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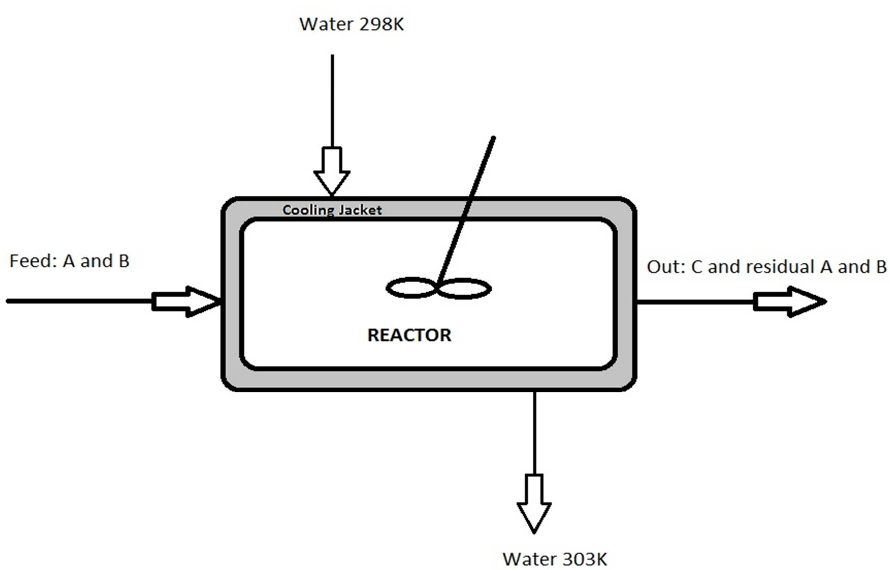
ME 575

Optimization of a Chemical Reactor

Problem Statement

A company has hired your optimization firm to design a new reactor which will maximize their profit. The Chemicals are proprietary, but referring to them as A, B and C, the company has given you enough information to do the job. Chemical A and B produce chemical C in the following reaction:

$$A + B \rightarrow C$$



A continuous-stirred tank reactor (CSTR) has a flow of A and B going into it to form C. The reactor is kept at a constant temperature by a cooling jacket surrounding the reactor. The profitability of this design is based on how pure the C is coming from the reactor. To maximize profit you need to provide the optimal **reactor volume, reactor temperature, mass flow of water through the cooling jacket, and feed rate of compounds A and B.**

Modeling

The Reaction

The reaction rate is based on temperature based on the Arrhenius equation.

$$k = A \exp(-E/R*T) \quad (1)$$

Where A is a pre-exponential factor, E is the activation energy, R is the gas constant, and T is the reactor temperature in K. The k from the Arrhenius equation the then plugged into the rate law that determines the rate of the reactions. The rate for this reaction is:

$$rA = -k* CA0*(1-XA) * (CB0 – CA0 * XA) \quad (2)$$

In units of mols/(Liter*min). Where k is the rate of the reaction, CA0 is the initial concentration of A, XA is the conversion of A, and CB0 is the initial concentration of B.

The temperature of the reactor is determined by the heat of the inlet stream and has an associated cost to increase it. The products must also be cooled soon after the reaction and there is a cost associated with the cooling as well. Remember that concentration is in units of moles per volume so you will have to determine a feed stream flow rate as well.

The volume of the reactor is based on the design equation for a CSTR:

$$Vr = -Fao * XA / rA / 1000 \quad (3)$$

In units of m^3, where Fao is the initial molar flow of A (mol/min).

The Cooling Jacket

The temperature of the cooling water will enter at 25^oC and the temperature of the water leaving the cooling jacket is set at 30^oC due to environmental regulations so the cooling water flow rate must be found to keep the reactor temperature constant.

The reaction produces 208.95 kJ/mol of A reacting. This is known as the heat of reaction. That much heat must be removed to keep the reaction at a constant temperature as seen in the equation:

$$Q = rA * Vr * H \quad (4)$$

Where Q is the heat to be removed from the reactor, rA is the reaction rate, Vr is the volume of the reactor in m^3 and H is the heat of reaction. The area of the heat exchanger can be calculated by

$$Q=U*A*\Delta T \quad (5)$$

Where Q is the overall heat transferred, U is the overall heat transfer coefficient, A is the area of the cooling jacket and ΔT is the log mean temperature difference:

$$\Delta T=((Th2 - Tc2)-(Th1-Tc2))/\ln((Th2 - Tc2)/(Th1-Tc2)) \qquad (6)$$

This is very similar to what was done for the heat pump assignment so look on the course website for additional help.

Finances

The cost operating costs as well as the profit should take into account the present value similar to the in class discussion. The worksheet with the equations is available on the class website.

<u>Data</u>
Pre-exponential factor for the reaction is **377.359 (L/mol*min)**
Activation energy for the reaction is **11237 (cal/mol)**
The gas constant is **1.986 (cal/mol*K)**
Cooling water enters the cooling jacket at **298K** and exits at **303K**
The U value of the cooling jacket is **500 J/(min*m^2*K)**
Cost per area of the cooling jacket is **$200/$m^2$**
The cost of A is **$2/mol** and B is **$1/mol**
The reactor costs **$1000/(Liter^2)** to construct
The product can be sold for $**130 for every 10% conversion**
The cost to increase the feed stream temperature is **$1/(K*L/min)**
The cost to decrease the outlet stream temperature is **$1/(K*L/min)**
The process runs for **12 hours/day**
The economic life of the process is **8 years**
The interest rate is **5%**

<u>Report</u>

For this problem, provide an executive summary of main optimization results (include values for design variables and objective and indicate which constraints are binding) for the two cases. Include analysis to show that the solution is at an optimal solution. Some of things that you may want to include are:

1) A table including the optimal solution values

2) A contour plot of the design space showing the objective and constraints as a function of reactor temperature and conversion with the feasible region shaded and optimum marked

3) A discussion of any observations or comments about the model, process of optimization or the design space. Do you feel this is a global optimum?

4) Appendix: listing of your model file