L5 Inhibitor Interactions

Euler’s Method for solving ODEs

- This is the simplest approximation method.


For \( \frac{dy}{dt} = f(y) \):

- \( y_{n+1} = y_n + h f(y_n) \), where \( h \) is the step size.

Take the function \( \frac{dy}{dt} = ky \)

- Its approximation is:

\[
\begin{align*}
    y_{n+1} &= y_n + dt \cdot ky_n \\
    y_{n+1} &= y_n + dt \cdot k
\end{align*}
\]

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.

Inhibitor effect at high inhibitor conc

Inhibitor effect at low inhibitor conc

Effects of an inhibitor

- Substrate
- Inhibitor
- Product

Your next assignment will have a question on this system.

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 CO₂.
  - Excessive alcohol will kill yeast cells.

**Assumptions:**

- the rates of sugar consumption, CO₂ 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.

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**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 CO₂

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**Differential Eq. Required**

\[
\frac{dS}{dt} = -abSY - aeSY \\
\frac{dY}{dt} = acSY - dYA \\
\frac{dA}{dt} = abSY
\]

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**Model Output**

Model output showing the concentration and cell number over time with initial values:
- Sugar (e.g., 52000 mg)
- Alcohol (0)
- Yeast (e.g., 100 mg)
- Volume (20 L)