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Hydrolysis of Acetic Anhydride in a CSTR

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Hydrolysis of Acetic Anhydride in a CSTR

Abstract

To find the optimal reactor volume and temperature for the hydrolysis of acetic anhydride at the lowest possible cost with a 90% conversion of acetic anhydride, a formula for the total cost of the reaction was created. Then, the first derivative was taken to find a value for the temperature. This value was then inputted into the second derivative of the equation to find the sign of the value which would indicate whether that point was a minima or maxima value. The minima value would then be the lowest total cost for the optimum reaction to take place.

Keywords

chemical engineering, continuous stirred tank reactor, hydrolysis reaction

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PROBLEM STATEMENT

One of the reactor models used in engineering is the CSTR (Continuous stirred tank reactor). A CSTR is to be used for the hydrolysis of acetic anhydride (species A) as shown in the figure below.

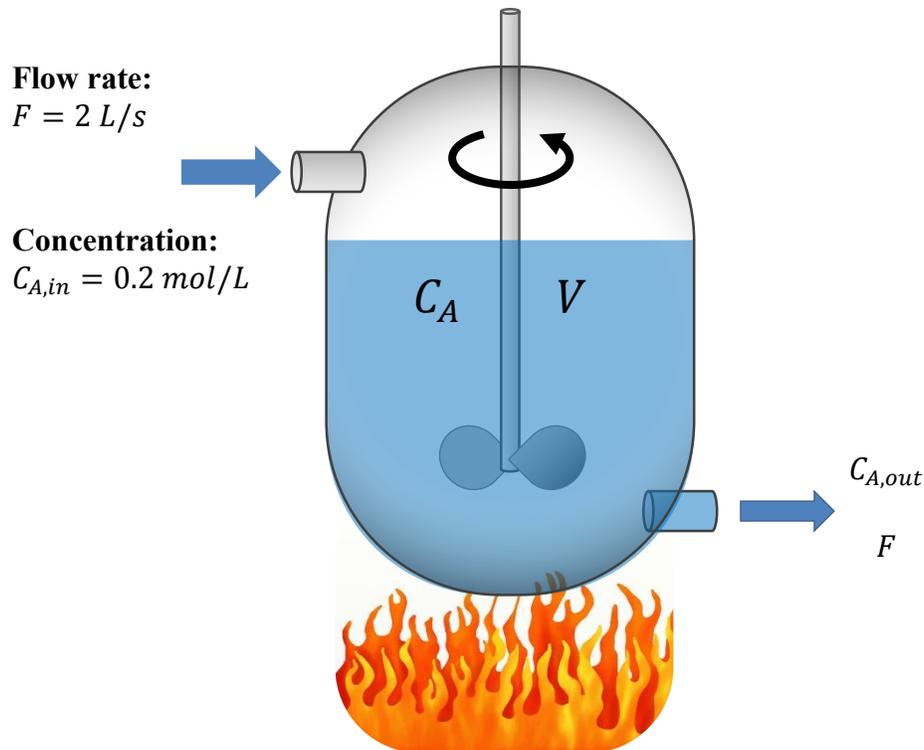


Figure 1: Design and settings of the continuous stirred tank reactor

Since the feed solution is fairly dilute (0.2 mol/L) in acetic anhydride, the reaction can be assumed to be first order in species A. As a result, the design equation for the CSTR is:

$$C_{A,out} = \frac{C_{A,in}}{1 + \frac{kV}{F}}$$

where $C_{A,out}$ is the concentration of the reactant leaving the reactor and $C_{A,in}$ is the concentration of reactant entering the reactor. F is the volumetric flow rate of liquid through the

reactor, V is the reactor volume and k is the reaction rate constant. The rate constant depends on temperature according to the Arrhenius relationship:

$$k(T) = 4 \cdot 10^5 e^{-5620/T} \quad (1)$$

where T is the temperature in Kelvin and k has units of s^{-1} . The cost of a reactor (expressed as a prorated *annual* cost) is:

$$\text{Reactor cost (\$/yr)} = 53 V, \text{ where } V \text{ is in } L$$

There is a cost associated with heating the reactor as well. On an annual basis, this is:

$$\text{Heating cost (\$/yr)} = 1080 (T - 298), \text{ where } T \text{ is in } K$$

The company desires a 90% conversion of acetic anhydride in the reactor. We determine the optimal reactor volume V and temperature T as well as the associated annual reactor cost, annual heating cost and total annual cost.

MOTIVATION

Engineers have to be concerned with the economic aspects of production because when they are employed by a company, the company expects that they maximize production yield while minimizing the cost of production. Finding the lowest cost for this reaction would ensure the most economically efficient way to convert the acetic anhydride.

CSTR is a machine commonly found in the chemical engineering industry that runs steadily mixing reactant to form products to create a uniform solution throughout the reactor so that the exit stream has the same composition (Michigan). The advantages to using a CSTR are that the reaction is continuous, easy to control, allows effective temperature control, and it has a low operating cost. This machine will facilitate the process of creating the most efficient chemical reaction. A schematic of a CSTR (Pugliesi) can be seen below (species B).

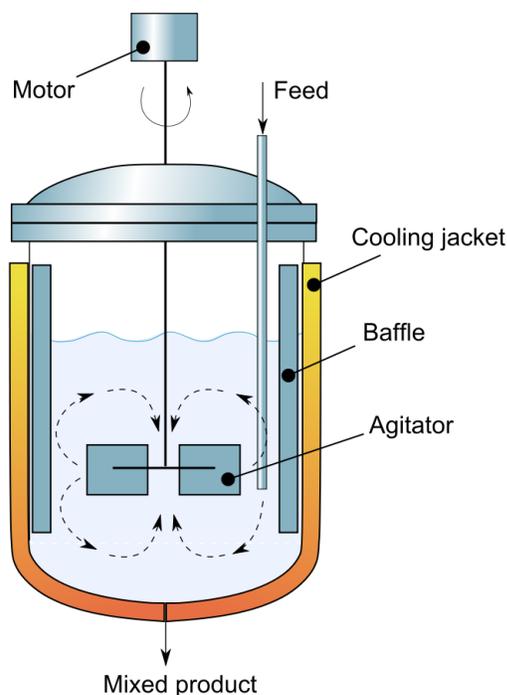


Figure 2: Schematic of the continuous stirred tank reactor for Species B (Pugliesi).

Another important reason to use the lowest temperature and volume of reactant beside costs would be to lessen the impact these chemical processes can have on the environment. Finding the lowest temperature at which a reaction could take place would be energy efficient which would decrease pollution caused by the use of fossil fuels that harm the environment (Top 5 Reasons to be Energy Efficient).

MATHEMATICAL DESCRIPTION AND SOLUTION APPROACH

We began by making an equation for the total cost of the reaction by combining the equations for the cost of the reactor with the associated cost of heating. Given the annual reactor cost and annual heating cost given above, the total cost for the reactor is expressed by:

$$\text{Total Cost (\$/yr)} = 53V + 1080 (T - 298) \quad (2)$$

The optimum reactor volume and temperature would be the one that produces the reaction at the lowest cost to the company with a 90% conversion of the acetic anhydride.

In order to fulfill the first requirement, we refer to the design equation for the CSTR:

$$C_{A,out} = \frac{C_{A,in}}{1 + \frac{kV}{F}} \quad (3)$$

With a 0.2 mol solution going into the reactor, a 0.02 mol solution must come out of the reactor to fulfill the 90% conversion of acetic anhydride that the company desires.

Substituting $F = 2 \text{ L/s}$, $C_{A,in} = 0.2 \text{ mol}$, $C_{A,out} = 0.02 \text{ mol}$, and (1) into (3) yields the relationship between V and T , i.e.,

$$V = 4.5 \cdot 10^{-5} e^{5620/T} \quad \text{and} \quad T = \frac{5620}{\ln\left(\frac{4.5 \cdot 10^{-5}}{V}\right)} \quad (4)$$

Equation (4) in terms of V can be substituted into the total cost equation (2), and T can be chosen to minimize the cost at which the reaction would take place. If $f(T)$ is the total cost of the reaction per year

$$f(T) = 53 (4.5 \cdot 10^{-5} e^{5620/T}) + 1080 (T - 298) \quad (5)$$

then

$$f'(T) = 1080 - 13.4037 T^{-2} e^{5620/T}. \quad (6)$$

An extremal operation cost occurs when $f'(T) = 0$, which holds at $T^* = 349.074$. The second derivative,

$$f''(T) = 26.8074 (T + 2810) T^{-4} e^{5620/T} \quad (7)$$

gives $f''(T^*) = 55.998 > 0$, so the critical value T^* is the temperature that yields the minimal yearly operating cost of the reactor.

DISCUSSION

The objectives outlined by the company were met. A 90% conversion of acetic anhydride at the lowest possible cost to the company was determined by creating a total cost equation using the combined cost of the reactor and the associated heating cost. Then we created an equation from the design equation of the CSTR that related V in terms of T to substitute back into the total cost equation thus eliminating one of the variables from the equation. In order to find the lowest possible cost, the minimum values of the function had to be determined.

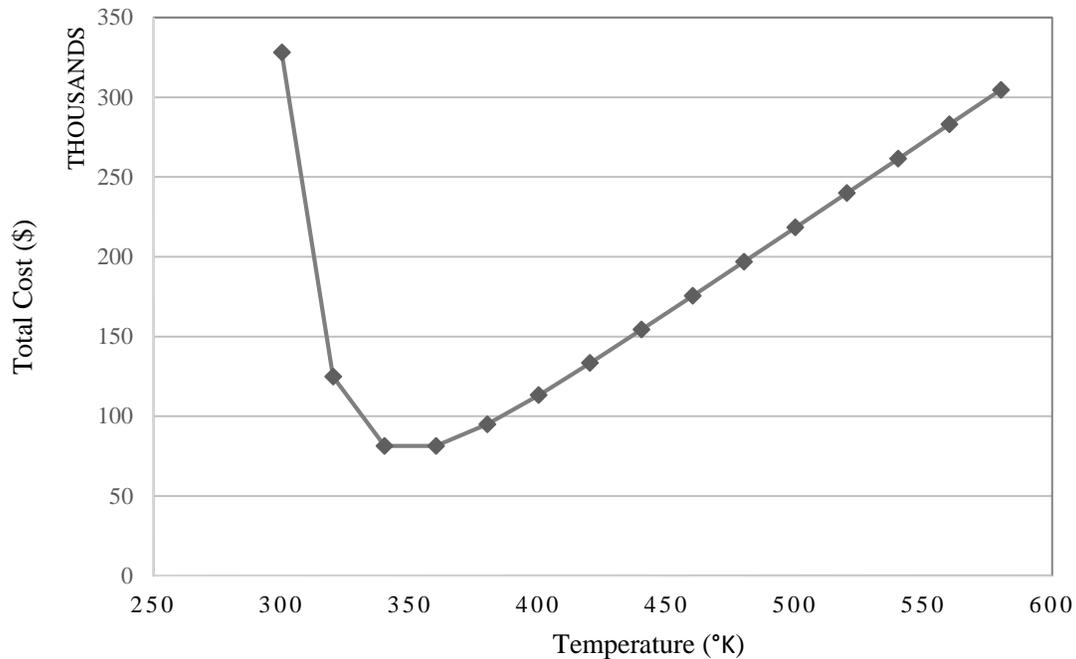


Figure 3: The total annual cost to operate the CSTR shown as a function of temperature. The minimal cost occurs at 349°K.

To do this, we determined the values of T where the first derivative equaled 0. This value was then substituted into the second derivative to find the sign of the inflection point. Because the value of the inflection point was positive, the initial value of T was determined to be a minimum. This value for T was then substituted into the volume equation to find the optimal

volume of the reactant. The values for V and T were then substituted back into the costs equations to find the annual cost of the reactor, the associated heating cost, and the total cost.

CONCLUSION AND RECOMMENDATIONS

Using 441.814 L of reactant at 394.074°K is the optimum temperature and volume for the reaction because it converts 90% of the acetic anhydride at the lowest cost. The annual cost of the reactor using 441.814 L would be \$23,416.14 per year while the associated heating cost of the reactor would be \$55,159.92 per year. Together, these expenses yield a total annual cost of 78,576.06 dollars per year. In the future, we would find the optimal combination of volume of reactant to heat of reaction that yields a 99% conversion of acetic anhydride at the lowest cost because this would develop an even more efficient process that would save money for the company while maximizing production as well as protecting the environment.

NOMENCLATURE

Symbol	Description	Value
F	Volumetric Flow Rate	$2 L / s$
k	Reaction rate constant	$0.407 / s$
M	Molarity of acetic anhydride	mol / L
T^*	Optimal operating temperature of the CSTR	$349.074^{\circ}K$
V	Volume of reactant	$441.82 L$
$f(T^*)$	Minimum annual operating cost of the CSTR	$\$78,576.06$

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