

Dynamic Optimization of a Catalyzed Reaction

The objective is to maximize the amount of **C** (or x_3) at the final time by adjusting the mixture of catalysts (u). The reactor is full of species **A** initially and proceeds until $t_f = 4$. The reactions include a reversible step from species **A** to intermediate species **B**, dependent on fraction of catalyst 1 and an irreversible step from **B** to **C**, dependent on the fraction of catalyst 2. The value of u is the fraction of catalyst 1 and $(1-u)$ is the fraction of catalyst 2.

$$\max_u x_3(t_f)$$

$$\text{s. t. } \frac{dx_1(t)}{dt} = -u (k_1 x_1(t) - k_2 x_2(t))$$

$$\frac{dx_2(t)}{dt} = u (k_1 x_1(t) - k_2 x_2(t)) - (1-u) k_3 x_2(t)$$

$$x_3(t) = 1 - x_1(t) - x_2(t)$$

$$x(0) = [1, 0]$$

$$0 \leq u(t) \leq 1$$

$$k_1 = 1, k_2 = 10, k_3 = 1$$