# Bio-Systems Modeling and Control

## Lecture 19

## Enzymes

## Brief Introduction

# References for this Introduction

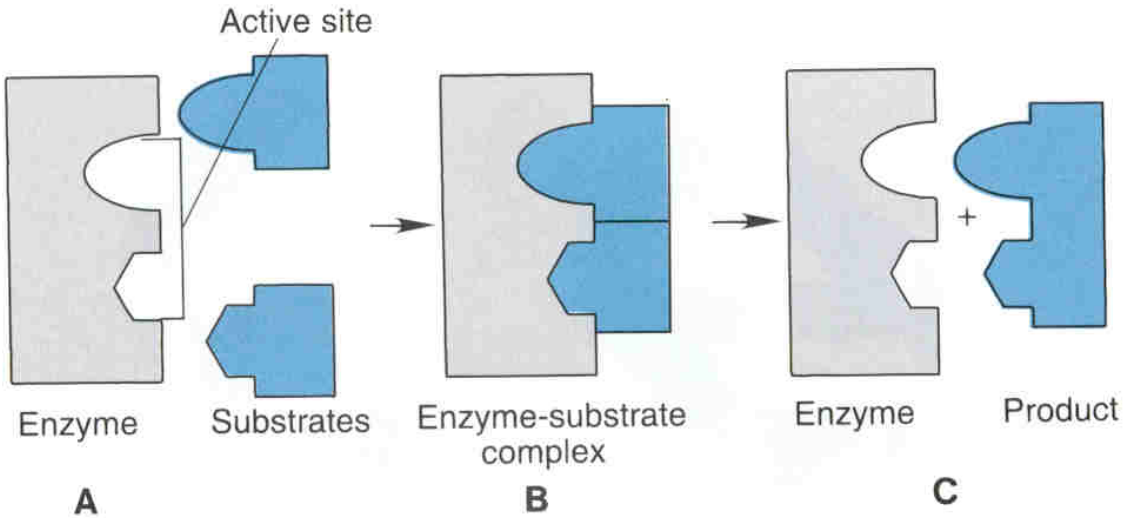

- Edward K. Yeargers, Ronald W. Shonkwiler & James V. Herod “An Introduction to the Mathematics of Biology” (With Computer Algebra Models), Birkhauser 1996.
- Valerie C. Scanlon & Tina Sanders “Essentials of Anatomy and Physiology” Third Edition, 1999 F. A. Davis Company

# Enzymes is a Class of Proteins that Act as Catalysts

- Enzyme Catalysts – can speed up the rate of biochemical reactions, sometimes by a huge factor (up to $10^{13}$ faster).
- Each enzyme is specific. It will catalyze only one type of reaction.
- There are many chemical reactions that take place in the body, and therefore we have thousands of enzymes.

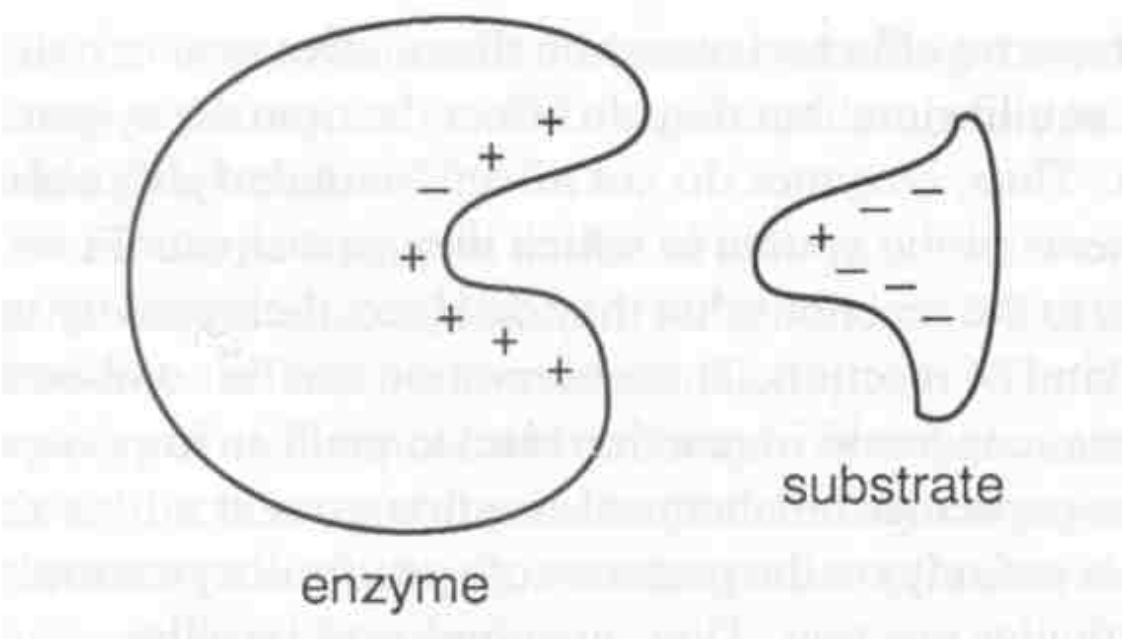
# Enzyme Functioning Idea – “Active Site Theory” (Lock-Key Mechanism)

From Scanlon & Sanders:




- There must be a match in geometric shape and electrical charge between an active site of an enzyme and a substrate molecule.
- “Substrates” – the reacting molecules.

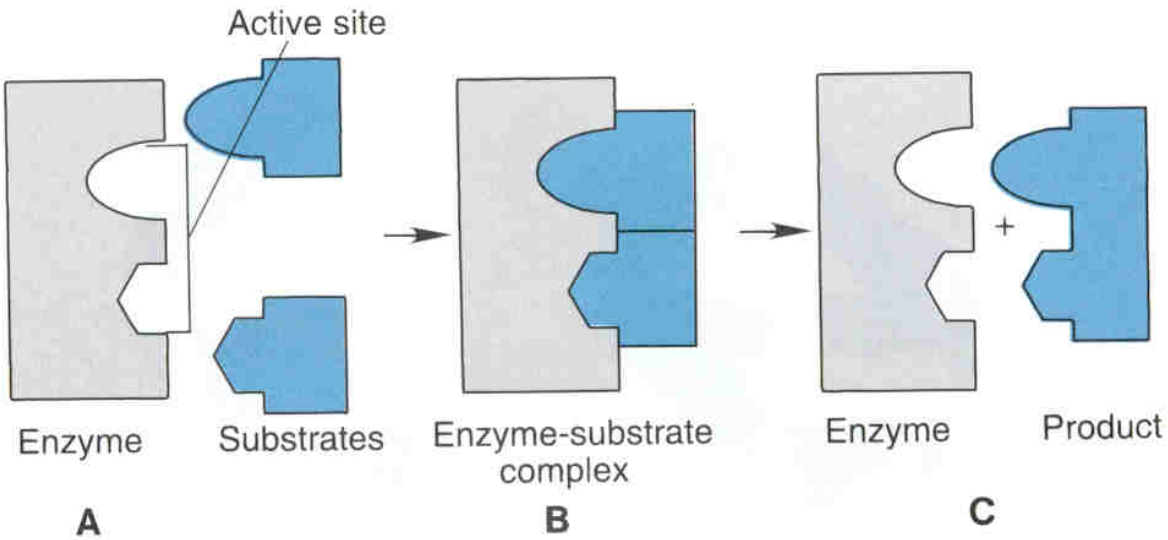
# Complementary Shapes and Electrical Charge Distributions:




[From Yeargers et al.]

# Enzyme-Catalyzed Reaction Steps

From Scanlon & Sanders:




- First an enzyme-substrates complex is created.
- Then, substrates bond to each other, while being at the complex.
- Finally, product is released, leaving the enzyme unchanged and ready to catalyze again.

# Ability of enzymes to function may be limited or destroyed by changes in the intracellular or extra-cellular fluids in which they are found

- Changes in pH are crucial.
- The pH of intracellular fluid is around 6.8.
- Decrease of pH means that more $H^+$ ions are present. These may react with the active sites of the enzyme, changing their shapes
- This state of “acidosis” may cause cell’s death as enzymes are unable to function properly.

## Ability of enzymes to function may be limited or destroyed by changes in the intracellular or extra-cellular fluids in which they are found

- Changes in temperature are also crucial.
- Most human enzymes have their optimum functioning in the normal range of body temperature ($97^0$ to $99^0$F or $36^0$ to $38^0$C).
- At T=$106^0$F some chemical bonds, that maintain the shapes of enzymes, may break. Enzyme becomes “denatured” and basically useless.

# More Comments about Enzymes:

- A reaction must be able to proceed in the absence of a catalyst. Only then, a catalyst can really help.
- Catalysts have no effect whatever on the relative concentrations of reactants and products at equilibrium.
- Enzymes do not affect the underlying chemistry or net energetic requirements for the process in which they participate.

# More comments about enzymes (cont'd):

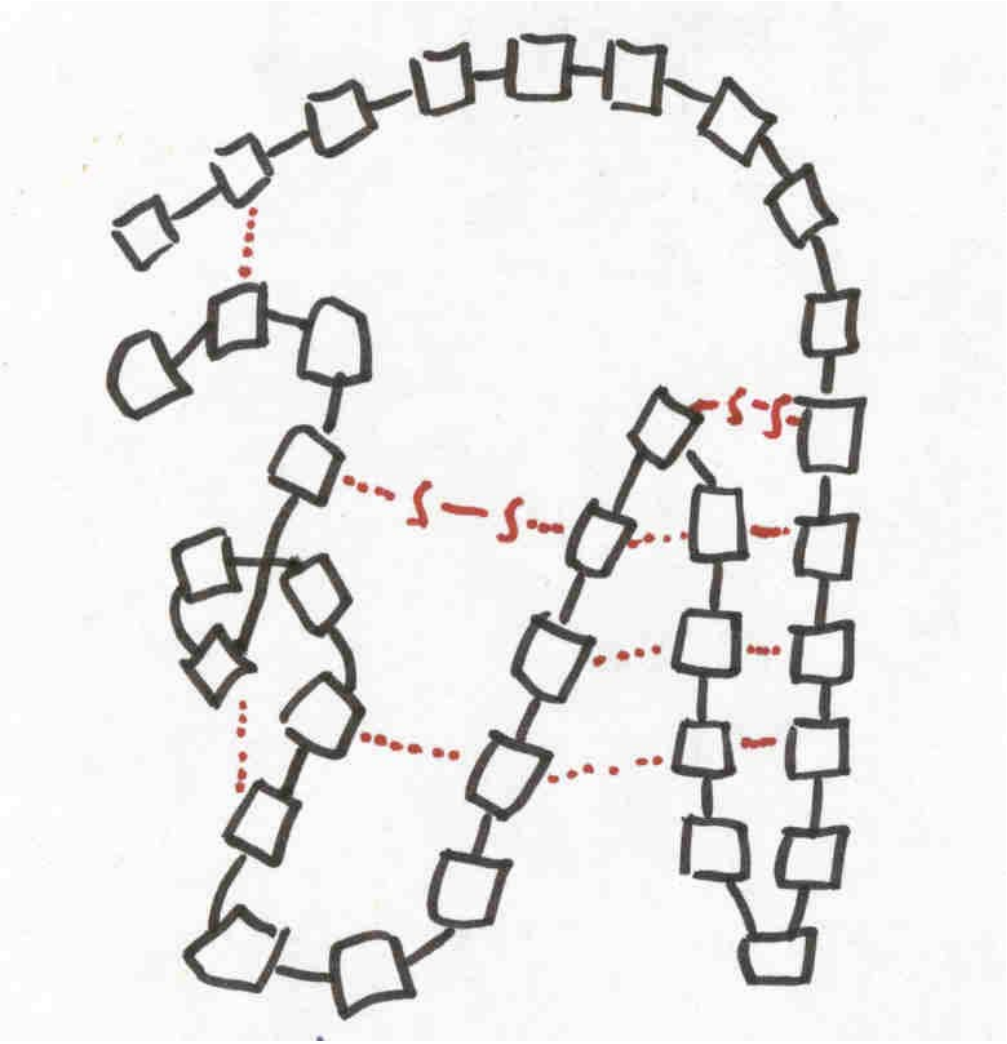
- Enzymes are very specific as to the reactions that they catalyze, their activity usually being limited to a single kind of reaction.
- Whether or not a particular biochemical reaction goes at a high enough rate, depends entirely on the presence of specific enzyme molecules that can catalyze that particular reaction.

# More comments about enzymes (cont'd):

- Enzymes act like valves, facilitating only the reactions appropriate to a particular cell. No other reactions proceed fast enough to be significant.
- The geometric shape of a protein, depends, in part, on many H-bonds (and other sulfur bonds) that hold the polypeptide folded in a certain 3D shape.

# 3D Shape of an Enzyme

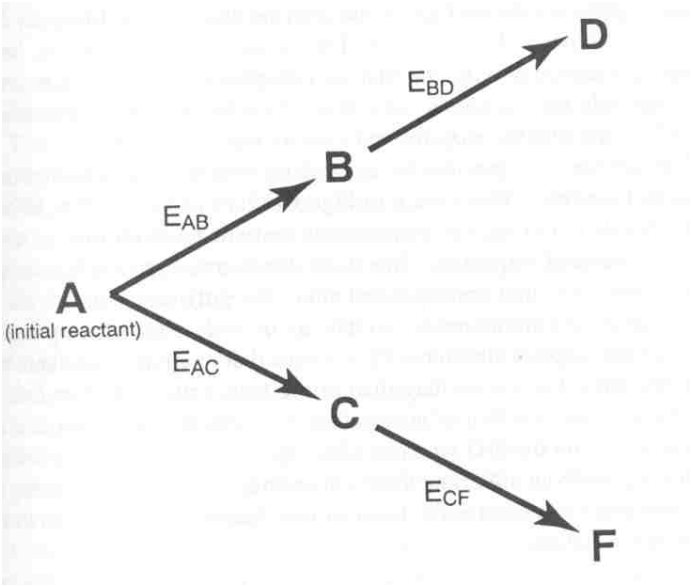
Shape affected by H-bonds and Sulfur-bonds etc



Based on Yeargers

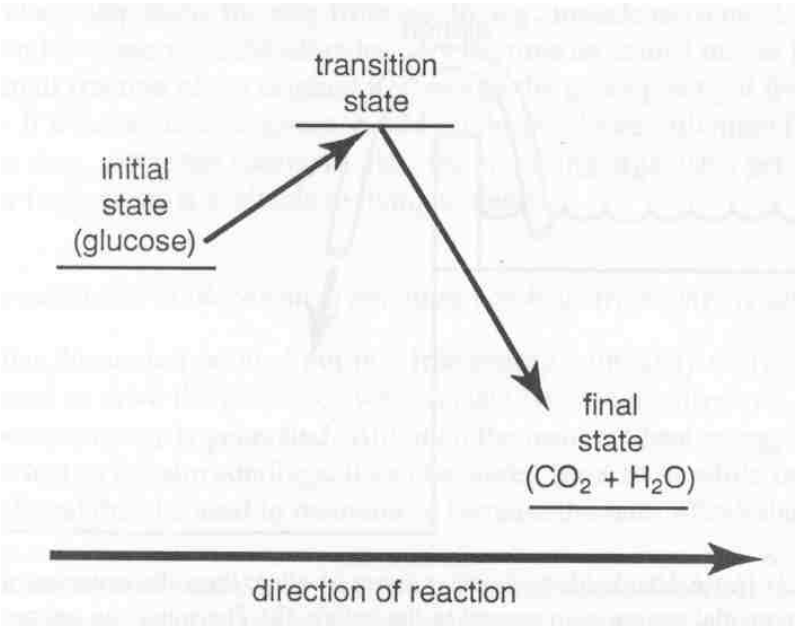
# It is the enzyme, and not the initial reactant that determine what the end product will be

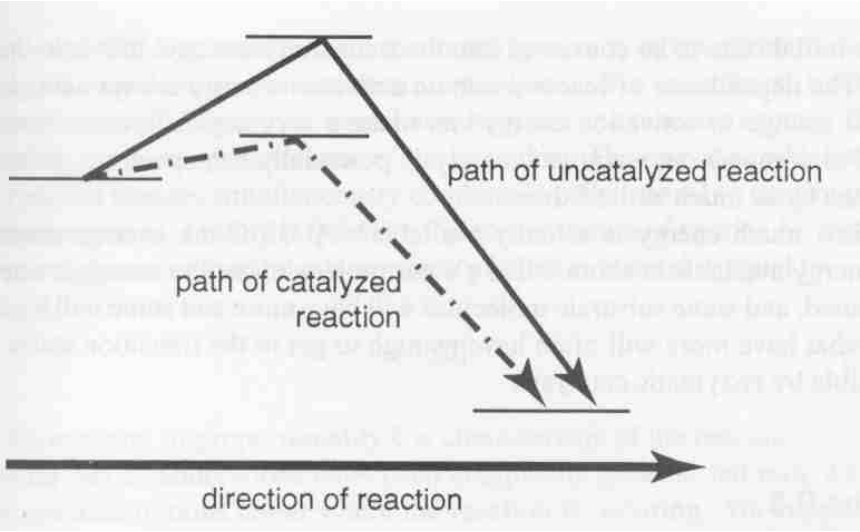
From Yeargers et al

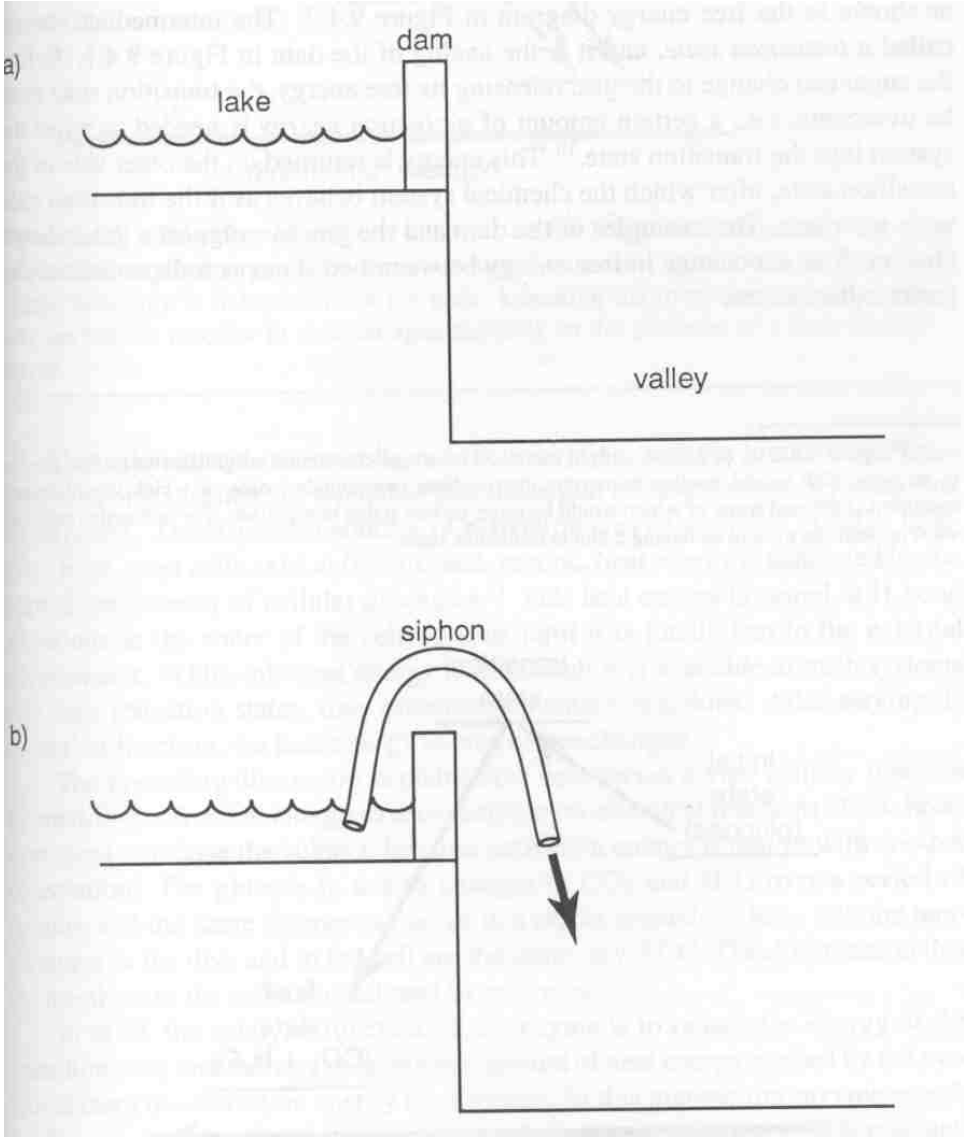



- E (above) are various enzymes.
- A is the initial reactant that can evolve into products B,C,D and/or F.
- It depends if enzyme exists at a given time.

# Enzyme lowers the energy of the transition state but the overall reaction's energy change is independent of the enzyme




[From Yeargers et al]

Lake analogy to the fact that overall energy change is unaffected by the catalyzing