3.0 DISCUSSION

A reversible reaction is a chemical reaction that results in an equilibrium mixture of reactants and products. For a reaction involving two reactants and two products this can be expressed symbolically as

$$aA + bB \rightleftharpoons cC + dD$$

A and B can react to form C and D or, in the reverse reaction, C and D can react to form A and B. This is distinct from reversible process in thermodynamics.

The concentrations of reactants and products in an equilibrium mixture are determined by the analytical concentrations of the reagents (A and B or C and D) and the equilibrium constant K_c. The magnitude of the equilibrium constant depends on the Gibbs free energy change for the reaction. So, when the free energy change is large (more than about 30 kJ mol^{-1}), then the equilibrium constant is large (log K > 3) and the concentrations of the reactants at equilibrium are very small. Such a reaction is sometimes considered to be an irreversible reaction, although in reality small amounts of the reactants are still expected to be present in the reacting system. A truly irreversible chemical reaction is usually achieved when one of the products exits the reacting system, for example, as does carbon dioxide (volatile) in the reaction. In this case, the reversible reaction is between acetic acid and ethyl acetate, such that:

$$AcA_{(l)} + EtOH_{(l)} \leftrightarrow EtAc_{(l)} + H_2O_{(l)}$$

To make this endothermic reaction irreversible, the water must be removed from the system at all times. However, in CSTR, which has a closed top, this is not possible. So the reaction's conversion becomes a percentage of the equilibrium reaction, which changes between 80-90% in ideal cases. 80% of the equilibrium conversion was assumed for this report. The reaction's conversion depends on many factors, such as temperature, the weight percentage of the catalyst in reaction (the catalyst in this reaction is H_2SO_4, with a weight percentage of 1.91%), presence of inert in the system, purity of the components and whether the tank is perfectly mixed. In this report, the components were taken as aqueous solutions, with mole percentage of acetic acid being 96%, and that of ethanol's percentage being 96.5%. These factors also affect the reactor tank's volume, due to the CSTR design equation. With mole balance and CSTR design equation, the inlet and outlet molar rates were calculated, and the inlet water of the solutions was added to the effluent water.

Concentrations were calculated from the rate equation. The k values of the rate equation depend on temperature and the weight percentage of the catalyst in the system. Upon finding these k and concentration values the rate of acetic acid's formation was calculated. After finding the rate, the reaction volume was calculated as 2.983 m^3.

The safety factor was added to the reaction volume and the tank volume was found as 3.43 m^3. After finding the volume, the diameter and the height of the tank was calculated as 1.5 and 1.95 m respectively. The diameter of the agitator was calculated as 0.5 m.

To heat the coil, many options are available. One can heat the components at a separate heat exchanger before feeding to the reactor, a jacket can be used, or a certain number of coils can be installed in the reactor. Choosing the heating fluid is very important, because choosing saturated steam (hence using steam generator) might cause additional expenses. Saturated steam is used in bigger industries in order to take advantage of its heating, and to generate electricity by means of steam turbines. Hot oil is a cheaper fluid to obtain, and for this reason hot oil was used as heating fluid. The velocity of the hot oil affects the heating of the reactor, as the velocity affects the Reynold's number, the Nusselt number, and the convection heat coefficient as a result. The pipes and pumps can be picked to obtain the desired mass flow rate. The Nusselt number of the jacket and coils were calculated using the Chilton-Drew-Jebend's correlation. The wall thickness of the jacket and reactor affects heat transfer because the mass flow rate, the heat transfer area and the temperature difference change.

The jacket was calculated first, which can be seen in appendix. To calculate the heat requirement for this endothermic reaction, hypothetical steps formed such that the reactor's temperature, which was 75°C, was virtually dropped down to 25°C; and the reaction take place in this temperature. The products and the remaining components are then heated up to 75°C. Since the temperature of the entering and exiting components were 75°C, the only remaining factor was ΔH_{rxn} in energy balance equation. The formation enthalpies at 25°C were found from references. The velocity of hot oil was assumed as 0.6 m/s, and then the temperature difference was calculated between the entrance and the exit of the jacket as 2.05 ^{0}C. If a higher velocity had been assumed, the mass flow rate would increase, required heat transfer area decrease and the pressure drop would change, a pump and pipe with a bigger diameter would be needed and this would cause more expensive operations and the temperature difference will be affected.

After finding the velocity and mass flow rate, using the correlations, h_o was calculated as 921.845 W/m^2K. The viscosity, specific heat and thermal conductivity of hot oil were taken at 200°C. With these data, h_i was calculated as 574.043 W/m^2K. After that U_o was found as 347.32 W/m^2K, and the area necessary for heating was calculated as 6.36 m^2. The jacket satisfies the reactor.

The same steps were followed for the coil, only that the number of coils was additionally calculated as 6, with the coils being a certain distance such as 20 cm away from the tank wall. Using coil for this reactor is a better option, because coil has a smaller area which lessens the required amount of hot oil as 3.536 kg/s , therefore making the reaction costly efficient.

In the agitation systems, we chose open turbine agitator with six-bladed impeller with four baffles. We chose our propeller speed as 2 rps, and the motor power needed was calculated as 4.441 kW. The safety factor and efficiency were also added for finding the actual power.

NOMENCLATURE

F_i :	Molar flowrate of i^{th} component	[kmol/min]
X:	Conversion	
T :	Temperature	[^oC]
C_i:	Concentration of i^{th} component	[kmol/m^3]
D_T:	Tank diameter	[m]
H_T:	Height of tank	[m]
N:	Rotational speed	[rps]
N_P:	Power number	
E:	Distance between reactor bottom and impeller	[m]
$D^{'}$:	Diameter of one coil	[m]
P_o:	Operating power	[W]
Q :	Heat taken/given from the reactor	[W]
U_0:	Overall heat transfer coefficient	[W/m^2.K]
D_{ji}:	Inner diameter of jacket	[m]
D_{jo}:	Outer diameter of jacket	[m]
G:	Mass flux	[kg/m^2.s]
Re:	Reynolds number	
V_{tank} :	Volume of tank	[m^3]
V_{liq} :	Volume of reaction mixture	[m^3]
d_{ag}:	Agitator diameter	[m]
$-r_A$:	Rate of reaction with respect to component A	[kmol/m^3min]
k :	Specific reaction rate	
$\dot{m}_i$:	Mass flowrate of i^{th} component	[kg/h]
d_o:	Outer diameter of coil	[m]
d_i:	Inner diameter of coil	[m]
h_i:	Convective heat transfer coefficient inner fluid	[W/m^2.K]
h_o:	Convective heat transfer coefficient outer fluid	[W/m^2.K]

Greeks

ρ :	Density	[kg/m^3]
μ :	Viscosity	[Pa.s]
υ_i :	Volumetric flowrate of i^{th} component	[m^3/min]
η :	Efficiency	
ΔH:	Enthalpy of out/ in/ reaction	[W]

Subscripts

i: i^{th} component

i: Inner

o: Outer

ag: Agitator

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Calculation of the Volume of the CSTR

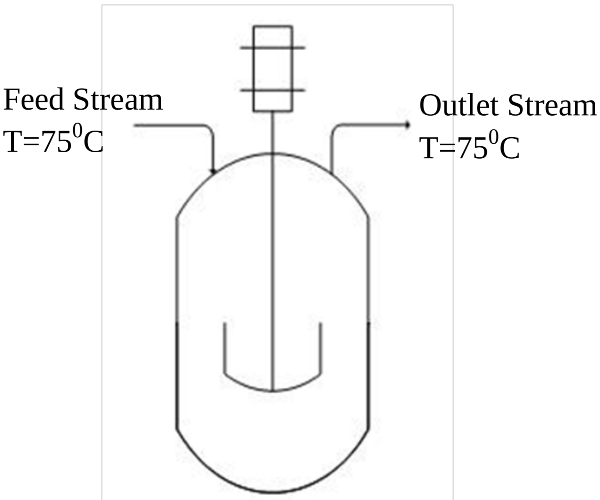

Figure 1. A typical CSTR

$$CH_3COOH + C_2H_5OH \underset{k_2}{\overset{k_1}{\rightleftharpoons}} CH_3CO_2C_2H_5 + H_2O$$

$$A \quad + \quad B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C \quad + \quad D$$

$T_{reaction} = 75\ {}^0C \quad , \quad \theta_B = 1.1$

$k_1 = 22.63*10^{-3}\ 1/min \quad , \quad k_2 = 1.55*10^{-3}\ m^3/kmol.min$ Reference 8

$-r_A = k_1 * C_A^{0.5} C_B^{0.5} - k_2 C_C C_D \quad ; \quad -r_A = 22.63*10^{-3} * C_A^{0.5} C_B^{0.5} - 1.55*10^{-3} C_C C_D$

Name	**Composition**	**Initial**	**Change**	**Remaining**
Acetic Acid	A	F_{A_0}	$-F_{A_0} * x$	$F_A = F_{A_0}(1-x)$
Ethanol	B	F_{B_0}	$-F_{A_0} * x$	$F_B = F_{A_0}(\theta_B - x)$
Ethyl Acetate	C	—	$+F_{A_0} * x$	$F_C = F_{A_0} * x$
Water	D	F_{D_0}	$+F_{A_0} * x$	$F_D = F_{A_0}(\theta_D - x)$

$$F_C = 21000 \frac{ton}{year} * \frac{1\ year}{365\ day} * \frac{1\ day}{24\ h} * \frac{1\ h}{60\ min} * \frac{1000\ kg}{1\ ton}$$

where did these values come from?

$$F_C = 39.954\ kg/min \quad , \quad F_C = 39.954 \frac{kg}{min} * \frac{kmol}{88.1\ kg} = 0.453\ kmol/min$$

$$\mathbf{x = x_e * 0.8 \quad , \quad x_e = 0.52} \quad ; \quad x = 0.52 * 0.8 = 0.416$$

$$F_C = F_{A_0} * x \quad ; \quad 0.453 = F_{A_0} * 0.416 \quad , \quad F_{A_0} = 1.09\ kmol/min$$

$$F_{A_0} = F_{A_{0,feed}} * 0.96 \quad ; \quad 1.09 = F_{A_{0,feed}} * 0.96 \quad ; \quad F_{A_{0,feed}} = 1.135\ kmol/min$$

$$\theta_B = 1.1 = \frac{F_{B_0}}{F_{A_0}} \quad F_{B_0} = 1.09*1.1 = 1.199 \ \ kmol/min$$

$$F_B = F_{A_0}(\theta_B - x) \ \ , \ \ F_B = 1.09(1.1-0.416) \ \ ; \ \ F_B = 0.745 \ \ kmol/min$$

$$F_{B_0} = F_{B_{0,feed}} * 0.965 \ \ , \ \ 1.199 = F_{B_{0,feed}} * 0.965 \ \ , \ \ F_{B_{0,feed}} = 1.242 \ \ kmol/min$$

$$F_{H_2O,from\ AcA} = F_{A_{0,feed}} - F_{A_0} = 1.135 - 1.09 = 0.0454 \ \ kmol/min$$

$$F_{H_2O,from\ EtOH} = F_{B_{0,feed}} - F_{B_0} = 1.242 - 1.199 = 0.0435 \ \ kmol/min$$

$$F_{H_2O,feed} = F_{H_2O,from\ AcA} + F_{H_2O,from\ EtOH} = 0.0454 + 0.0435 \ \ ; \ \ F_{D_0} = F_{H_2O,feed} = 0.0889 \ \ kmol/min$$

$$F_D = F_{D_0} + F_{A_0} x \ \ ; \ \ F_D = 0.0889 + 1.09*0.416 \ \ ; \ \ F_D = 0.542 \ \ kmol/min$$

$$F_A = F_{A_0}(1-x) \ \ , \ \ F_A = 1.09(1-0.416) \ \ ; \ \ F_A = 0.636 \ \ kmol/min$$

See in Table 7

$$F_{Total} = F_A + F_B + F_C + F_D \ \ , \ \ F_{Total} = 0.636 + 0.745 + 0.453 + 0.542 \ \ ; \ \ F_{Total} = 2.376 \ \ kmol/min$$

$$Design\ Equaition\ of\ the\ CSTR \ \ ; \ \ V = \frac{F_{A_0} x}{-r_A} \ \ , \ \ (\nu = \nu_0 \ in\ liquid\ phase)$$

$$C_{A_0} = \frac{F_{A_0}}{\nu_0} \ \ , \ \ C_{A_0} = \frac{F_{A_0}}{F_{A_0} * M_{w,A} * 1/\rho_A} \ \ , \ \ C_{A_0} = \frac{\rho_A}{M_{w,A}}$$

Reference 7

$$\theta_B = 1.1 \quad , \quad \theta_D = \frac{F_{D_0}}{F_{A_0}} = \frac{0.0889}{1.09} = 0.0815$$

$$C_{A_0} = \frac{1050 \ \ kg/m^3}{60.05 \ \ kg/kmol} \ \ ; \ \ C_{A_0} = 17.485 \ \ kmol/m^3$$

$$C_A = C_{A_0}(1-x) = 17.485(1-0.416) \ \ ; \quad C_A = 10.211 kmol/m^3$$

$$C_B = C_{A_0}(\theta_B - x) = 17.485(1.1-0.416) \ \ ; \quad C_B = 11.959 kmol/m^3$$

$$C_C = C_{A_0} x = 17.485*0.416 \ \ ; \quad C_C = 7.273 kmol/m^3$$

$$C_D = C_{A_0}(\theta_D + x) = 17.485(0.0815+0.416) \ \ ; \ \ C_D = 8.698 \ \ kmol/m^3$$

See in Table 8

$$-r_A = 22.63*10^{-3}*10.211^{0.5}*11.959^{0.5} - 1.55*10^{-3}*7.273*8.698$$

$$-r_A = 0.152 \ \ kmol/m^3.min$$