Computer Lab – Optimization of Temperature in Enzymatic Reactors (Batch & Chemostat)

Background
The enzymatic hydrolysis of lactose in milk can be carried out in an isothermal batch reactor or an isothermal CSTR to provide milk to lactose intolerant individuals. The enzyme lactase for this reaction is competitively inhibited by one of the two products, galactose. Lactose is a disaccharide with one galactose sugar molecule bound to one glucose sugar molecule. The lactase catalyzed reaction is

\[
\text{LACTOSE} + \text{H}_2\text{O} \rightarrow \text{GALACTOSE} + \text{GLUCOSE}
\]

The inhibition constant, \(K_i\) for galactose has the same value as the Michaelis-Menten constant, \(K_m\).

The rate expression for this reaction is thus given by,

\[
\frac{d[P]}{dt} = \frac{V_m [S]}{K_m \left(1 + \frac{[I]}{K_i} \right) + [S]} = \frac{k_2 [E]_0 [S]}{K_m \left(1 + \frac{[I]}{K_i} \right) + [S]} = \frac{k_2 [E]_0 [S]}{K_m + [I] + [S]}
\]

where the initial condition (for a batch reactor) or inlet condition (for a CSTR) of the enzyme concentration are such that,

\[
k_2 [E]_0 = 2.71 \times 10^6 \, e^{-5630/T}
\]

\[
K_m = 2.77 \times 10^2 \, e^{-3210/T}
\]

in units of gmol/L·h with \(T\) in Kelvin.

You should also consider enzyme degradation. The enzyme degradation with time is described by

\[
E_0 (T, t) = [E]_0 \, e^{-k_d t}
\]

\[
k_d = 6.14 \times 10^{20} \, e^{-15923/T}
\]

where concentrations are in units of gmol/L and \(k_d\) in units of h⁻¹.
Computer Simulation Assignment

A. Create a computer model, using modeling software of your choice and that is available in the department’s computer lab, to determine the optimal constant temperature (°C) of operation for a batch reactor that will hydrolyze 90% of the lactose in milk with an initial concentration of 0.1 g.mol/L. What is the needed reaction time for this batch reactor operating at this optimal temperature?

B. For the optimal temperature determined in part A, show a plot of percent lactose hydrolyzed as a function of time.

C. Repeat parts A and B for 80% hydrolysis of lactose.

D. Consider the steady-state operation of a chemostat (CSTR) with continuous feed of milk having a lactose concentration that is the same as analyzed in the batch reactor model. 80% of the lactose is to be hydrolyzed in the chemostat. The deactivation time for the enzyme in the chemostat feed stream may be considered to be the residence time in the chemostat. 100 L of milk are to be treated per hour. What is the optimal temperature (°C) and needed volume (liters) of the reactor?

Note – you will need to consider material balances for enzymatic reactions in both the batch reactor and CSTR. This involves the solution of simultaneous ordinary differential equations and solution of a nonlinear algebraic equation with optimization.

Prepare a summary report (brief Technical Memorandum format) of your results. In your report, include the plots or other appropriate model results, and include portions of the model as needed to support the analyses. Answer questions that are asked in parts A through D and discuss any unusual modeling requirements in order to solve this problem. The report is to focus on the results of your analysis – you may repeat the equations given here & show the development of the system of equations but do so in the Appendix.