Heat Flow and Process Engineering Optimization

Background
As a research chemist working for the Bear Creek Chemical Company, Dr. Ann Sar-Key was experimenting with an allyamine, C₃H₅NH₂ (Molar mass 57.11 g/mol). One afternoon, the heating mantle controlling the temperature of the reaction unexpectedly rose 35°C, and overflowed the reaction vessel while Dr. Sar-Key was at lunch. The resulting polymer covered a plastic spoon that was nearby in the hood. After returning from lunch, she noticed that an accident occurred in the fume hood. Upon further investigation, Dr. Sar-Key observed that the spoon was covered in the polymer solution and was now much harder to bend than before. Upon further testing, the “accident” produced a coating that increased the strength of a plastic material by over 4 times. “Eureka!” The coating and its properties were discussed with management and then described to the marketing department to sell. Within days of the launch of the coating, the demand by the “We Make Playgrounds” materials company was high and there was a need to upscale the reaction for production.

The reaction to make the coating is an exothermic polymerization reaction that required an aqueous (with water) solution of C₃H₅NH₂ catalyzed by the addition of 3.0M HCl and releases 75.0 kJ/mol of energy. Upon further study, the reaction had to occur at 90°C ± 5°C to produce the desired polymer needed in the coating. If the temperature is not kept within the range, the reaction will not have the activation energy needed to produce the polymer, or will cause the polymer to decompose. During a small scale reaction on the benchtop, the heat of the reaction did not increase the temperature of the reaction mixture to the point of denaturing the polymer. This is not the case in upscaling the reaction. Careful planning must be engineered to properly manufacture the coating on a large scale. The heat generated during the reaction must be removed as the polymer is produced to keep the temperature of the reaction within the proper range.

Upon discussion with the manufacturing plant engineers, their largest concern was with the heat that was generated during the reaction and how to keep it from causing the temperature to go out of the acceptable reaction range and ruin the product. There are three areas of concern:

1. The large scale heat of reaction.
2. The heat gained by the reaction vessel from the reaction.
3. The cooling material used in the heat sink to remove the heat from the reaction vessel.

Your task is to examine 1 of these areas, calculate the necessary information and make an informed choice as to which material you should use to answer your task. In the end, the three independent groups will come together, as a team, to discuss and confirm your choices.
Calculations

**Team #1: Heat of reaction and solution concentration calculations**
Given that the reaction generates 75 kJ/mol of heat, you have the option of making 500 L of 1.0M solution in a single batch or you can make 300 L of a 3.0M solution. Using the heat equation, \( q = mc\Delta T \), determine which reaction gives a more ideal temperature change. The specific heat of water is 4.18 J/g\(^0\text{C}\) = 4.18 kJ/kg\(^0\text{C}\)

Summary Questions

1. Describe the thinking process of your group, given your task. How did you decide what would be the best solution to your problem? What factors did your group members consider when determining your answer?

2. When you got together with other groups to determine the total plan for the upscale problem, what materials did you decide to use? Describe how the heat flows through each step of the process.

3. Would the most efficient answer change with a different temperature change of the reaction?

4. Would the most efficient answer change with a different temperature change of the coolant?

Conclusion
This activity made a couple of assumptions that are unrealistic to an industrial process. One is that the heat transfer is instantaneous, when in real life, heat transfer takes time. Describe how your answers to each part of the process would be different if you were to factor in the amount of time it takes for heat to transfer from one aspect of the process to another. Be sure to address each part of the process, including the reaction, the reaction vessel, and the heat sink. What physical characteristics affect the rate of heat flow from one material to another?
Calculations

**Team #2 Heat transfer from the reaction solution to the reactor vessel**

Assuming that 37,500 kJ of heat is released from the reaction to the reaction vessel, select the best material for the reaction vessel (steel or glass). Describe which reaction vessel material would be a better choice and be sure to justify why, including a description of how the heat is flowing in the reaction. Use the equation, \( q = mC\Delta T \), solving for the change in temperature of the reaction vessel.

<table>
<thead>
<tr>
<th>Reaction Vessel Material</th>
<th>Specific Heat (kJ/kg(^0)C)</th>
<th>Mass of 500-L Vessel (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel</td>
<td>0.490</td>
<td>23,000</td>
</tr>
<tr>
<td>Pyrex Glass</td>
<td>0.753</td>
<td>6400</td>
</tr>
</tbody>
</table>

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Team #3 Heat absorption of a coolant
Select the most efficient coolant to cool the reaction vessel from part #2. Typically coolant flows through pipes that are coiled around the reaction vessel. The goal of this part is to remove as much heat with the least amount of coolant. This will minimize the coolant flow rate required through the coolant pipes.

There are three choices of coolants:

<table>
<thead>
<tr>
<th>COOLANT</th>
<th>SPECIFIC HEAT (J/g °C)</th>
<th>DENSITY (g/ mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>4.184</td>
<td>1.0000</td>
</tr>
<tr>
<td>air</td>
<td>1.005</td>
<td>0.0013</td>
</tr>
<tr>
<td>1:1 propylene glycol: H2O</td>
<td>3.765</td>
<td>1.0030</td>
</tr>
</tbody>
</table>

Assume that the coolant begins at a temperature of 20°C and the maximum temperature for the coolant is 50°C. Also assume that the heat transfer occurs instantaneously and there are no calculations based on cooling time. You may select a temperature change within this range to make calculations of coolant mass. Calculate the mass of each coolant required to remove 37,500 kJ of heat from the walls of the reaction vessel. Calculate the volume of coolant required. Select the most efficient coolant and explain your selection based on your calculations. Would this selection change with a different temperature change?

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