A First Course on Kinetics and Reaction Engineering

Example 20.2

Problem Purpose

This example illustrates the optimization of a batch reactor operating protocol for a simple situation.

Problem Statement

Consider the batch reactor process described in Example 20.1. What coolant flow rate in step 2 will maximize the net rate of production of B?

Problem Solution

The models for each of the two processing steps are the same as in Example 20.1. However, in this problem, we want to choose a value for the coolant flow rate in the second processing step that results in the maximum net rate of production of B. There are a few ways to do this; here I simply evaluated the models from example 20.1 using different coolant flow rates. I then plotted the net rate of production of B versus the coolant flow rate, as shown in Figure 1.
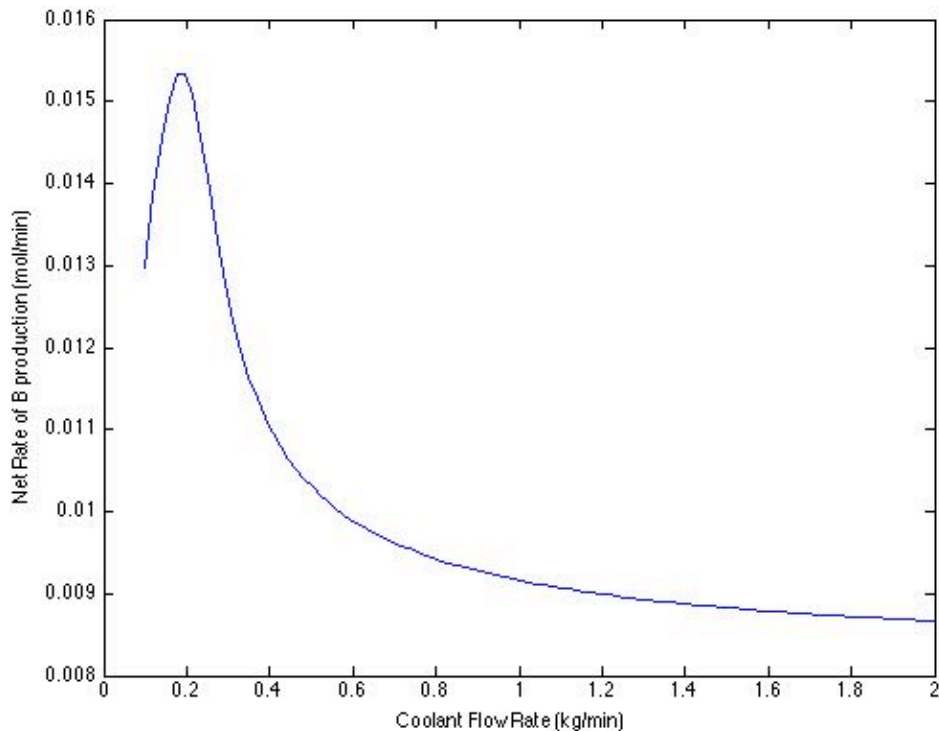

Figure 1. Net rate of production of B as a function of the coolant flow rate in the second processing step.

The figure shows that the net rate of production of B reaches a maximum value of ca. 0.015 mol min^{-1} at a coolant flow rate of ca. 0.2 kg min^{-1}. When that coolant flow rate is used, the reaction volume reaches a maximum temperature of ca. 81ºC during the second processing step. It is interesting to consider the reason for the maximum seen in Figure 1. In the second processing step, varying the cooling rate will have two effects. First, for lower coolant flow rates, the temperature will rise faster and reach a higher maximum value. This is good, in that the product B will be produced at a faster rate and therefore in greater quantity. It is bad, however, because it will take longer to cool the reaction volume down to 25 ºC after the temperature has reached its maximum. During the cooling phase, the rate is decreasing both because the amount of reactant is decreasing and because the temperature is decreasing, so relatively little B is being produced, but the processing time is increasing. In contrast, at high coolant flow rates, this cooling phase is much faster, but the maximum reaction temperature is not as large, and consequently less B is produced in the early part of the step. Hence, there is a maximum in the net rate of production of B.

Calculation Details Using MATLAB

The code used to model the first step in the protocol is exactly the same as the code used in Example 20.1, except the code to generate the plots was removed. The plotting code was also removed from the code for modeling the second processing step. Two additional modifications were made to the code for modeling the second processing step. First, the code was changed so that the coolant flow rate is passed in as an argument instead of being entered within the code as a constant. Doing this makes it easier to make repeated runs with different coolant flow rates. The second modification wasn't required, but I decided to enter some code to determine the maximum temperature reached during this processing step and return it along with the final elapsed time and dependent variable values.

As in Example 20.1, a third function was written to integrate the models for the two steps. It begins by declaring variables to hold the data for plotting and the coolant flow and net rate of production of B at the maximum. A range of coolant flow rates is then divided into 100 equally spaced points, and the model equations are solved for each flow rate. The net rate is then computed for each flow rate, and if the rate represents a new maximum it is saved along with the corresponding coolant flow and the maximum temperature during the step. Once this has been done for all of the flow rates, the maximum net production rate is displayed along with the corresponding coolant flow and maximum temperature. Finally, the plot shown as Figure 1 is generated. The code is shown in Listing 5. When it is run, it generates the plot and produces the output shown in Listing 6.

```
% Function to solve the design equations for Example 20.2 from "A First
% Course on Kinetics and Reaction Engineering" for both steps of the
% operating protocol
function Example_20_2
    % Define variables for plotting
    m = linspace(0.1,2.0);
    r_net = zeros(100,1);
    mmax = 0;
    rmax = 0;
    Tmax = 0;

    % Calculate the net rate for each coolant flow rate
    for i=1:100
        [tf1,zf1] = Example_20_2_a;
        [tf2,zf2,Tm] = Example_20_2_b(m(i),zf1);
        r_net(i) = zf2(2)/4/(tf1 + tf2 + 25);
        if(r_net(i) > rmax)
            rmax = r_net(i);
            mmax = m(i);
            Tmax = Tm;
        end
    end

    % Report optimum flow rate
    display(['Optimum coolant flow (kg/min): ',num2str(mmax)])

    % Report maximum rate
    display(['Maximum net rate of B production (mol/L/min):
        ',num2str(rmax)])

    % Report maximum reaction temperature
    display(['Maximum reaction temperature (deg C) at optimum flow:
        ',num2str(Tmax-273.15)])

    % Plot the results
    figure
    plot(m,r_net)
    xlabel('Coolant Flow Rate (kg/min)')
    ylabel('Net Rate of B production (mol/min)')

end % of Example_20_2
```

Listing 5. Contents of the function Example_20_2.

```
>> Example_20_2
Optimum coolant flow (kg/min): 0.19596
Maximum net rate of B production (mol/min): 0.015341
Maximum reaction temperature (deg C) at optimum flow: 81.1642
```

Listing 6. Output from the execution of Example_20_2.