

- 3) (25 pts) A continuous stir tank reactor (CSTR) is used to produce a product **P** from chemicals **A** and **B**. The reaction is $\mathbf{A} + \mathbf{B} \rightarrow \mathbf{P}$. **A** is in excess and the rate of decomposition of **B** is given by:

$$r_b = \frac{k_1 x_2}{(1 + k_2 x_2)^2}$$

where k_1 and k_2 are constants and x_2 is the product concentration.

The equations describing the system are given by:

$$\begin{aligned} \frac{dx_1}{dt} &= u_1 + u_2 - 0.2\sqrt{x_1} \\ \frac{dx_2}{dt} &= (C_{b1} - x_2) \frac{u_1}{x_1} + (C_{b2} - x_2) \frac{u_2}{x_1} - \frac{k_1 x_2}{(1 + k_2 x_2)^2} \end{aligned}$$

The parameters are: $C_{b1} = 24.9$, $C_{b2} = 0.1$, $k_1 = k_2 = 1$, and $u_1 = u_2 = 1$.

The initial conditions are: $x_1(0) = 10$ and $x_2(0) = 0$.

- First, simulate the equation for x_1 only since it does not depend on x_2 . Note the steady-state value that you find for x_1 .
- In the model for x_2 , initialize the integrator for x_1 to the steady-state value you found in part (a) and initialize $x_2(0) = 0$. Run the simulation for 1000 seconds to determine $x_2(t)$ and the steady-state value of x_2 .
- Repeat the simulation for x_2 using an initial value $x_2(0) = 10$. Note the new steady-state value you find for x_2 .
- Both of the previous cases are stable. There is another steady state corresponding to everything else being the same and the steady states for x_2 and x_1 being $x_2 = 2.793$ and $x_1 = 100$. This is an unstable steady state. Demonstrate this by setting the initial value of the integrator for x_2 to $x_2(0) = 2.80$ and show that the simulation goes to the upper steady-state value. Repeat the simulation with $x_2(0) = 2.79$ and show that it goes to the lower steady-state value. This means that any small fluctuation will cause the system to fall to steady state of part (b) or rise to the steady state of part (c).
- Demonstrate that the steady state with $x_2 = 2.793$ is unstable by linearizing the equation for x_2 about the steady-state values and showing that the linear system that results is unstable. You can do this by either solving the differential equation or by simulating the system with a small initial Δx_2 .