# REB, The Course
# Class 13 Learning Activity Solution

Cells are growing in an isothermal, steady-state CSTR. The effective reaction, in mass units, is given in equation (1). The reaction is auto-catalytic, and the rate is accurately described by the Monod equation, equation (2), with $V_{max}$ equal to 0.014 min$^{-1}$ and $K_m$ equal to 0.001 g cm$^{-3}$. Through an appropriate startup process, the 4.43 L reactor can operate at steady-state with no cell mass in the feed. Specifically, if 60 cm$^3$ min$^{-1}$ of feed containing only substrate at a concentration of 0.04 g cm$^{-3}$, the steady-state product stream contains substrate at a concentration of 2.97 x 10$^{-2}$ g cm$^{-3}$ and cell mass at at concentration of 4.68 x 10$^{-3}$ g cm$^{-3}$. However, reactor operation is parametrically sensitive to the volumetric flow rate. Show that to be true by calculating the transient outlet concentration of cell mass as a function of time if the inlet volumetric flow rate changes from 60 to 61 cm$^3$ min$^{-1}$.

$$2.2\,S \rightarrow X \tag{1}$$

$$r_1 = \frac{V_{max} C_S C_X}{K_m + C_S} \tag{2}$$

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***Assignment Summary***

<u>Reaction</u>

$$2.2\,S \rightarrow X \tag{1}$$

<u>Rate Expressions</u>

$$r_1 = \frac{V_{max} C_S C_X}{K_m + C_S} \tag{2}$$

<u>Reactor</u>: Liquid-phase, isothermal, transient

Given Constants: $V_{max}$ = 0.014 min$^{-1}$, $K_m$ = 0.001 g cm$^{-3}$, $V$ = 4.43 L, $\dot{V}_{in}$ = 61 cm$^3$ min$^{-1}$, $C_{S,in}$ = 0.04 g cm$^{-3}$, $C_{X,in}$ = 0 g cm$^{-3}$, $C_{S,0}$ = 2.97 x 10$^{-2}$ g cm$^{-3}$ , and $C_{X,0}$ = 4.68 x 10$^{-3}$ g cm$^{-3}$.

Deliverables: $\underline{C_X}$ vs. $\underline{t}$ as a graph

***Formulation of the Equations***

Reactor Model Equations:

$$\frac{d\dot{m}_S}{dt} = \frac{\dot{V}}{V}\left(\dot{m}_{S,in} - \dot{m}_S - 2.2Vr_1\right) \tag{3}$$

$$\frac{d\dot{m}_X}{dt} = \frac{\dot{V}}{V}\left(\dot{m}_{X,in} - \dot{m}_X + Vr_1\right) \tag{4}$$

Reactor Model Variables: $\underline{t}$, $\underline{\dot{m}}_S$, and $\underline{\dot{m}}_X$

Additional Computable Unknowns: $\dot{V}$, $\dot{m}_{S,in}$, $r_1$, $C_S$, $C_X$, and $\dot{m}_{X,in}$

$$\dot{V} = \dot{V}_{in} \tag{5}$$

$$\dot{m}_{i,in} = \dot{V}_{in}C_{i,in} \quad i = S \text{ and } X \tag{6}$$

$$C_i = \frac{\dot{m}_i}{\dot{V}} \quad i = S \text{ and } X \tag{7}$$

IVODE Solver Inputs:

1. Initial values of the reactor model variables shown in Table 1.
2. Stopping criterion that $t$ equals the final value shown in Tables 1.
3. Derivatives function that
    a. receives values of $t$, $\dot{m}_S$, and $\dot{m}_X$ at the start of an integration step
    b. returns the corresponding values of the reactor model derivatives

Table 1. Initial and final values of the design equation variables.

| Variable | Initial Value | Final Value |
|---|---|---|
| $t$ | 0 | $t_f$ = 60 min |
| $\dot{m}_S$ | $\dot{m}_{S,0} = \dot{V}C_{S,0}$ | |
| $\dot{m}_X$ | $\dot{m}_{X,0} = \dot{V}C_{X,0}$ | |

<u>Deliverables Equations</u>:

$$\underline{C}_X = \frac{\dot{m}_X}{\dot{V}} \tag{8}$$

### ***Implementation of the Calculations***

The Python script, activity_13.py, that was written to perform the calculations accompanies this solution.

### ***Results and Discussion***

The calculations were performed as described above. The final time, $t_f$, was adjusted so that the transient filled the graph. The results are shown in Figure 1.

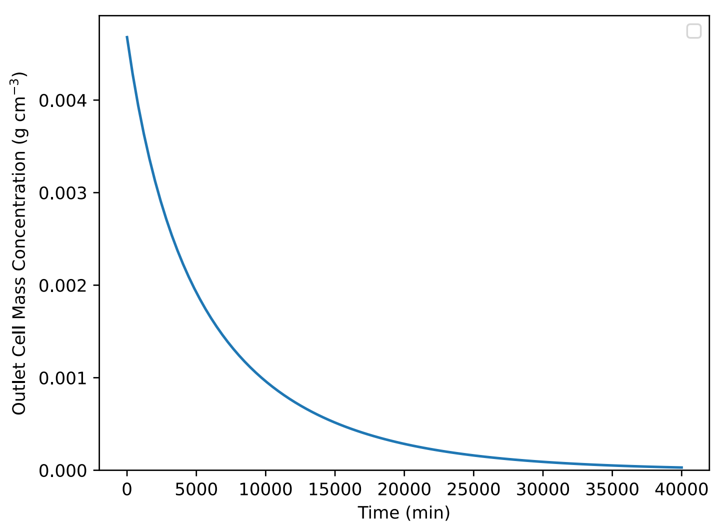


*Figure 1. Cell mass washout upon changing the feed rate from 60 to 61 cm$^3$ min$^{-1}$*

Cell growth is like an autocatalytic chemical reaction, the rate increases when the product concentration (in this case, cell mass) increases. It differs in that most autocatalytic chemical reactions have a small rate when no product is present. In contrast, cells can't grow if there aren't any present.

Indeed, a well-designed startup procedure would be needed to reach the initial steady state in this system. There is no cell mass in the feed. As a result of the startup procedure, the rate of cell mass production within the reactor exactly matches the rate at which cell mass is leaving the reactor.

This can result in a situation with extreme parametric sensitivity. Specifically, If the flow rate through the reactor is increased such that the cell mass leaves the reactor faster than it is generated within it, all of the cell mass eventually will be swept out of the reactor. This phenomenon, sometimes referred to as washout, is illustrated in this example. This reactor was producing cell mass at a steady state, until a small increase in flow rate caused all of the cell mass to be washed out of the reactor.

### ***Deliverables***

The initial steady state was parametrically sensitive to the volumetric flow rate, and when it was increased by less than 2%, from 60 to 61 $cm^3$ $min^{-1}$, the reactor contents were washed out.