Project 9 Solutions

In this project, we will solve a simple unconstrained optimization problem for a CSTR involving multiple reactions. Setting up the system of equations for the reaction network, we obtain:

$$Q \cdot (C_A - C_{Ao}) + V \cdot (k_1 C_A C_B) = 0$$

$$Q \cdot (C_B - C_{Bo}) + V \cdot (k_1 C_A C_B + k_1 C_B C_C) = 0$$

$$Q \cdot C_C - V \cdot (k_1 C_A C_B - k_2 C_B C_C) = 0$$

$$Q \cdot C_D = V \cdot k_2 C_B C_C$$

One way to simplify the type of system that we feed into the solver is by rendering all equations dimensionless. In this step, we perform the following substitution to remove all units from the equations

$C_i^* = \frac{C_i}{C_{Ao}}$, $k_1^* = \frac{k_1 C_{Ao} V}{Q}$ $k_2^* = \frac{k_2 C_{Ao} V}{Q}$ and $C_{Bo}^* = \frac{C_{Bo}}{C_{Ao}}$

The resulting system of equations is

$$C_A^* + k_1^* C_A^* C_B^* - 1 = 0$$

$$C_B^* + k_1^* C_A^* C_B^* + k_2^* C_B^* C_C^* - C_{Bo}^* = 0$$

$$C_C^* - k_1^* C_A^* C_B^* + k_2^* C_B^* C_C^* = 0$$

$$C_D^* = k_2^* C_B^* C_C^*$$

One interesting aspect to notice is that the equation for concentration of D is explicit for the concentrations of B and C; thus, it does not need to be incorporated into the system of equations that we will solve.

Contents

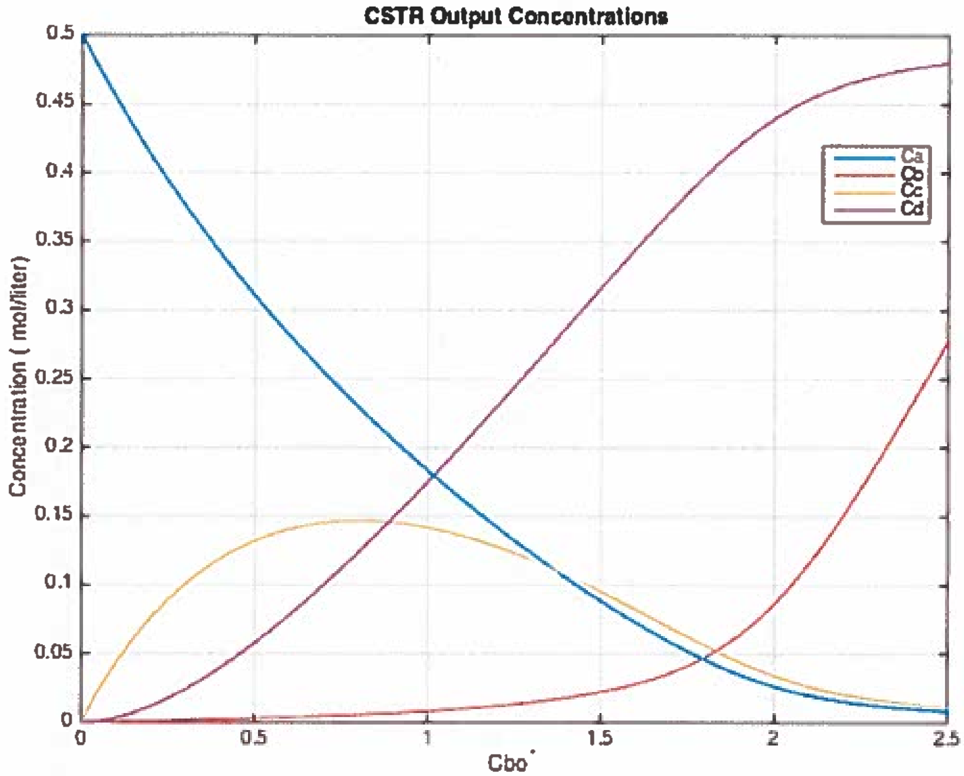
Part 1. Specify the parameters for the problem.

```
% We start by defining all of the relevant constants to be used later on
% in the problem, including the dimensionless variables.
clear
clc

% Initial volume and flowrate
V = 1000; % [L]
Q = 0.1; % [L/s]

% Reaction rate constants
k1 = 0.021; % [L/mol s]
k2 = 0.015; % [L/mol s]
```

```
% Initial concentration of A.
Cao = 0.5; % [mol/L]

% Dimensionless constants.
k1_d = (k1 * Cao * V)/Q;
k2_d = (k2 * Cao * V)/Q;
```

Part 2. Plot the concentrations for different feed rates for B.

```
% In this step, we specify the dimensionalized system of equations. In this
% part, we specify a range of values for the feed rate of B in order to
% generate a plot containing the concentration of all species.
Eqns_d = @(x,Cbo_d) [ x(1) + k1_d * x(1) * x(2) - 1; ...
                    x(2) + k1_d * x(1) * x(2) + k2_d * x(2) * x(3) - Cbo_d; ...
                    x(3) - k1_d * x(1) * x(2) + k2_d * x(2) * x(3)];

% Sepcify a vector for dimensionless Cbo.
Cbo_d = 0:0.05:2.5;

% Initial guess and solver options.
options = optimoptions('fsolve','Display','off');
xguess = 0.25 * ones(1,3);

% Construct a for loop to specify concentrations for different feed
% concentrations of B.
for i = 1 : length(Cbo_d)
    x_plot = fsolve(@(x) Eqns_d(x,Cbo_d(i)), xguess, options);
    Call(:,i) = [x_plot, k2_d * x_plot(2) * x_plot(3)];
end

% Plot the results.
figure(1)
plot(Cbo_d,Call*Cao)
xlabel('Cbo^{*}')
ylabel('Concentration ( mol/liter)')
legend('Ca','Cb','Cc','Cd','location','best')
title('CSTR Output Concentrations')
grid on
```

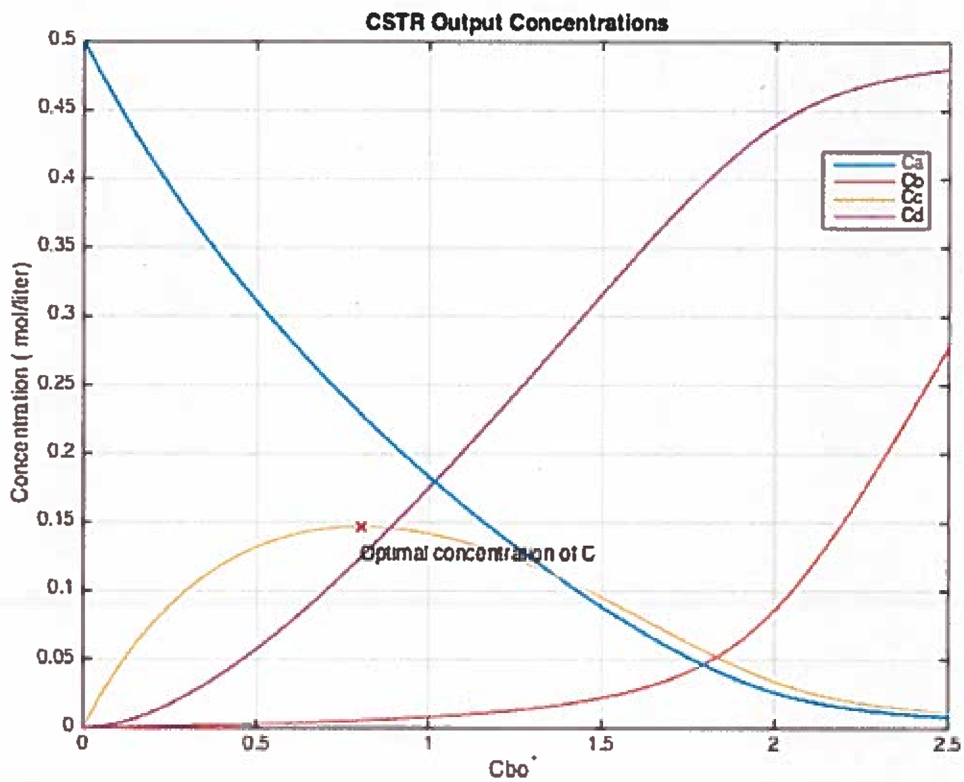


Part 3. Solve for optimal initial concentration of C.

```
% Call the optimization solver to handle the problem. The objective
% function in this case will be to maximize the concentration of C. The
% initial guesses are selected such that they scale with the rest of the
% variables.
x0 = 0.25;
options = optimset('Display','off');
xopt = fminsearch(@(Cbo_d) Objective(Cbo_d,Eqns_d), x0 , options);

% Now, let's substitute the optimal answer for Cbo into the original
% problem and see what the concentrations look like.
x_final = fsolve(@(x) Eqns_d(x,xopt), xguess, options);

% Calculate nondimensional concentrations.
C_nd = Cao * x_final;

% Finally, we display all results and update the graph to indicate where
% the optimum concentration of C was found.
format short e

disp(['The optimal value for Cbo is ', num2str(xopt*Cao)])
disp('     ')

disp('The optimal concentrations for each species are ')
table = str2mat('Ca ', 'Cb ', 'Cc ', 'Cd  ');
table = [table,str2mat(num2str(C_nd(1)),num2str(C_nd(2)),num2str(C_nd(3)), num2str((V*k2*C_nd(2
disp(table)
```

```
figure(1)
hold on
plot(xopt,C_nd(3),'xr')
hold off
text(xopt,0.85*C_nd(3),'Optimal concentration of C')
```

```
The optimal value for Cbo is 0.40073

The optimal concentrations for each species are
Ca   0.22902
Cb   0.0056343
Cc   0.14686
Cd   0.12412
```



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```
function f = Objective(Cbo_d, Eqns_d)
% In this project, we will learn how to formulate an objective function.
% These functions are used in practice to specify optimization objectives,
% such as maximizing a certain desired quantity.

% The first part will be to solve the problem and find concentrations for
% all the desired species given a value of Cbo using fsolve.
options = optimoptions('fsolve','Display','off');
xguess = 0.25 * ones(1,3);
x_obj = fsolve(@(x) Eqns_d(x,Cbo_d), xguess, options);

% Our objective will be to maximize the amount of Cbo.
f = - x_obj(3);
```