Introduction to Chemical Engineering

Chapter 14

Case Studies
(*Integrating It All Together*)

14.2 Case study 1: manufacture of aspirin

Project Description

In the manufacture of aspirin, acetylsalicylic acid (ASA, the active ingredient in aspirin) is synthesized using the reaction

$$\text{salicylic acid} + \text{acetic anhydride} \rightarrow \text{acetylsalicylic acid} + \text{acetic acid}$$

The presence of phosphoric acid catalyzes the irreversible reaction, which proceeds with kinetics that are first-order with respect to salicylic acid concentration ($k_{reaction} = 0.5\ s^{-1}$). Further, the reaction is exothermic (ΔH_{react} = -85,800 $J/gmol$ of salicylic acid reacted). A simplified process is described below:

The following three streams will be continuously fed to a reactor at 70°C:

Feed stream	Component	Flow rate
1	Crystalline salicylic acid	2000 kg/hr
2	Liquid acetic anhydride (pure)	5000 L/hr
3	Liquid concentrated (95%) phosphoric acid	1250 L/hr

The salicylic acid will enter the reactor as a crystalline solid but will dissolve in the acetic anhydride.

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The reactor is a continuously stirred tank reactor, where 99.5% of the salicylic acid will be converted to acetylsalicylic acid (also dissolved). Furthermore, the contents of the reactor will be maintained at $70^\circ C$ in the reactor by a cooling jacket around the reactor (carrying cooling water as needed).

The outlet stream from the reactor will flow to a mixer where it will be joined by an additional stream of ultrapure water (22,000 L/hr, $25^\circ C$). The water will react with the excess acetic anhydride to form more acetic acid, according to the reaction

$$\text{acetic anhydride} + \text{water} \rightarrow 2(\text{acetic acid})$$

This reaction proceeds to 100% conversion in the mixer, so the sizing of a "reactor" for this step is not necessary. Further, this reaction is also exothermic, but the extent of this reaction is small enough in this case to justify neglecting the heat of the reaction.

The mixed product stream leaving the mixer will enter a centrifugal pump, which will boost the pressure to the value needed to pass through the remainder of the process (leaving the final filtration sequence at atmospheric pressure).

The stream leaving the pump will enter a product cooler (a heat exchanger) in which it will be cooled to $25^\circ C$ using cooling water as the other stream in the exchanger.

The water addition and cooling step will promote the crystallization of the acetylsalicylic acid (and any unreacted salicylic acid), and the stream will then enter a filtration sequence to separate the crystals (aspirin stream) from the other byproducts (acetic acid byproduct stream, which is sold).

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Technical Details

1. Individual Properties

	Salicylic Acid (liq)	Acetic Anhydride	Phsphoric Acid	Acetylsalicylic Acid (liq)	Acetic Acid	Water
Formula	$C_7H_6O_3$	$C_4H_6O_3$	H_3PO_4	$C_9H_8O_4$	$C_2H_4O_2$	H_2O
M.W.	138.1	102.1	98.0	180.2	60.1	18.0
M.P. ($^{\circ}C$)	159	-73	21	135	17	0
B.P. ($^{\circ}C$)	211	139	158	140	118	100
Density g/cm^3)	1.44	1.08	1.68	1.35	1.05	1.0

2. Treat the concentrated phosphoric acid (95% PA, 5% water) as pure phosphoric acid.
3. Assume the following stream heat capacities:

reactor outlet stream	1.67 $J/g^{\circ}C$
ultrapure water and cooling water streams	4.184 $J/g^{\circ}C$
mixer outlet stream	3.41 $J/g^{\circ}C$

4. To determine the mixer outlet temperature, construct separate heat balances on the ultrapure water stream and reactor outlet stream. The outlet temperatures of both streams must be the same, and the heat needed to cool the reactor outlet stream from its entering temperature must equal the heat to raise the ultrapure water temperature from its entering temperature.

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5. Cooling water is available at $18^\circ C$ and has a maximum return temperature of $40^\circ C$. In selecting the actual return cooling water temperature, assume that you want to minimize the cost of cooling water (even though this will affect the size and cost of the heat exchanger). However, a second and overriding constraint is the rule of thumb that the minimum temperature difference (either ΔT_1 or ΔT_2, see Figure 10.11) for a heat exchanger is $5^\circ C$.
6. Assume countercurrent, single-pass heat exchangers.
7. Assume that the separation system is isothermal (operates at constant temperature).
8. For the purposes of sizing the pump, the pressure drop due to friction in each of the units downstream of the pump is estimated to be as follows:

heat exchanger	22 *psi*
filtration sequence	260 *psi*

9. The separation system uses a complex scheme of multiple steps For this preliminary design, simply represent the separation system by a box labeled "Separation System."
10. The cost of the separation system can be approximated as $2.9 million (delivered price).
11. The following market costs/values apply:

Salicylic acid	$\$1.33/lb_m$
Acetic anhydride	$\$0.49/lb_m$
Phosphoric acid	$\$0.34/lb_m$
Ultrapure water	$\$0.03/lb_m$
Acetylsalicylic acid (aspirin)	$\$3.97/lb_m$
Acetic acid byproduct stream	$\$0.013/lb_m$

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12. The following utility costs apply:

cooling water	\$0.03/1000 gal
electricity	\$0.05/kW-hr

13. The total operating cost per year can be estimated as 1.55 times the sum of the feed cost, cooling water costs, and electricity costs (excluding the filtration sequence, for which these values are not known). In other words,

$$\textit{Operating cost} = 1.55\ (\textit{Feed cost} + \textit{cooling water cost} + \textit{Electricity cost})$$

13. The direct capital costs for the reactor, heat exchangers, and pump can be estimated from the formulas in Table 13.2 and using the current value of the *M&S* Index.
14. The current tax rate is 35%; we are allowed to depreciate out equipment over 10 years; and our company requires a minimum *ROI* of 0.15. In our case, 85% of the capital investment can be depreciated.

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Assignment

1. Draw a PFD for the process.
2. Perform material balances on the process, one unit at a time, to determine the component flows for each stream.
3. Perform energy balances to determine the unknown temperatures of the streams and/or the heat duties for the heat exchangers and reactor.
4. Calculate the amount of steam and cooling water needed for the heat exchanger(s) and reactor(s).
5. Design the reactor(s) – determine the reactor volume(s) needed to achieve the specified conversion.
6. Determine the work required for the pump assuming that the pump is 85% efficient (only 85% of the energy added to the pump is transferred to the fluid).
7. Size all heat exchangers using approximate values of U_0 from Table 10.4.

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8. Complete a stream table showing, for each stream, the mass flow rates of all components, the temperature, and the pressure. The stream table would be as follows:

	Process Feed	Reactor Outlet	Mixer Outlet	Pump Outlet	Cooler Outlet	Separator Outlet	
						#1	#2
Flows (*kg*/*hr*)							
Salicylic Acid (liq)							
Acetic Anhydride							
Phsphoric Acid							
Acetylsalicylic Acid (liq)							
Acetic Acid							
Water							
Temp ($^{\circ}C$)							
Pressure (*kPa*)							

9. Complete an equipment specification list containing the following kinds of information:
   Pumps: For each pump, provide the required horsepower
   Heat exchanger: For each exchanger, provide the heat duty (*Btu*/*hr*), area, A_0 (ft^2), and required steam (lb_m/hr)or cooling water (lb_m/hr)
   Reactor: For each reactor, provide the volume (*liters*), heat duty for the heating/cooling jacket (*Btu*/*hr*), and required flow (lb_m/hr) of steam or cooling water for the jacket.
8. Determine the *ROI* for this project.
9. Suggest three ways to potentially improve the economics of this process. Explain why you believe your suggestions may make a significant improvement.