Continuously Stirred Tank Reactor, part 3

The dimensionless model

$$x' = -x + \mathrm{Da}(1-x)e^{\frac{\beta x}{1+\delta x}}, \qquad x(0) = 0, \tag{1}$$

is widely applicable to continuously stirred tank reactors whenever the chemical reaction rate is simply proportional to the concentration of one of the reactants. The parameter δ is often small, so for now we consider only the problem

$$x' = -x + \mathrm{Da}(1-x)e^{\beta x}, \qquad x(0) = 0. \tag{2}$$

In principle, this first-order initial value problem can be studied by a combination of graphical, analytical, and numerical methods. Analytical methods are problematic. The differential equation is separable, but solving it results in an implicit solution formula involving a definite integral. This solution would have to be evaluated numerically in order to get a graph, but this would be far more difficult than just using a numerical method to solve the original differential equation.

The qualitative analysis is the focus of part 3, and the numerical analysis will be part 4.

Qualitative Analysis

We expect to run a continuously-stirred tank reactor for a long time, so the primary interest in the model is to determine equilibrium solutions and their stability. The problem has two parameters, which means that a thorough analysis would be a lot of work. We can do an interesting analysis by choosing $\beta = 5$ as a typical value (representing a chemical reaction that releases a large amount of heat) and studying the effect of the Damkohler number on the behavior of the system.

The equilibrium equation cannot be solved for the equilibrium x^*, but it can easily be solved for Da as a function of x^*. This formula can then be used to make a graph that shows how the equilibrium values depend on Da, using Da on the horizontal axis and x^* on the vertical axis. Your graph should show that there are three ranges for Da that correspond to different numbers of equilibria. The graph should show that the values 0.10, 0.08, and 0.06 can be used to illustrate the high, medium, and low cases.

Do an equilibrium stability analysis for each of the three illustrative values of Da. Display the results of the analysis using Matlab graphics. You can use the subplot command to make a single figure with four graphs, arranged in two rows and two columns. For the first graph, plot the equilibrium solutions as a function of Da. Use the range $0 \le \mathrm{Da} \le 0.2$ for a nice-looking graph. Add dashed vertical lines at the values used for the phase line plots to provide simple visual identification of the approximate equilibrium reaction progress values. The other three graphs should be plots of dx/dt as a function of x, each labeled with the corresponding value of Da. Add dashed lines for the x axis so that it is easy to see the equilibria and determine the direction of the phase line arrows. You don't actually need to plot the phase line; simply use the x' vs x plots to identify which equilibria are stable.

In your discussion of the results, focus on the question of which Da values make for a good reactor design. You will have to think about whether an intermediate value like $\mathrm{Da} = 0.08$ is good or not. Also explain the connection with the flow rate, which is the actual parameter the engineer can control. (Refer back to the original model derivation.) Use the equilibrium analysis to explain what happens if the flow rate is too large. You will need a different line of thought to explain what happens if the flow rate is too small. For this, think about the purpose of the chemical reactor and how you would use the original dimensional equation to determine the efficiency of the reactor.