Scilab for Chemical Engineers

TSEC - Online Certificate Course

CLASS PROJECT 1

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1 Ethanol Conversion Kinetics

Let's consider a CSTR where ethanol is produced through the fermentation of glucose by yeast. The main reaction can be written as:

$$\text{Glucose} \rightarrow \text{Ethanol} + CO_2$$

Let's denote:

- C_S: Concentration of glucose (substrate) (g/L)
- C_X: Concentration of biomass (yeast) (g/L)
- C_E: Concentration of ethanol (product) (g/L)
- F: Volumetric flow rate into and out of the reactor = 1 L/h
- V: Volume of the reactor = 10 L
- k: Reaction rate constant
- μ: Specific growth rate of yeast
- Y_{XS}: Yield coefficient for biomass from the substrate = 0.5
- Y_{XE}: Yield coefficient for ethanol from biomass = 0.1

Material Balance for Substrate (Glucose):

$$\frac{dC_S}{dt} = \frac{F(C_{S0} - C_S)}{V} - \mu \frac{C_X}{Y_{XS}}$$

Where C_{S0} is the inlet concentration of glucose.
Material Balance for Biomass (Yeast):

$$\frac{dC_X}{dt} = \frac{F(C_{X0} - C_X)}{V} + \mu C_X$$

Where C_{X0} is the inlet concentration of yeast (typically zero).
Material Balance for Ethanol (Product):

$$\frac{dC_E}{dt} = \frac{F(C_{E0} - C_E)}{V} + \mu \frac{C_X}{Y_{XE}}$$

Where C_{E0} is the inlet concentration of ethanol (typically zero).
The specific growth rate of yeast, μ, can be modeled as:

$$\mu = \frac{\mu_{max} C_S}{K_S + C_S}$$

Where: μ_{max} is the maximum specific growth rate = 0.4 h^{-1}. and K_S is the half-saturation constant = 1.
These differential equations describe the dynamic behavior of substrate, biomass, and ethanol concentrations within the CSTR. By solving these equations, we can predict the performance of the reactor under various operating conditions.

2 Ethanol Manufacturing

In the process of producing ethanol from glucose, glucose is first fermented in a Continuous Stirred-Tank Reactor (CSTR) where it is converted to ethanol and carbon dioxide by yeast.

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2 \quad (1)$$

The conversion rate of glucose to ethanol is 80%. The product stream from the CSTR is sent to a distillation unit. In this unit, 60% of the ethanol produced is recycled back to the reactor, and the distillation bottoms, which contain yeast and unreacted glucose, are recycled into the fermenter. The initial feed contains 10 moles/hr of glucose. The goal is to model this process and calculate the amount of ethanol produced and the amount of glucose recycled in each step.