords: Aspen Plus, Acetic Anhydride, Ketene, Acetone.

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استخدام برنامج Aspen Plus لتصميم وتمكين تكسير الأسيتون وتصنيع أنهيدريد الخل عالي النقاء

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الملخص
إن انتاج أنهيدريد الخليك من الاسيتون يحتاج الي تصميم نظام مناسب وفي ظروف تشغيلية محددة من درجة حرارة وضغط وذلك الي تكسير الاسيتون و تحليله إلى كيتين و ميثان ومن ثم تفاعل الكيتين المنتج مع حمض الأسيتيك وانتاج أنهيدريد الخليك . حيث ان هذا النظام يتكون من مفاعل plug-flow reactor (PFR) حيث ان في هذا المرحلة يتم تكسير الاسيتون الي كيتين وميثان عند درجة حرارة $762C^0$ وضغط 180 atm ومن عمود التصحيح Radfrac (RECTIF) وذلك الي فصل الكيتين عن الميثان و الاسيتون المتبقي من التفاعل , واخيرا اضافة مفاعل الخزان المقلوب المستمر Continuous Stirred Tank Reactor وذلك الي تفاعل الكيتين مع حمض الأسيتيك و انتاج انهيدريد الخليك و يثم التصميم النظام باستخدام برنامج V9 Aspen Plus.

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الكلمات المفتاحية: أسبن بلس، أنهيدريد الخليك، الكيتين، الأسيتون.

Introduction

One of the most significant intermediate organic molecules is acetic anhydride. Since it smells strongly of acetic acid and is a colourless liquid, it is also known as carboxylic methyl anhydride or ethanoic anhydride.

The production of aspirin is the most significant industry that uses acetic anhydride, although it is also used to make herbicides, acetyl peroxide bleach, and perfumes.

We need two phases to make acetic anhydride from acetone because the first step, which takes place inside the PFR reactor at a temperature of 762° C and a pressure of 1.8 atm, breaks down acetone and converts it into chitin and methane. The second stage took conducted within the continuous inverted tank at a temperature of 300 K and a pressure of 0.01 atmosphere pressure, where the resultant chitin combines with acetic acid to produce acetic anhydride as described in equation (2). A separation method is used to mediate the two phases and separate the chitin from the unreacted methane and acetone.

$CH_3\text{-}CO\text{-}CH_3 \rightarrow CH_2{=}CO + CH_4$ (1)

$CH_3COOH + C_2H_2O \rightarrow C_4H_6O$ (2)

Methodology

The following steps are involved in the design and development of a process simulation in ASPEN PLUS.

1- Chemical names are used to input the materials utilized in the manufacturing process.
2- Choose an exclusive technique for calculating the thermodynamics, kinematics, and transport process features of the NRTL (Non-Random-Two-Liquid) process, which describes the liquid-vapour equilibrium.
3- In the steady state, the process was difficult.
4- Use the following equation to determine the reaction rate constant and activation energy.

$$r = K' \exp -E/R[\frac{1}{T}]$$

$$In = 34.33 - \frac{43221}{T}$$

$$In\ k = A * e^{\frac{-E}{RT}}$$

E = 284521 KJ\Kmol

$K = 8.1972 \times 10^{14}\ s^{-1}$

T° is the reference temperature.

System design simulation for acetone cracking and acetic anhydride synthesis

This simulation features a plug-flow reactor where acetone enters through flow (1), is transformed to acetone by thermal cracking inside the reactor, and finally leaves through flow (2) with chitin. from the RadFrac rectification column as well. This column has one entrance stream, flow (2), one output stream for undissolved acetone, flow (3), one outlet for methane produced during the cracking process, and one outlet stream, flow (5). Additionally, a mixer is added to mix the chitin and acetic acid before they enter the RCSTR reactor. This mixer has two entrance flows—one for the chitin and the other for the acetic acid—and one outlet flow. Additionally, because chitin and acetic acid flow at the same rate. In the end, a continuous stirred tank reactor is added. This reactor has one flow, flow (7), which is the mixture's inlet, and one flow, flow (8), which is the stream for acetic anhydride production.

A schematic showing how acetone is broken down to create acetic anhydride

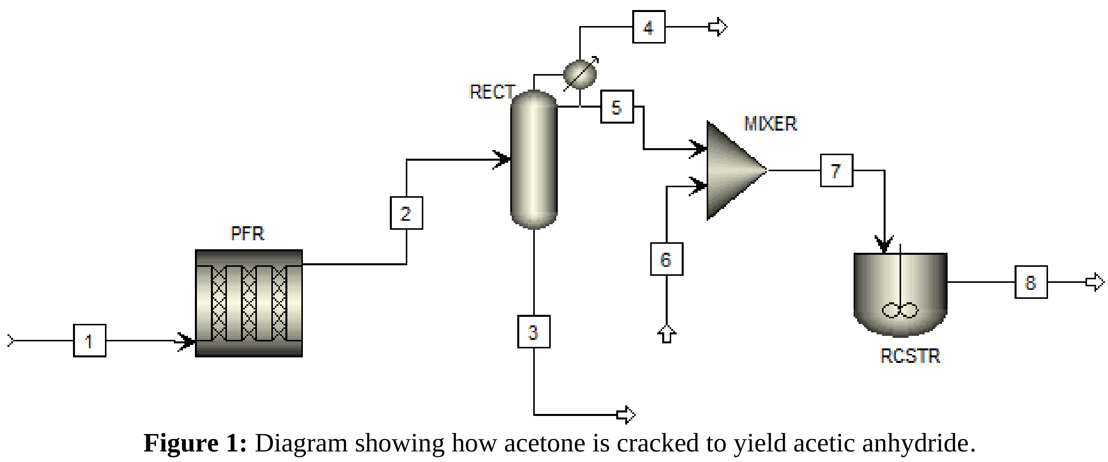

Figure 1: Diagram showing how acetone is cracked to yield acetic anhydride.

Results and discussion

The entire outcomes of the procedure to break down acetone and transform it into methane and chitin are displayed in the table below. Due to the PFR reactor's approximately 21% acetone cracking percentage and around 2760 kg/hr of acetic anhydride production

Table 1: Complete outcomes of the synthesis of acetic anhydride and acetone cracking.

Compound name	Acetone	Ketene	Methane	Acetic Acid	Acetic Anhydride
Chemical formula	C_3H_6O	C_2H_2O	CH_4	$C_2H_4O_2$	$C_4H_6O_3$
Unit	Kg/hr	Kg/hr	Kg/hr	Kg/hr	Kg/hr
Stream 1	8422	0	0	0	0
Stream 2	6668	1270	485	0	0
Stream 3	6668	17.00	0.82	0	0
Stream4	0	117.40	468.30	0	0
Stream 5	0	1136	15.50	0	0
Stream 6	0	0	0	1622	0
Stream 7	0	1136	15.50	1622	0
Stream 8	0	0.082	15.50	0.12	2760

Table1 indicates 8422Kg of acetone are given to the PFR in stream1, and that 1270Kg of chitin and 485Kg of methane are fed to stream2 following the acetone cracking process

We observe that the acetone mass flow.

The unreacted kg/hr (6668) indicates a 21% acetone conversion rate in PFR.

The distillation column indicates that stream 5's overall flow rate is (1151.5 kg/hr).

With a mass flow of 1136 kg/hr, the mass fraction of chitin in this stream was the biggest, and it reacted with ac etic acid in the continuous stirred tank reactor (CSTR).

In stream 6, the total mass flow to acetic acid is 1622 kg/hr.

Mass balance and processing enthalpy

plug flow reactor (PFR)

Table 2: Plug flow reactor mass balance and enthalpy

Total	Units	In	Out	Rel.diff
Mass flow	Kg/hr	8422	8422	$1.34e^{-14}$
Enthalpy	KJ/hr	$-1.775e^{+7}$	$-1.775e^{+7}$	$-3.954e^{-16}$

Because this reaction is occurring adiabatically, it is known that heat transfer is zero in the adiabatic state—Table 2 shows that the enthalpy of the entrance and output are equal.

RadFrac rectification column (RECT)

Table 3: Enthalpy and mass balance of the rectifying column RECT.

Total	Units	In	Out	Rel.diff
Mass flow	Kg/hr	8422	8422	$1.295e^{-15}$
Enthalpy	KJ/hr	$-1.775e^{+7}$	$-3.254e^{+7}$	0.455

As can be seen from Table 3, the temperature differential between the top and bottom of the adjustment column is the reason why the heat content of the input and outflow is not equal.

Continuous Stirred Tank Reactor (RCSTR)

Table 4: Mass balance and enthalpy of Continuous Stirred Tank Reactor.

Total	Units	In	Out	Rel.diff
Mass flow	Kg/hr	2773	2773	0
Enthalpy	KJ/hr	$-1.456e^{+7}$	$-1.5621e^{+7}$	0.071

Table 4 demonstrates that the heat content of the outflow and the entrance are nearly similar, with no appreciable difference between the two.

Conclusion

In order to break down acetone, turn it into methane and chitin, and produce highly pure acetic anhydride, a suitable system and model were created using the Aspen Plas V9 program. Additionally, the main reactor equipment in the cracking process was simulated and improved. Purification and separation of the resulting materials' simulation of separation equipment, followed by a simulation of the manufacturing reactor's equipment to get good results and have a high level of product purity, there are around 26,000 tons of acetic anhydride produced annually.

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