MATH1070

L5 Inhibitor Interactions

1

Euler's Method for solving ODEs

- This is the simplest approximation method.

http://www.physics.uq.edu.au/people/jones/ph362/cphys/node1.html

For $\frac{dy}{dt} = f(y)$; $\mathbf{y_{n+1} = y_n + hf(y_n)}$, where h is the step size.

Take the function $\frac{dy}{dt} = ky$

Its approximation is:

$$\frac{y_{i+1} - y_i}{dt} = ky_i$$

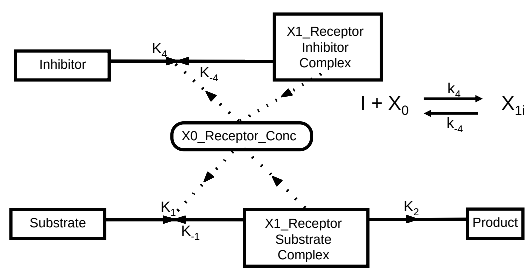
$$y_{i+1} - y_i = dt * ky_i$$

$$y_{i+1} = y_i + dt * ky_i$$

Effects of an inhibitor on enzyme kinetics

- An inhibitor may competitively bind with an enzyme required for a substrate.
- Under high concentrations of inhibitor and low concentrations of substrate (and limiting levels of enzyme) the conversion of substrate to product is very low.
- Competitive inhibition can be overcome at a sufficiently high substrate concentration.

Effects of an inhibitor

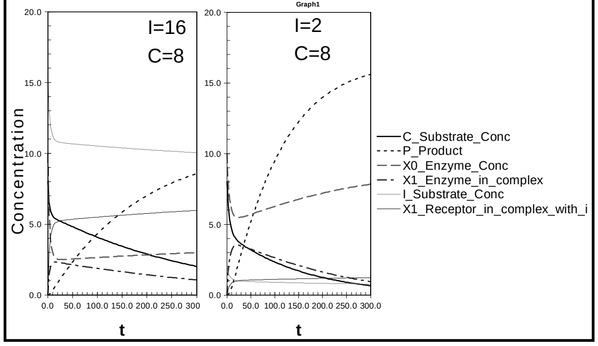


$$I + X_0 \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} X_{1i}$$

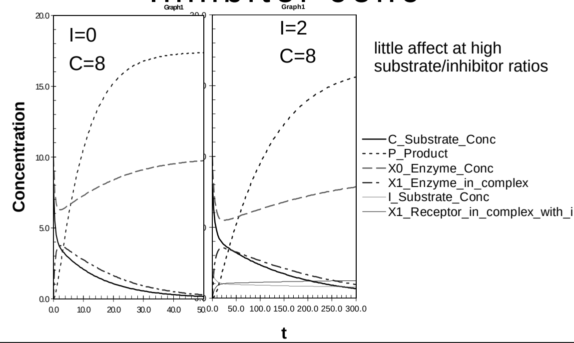
$$S + X_0 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} X_1 \xrightarrow{k_2} P + X_0$$

Your next assignment will have a question on this system

Inhibitor effect at high Inhibitor conc



Inhibitor effect at low Inhibitor conc



little affect at high substrate/inhibitor ratios

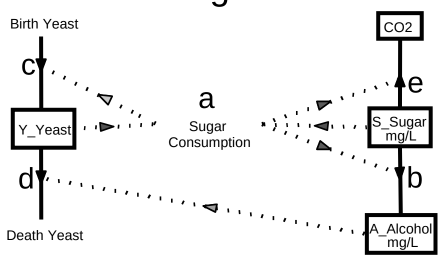
Beer Production

- An example that includes saturation and mass action.
- Simplification: brewing beer involves putting yeast and sugar in a vessel so that alcohol is produced as a by-product of the metabolism of yeast.
- FACTS:
  - There is a finite amount of sugar at the start.
  - Sugar enhances yeast formation through mass action with yeast but this causes sugar breakdown into fractions of alcohol and CO_2.
  - Excessive alcohol will kill yeast cells.

Beer Production

- Assumptions:
  - the rates of sugar consumption, CO_2 and alcohol production, and yeast mortality due to alcohol follow mass action laws.
  - rate of alcohol production is proportional to the rate of sugar consumption.

Beer Production Diagram



Solid lines represent flows; dashed lines represent influences

What parameters are required?

- a. Rate of sugar uptake & consumption by yeast
- b. Rate of alcohol produced from sugar consumption by yeast
- c. Rate of yeast cell formation per unit of sugar consumed
- d. Death rate of yeast cells per unit of alcohol
- e. Fraction of sugar breakdown that yields CO_2

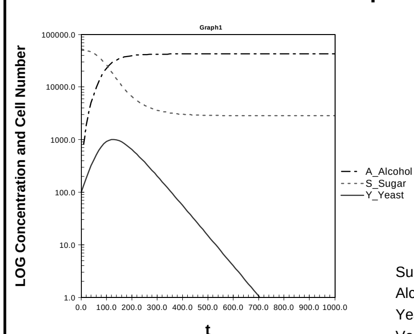
Differential Eq. Required

$$\frac{dS}{dt} = -abSY - aeSY$$

$$\frac{dY}{dt} = acSY - dYA$$

$$\frac{dA}{dt} = abSY$$

Model Output



Initial values
Sugar (e.g., 52000 mg)
Alcohol (0)
Yeast (e.g., 100 mg)
Volume (20 L)