Enzyme Reaction Simulation : Michaelis-Menten Kinetics

Introduction

Chemists are concerned with the laws of chemical interactions.

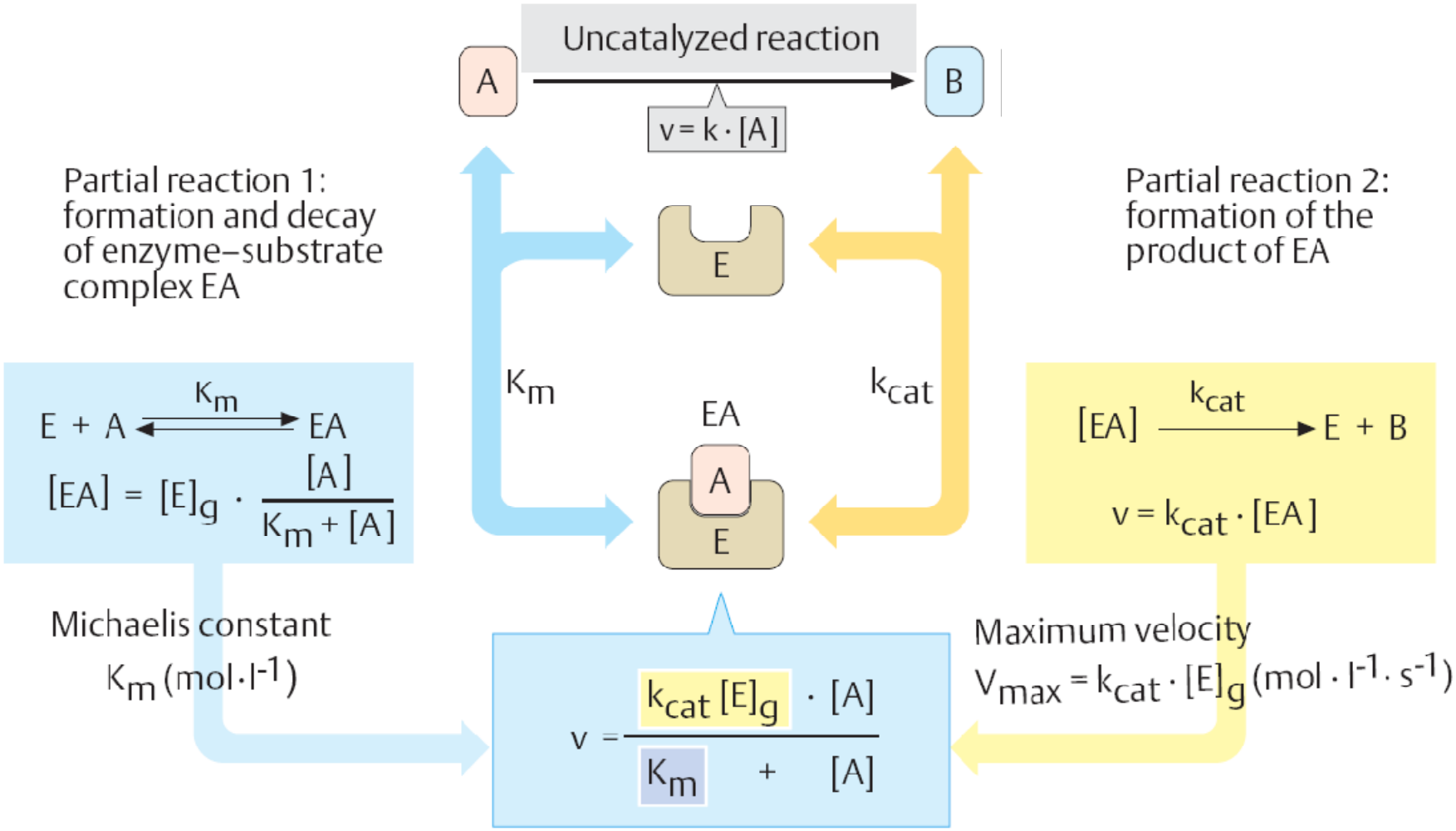
Two main approaches have been used to explain chemical reactivity: thermodynamic and kinetic. Theoretical analysis of the kinetics, or time course, of processes can provide valuable information concerning the underlying mechanisms responsible for these processes.

For this purpose it is necessary to construct a mathematical model that embodies the hypothesized mechanisms.

Whether or not the solutions of the resulting equations are consistent with the experimental data will either prove or disprove the hypothesis.

The task of a kineticist is to predict the rate of any reaction under a given set of experimental conditions. At best, a mechanism is proposed that is in qualitative and quantitative agreement with the known experimental kinetic measurements.

Michaelis-Menten Kinetics



ODEs from M-M Kinetics

Reaction Mechanism

$$E + S \underset{k_{-1}}{\overset{k_1}{\leftrightarrow}} ES \xrightarrow{k_2} E + P$$

E : enzyme, S : substrate, P : product,
ES : enzyme-substrate complex

$$\frac{d[S]}{dt} = -k_1[E][S] + k_{-1}[ES]$$

$$\frac{d[ES]}{dt} = k_1[E][S] - (k_{-1} + k_2)[ES]$$

$$\frac{d[P]}{dt} = k_2[ES]$$

S=y1

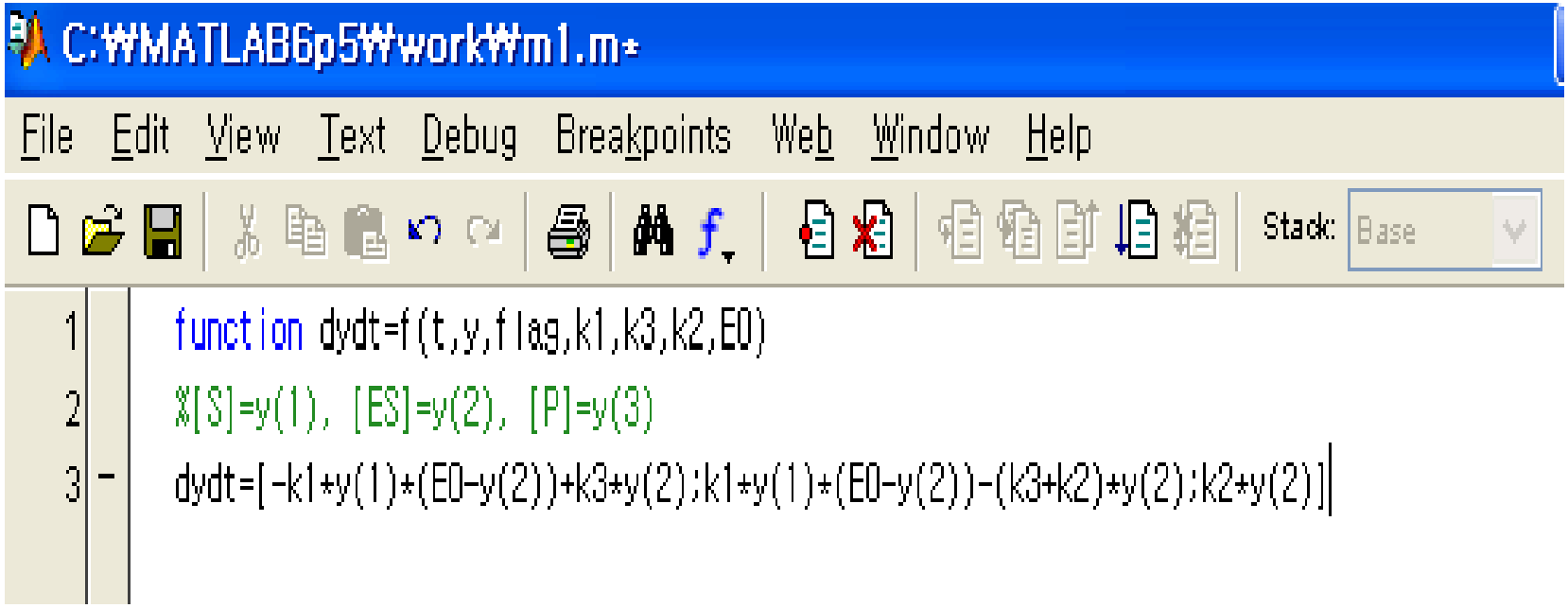
ES=y2

P=y3

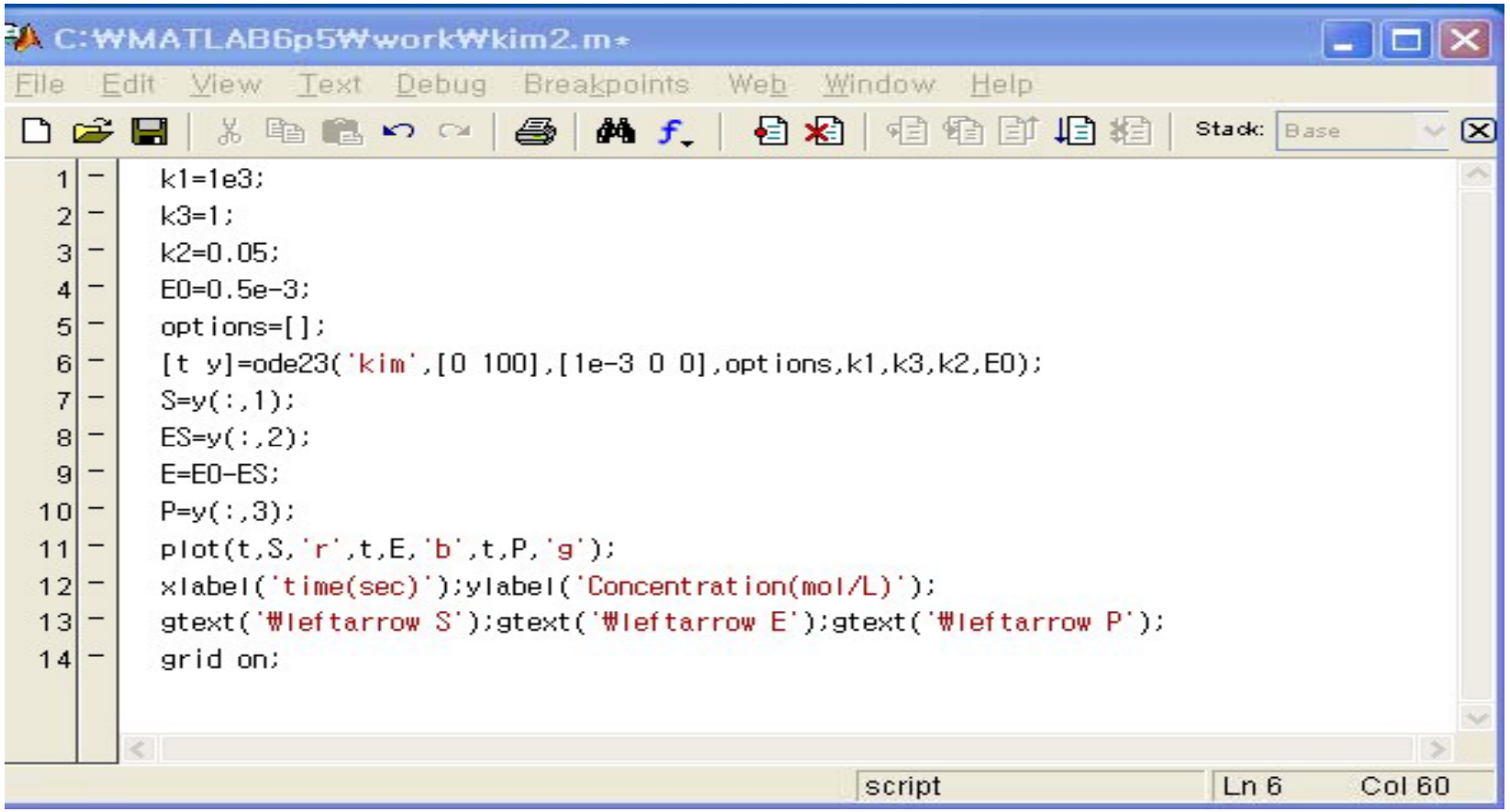
E=E0-ES

=E0-y2

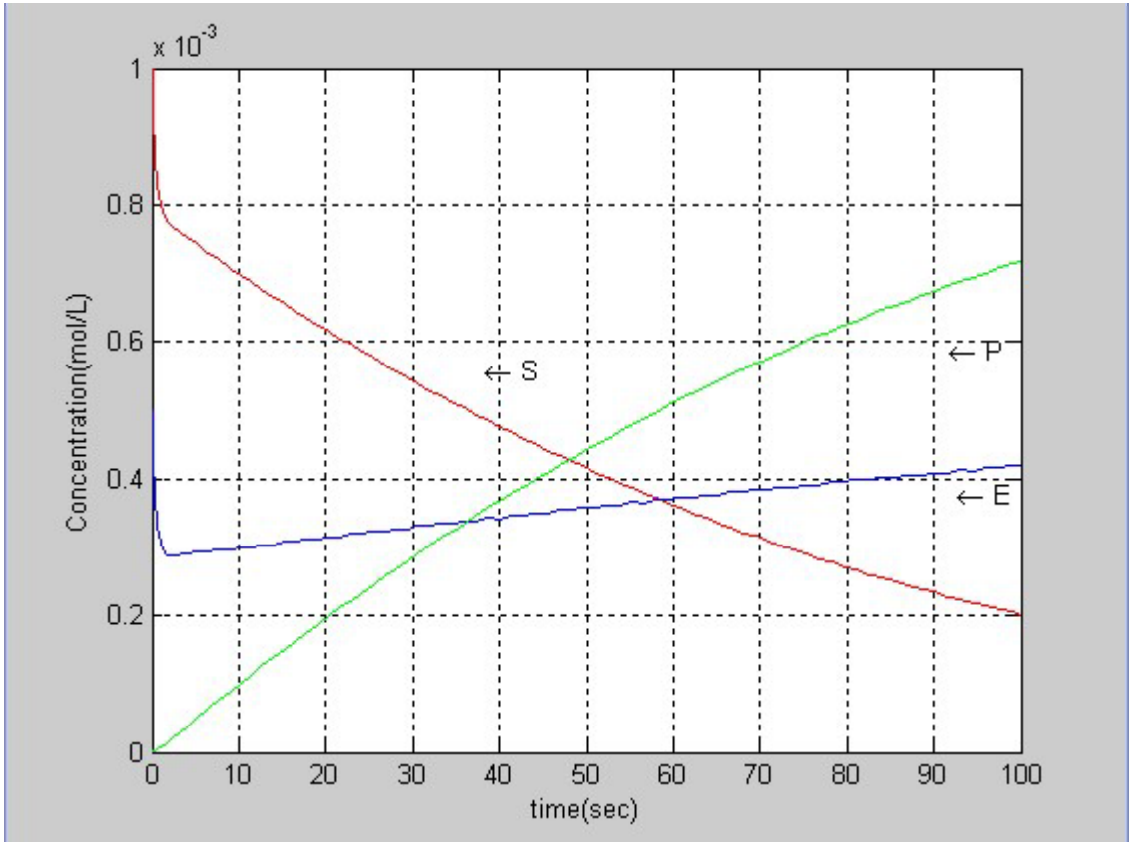
Matlab Program



Program (continued)

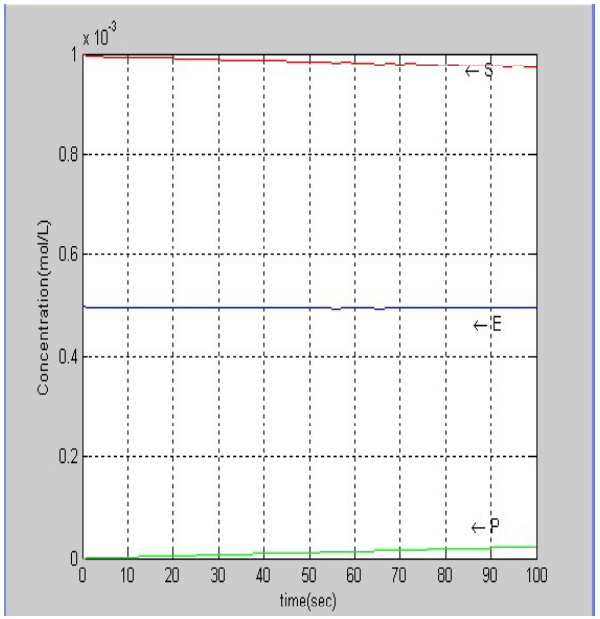


Simulation Results

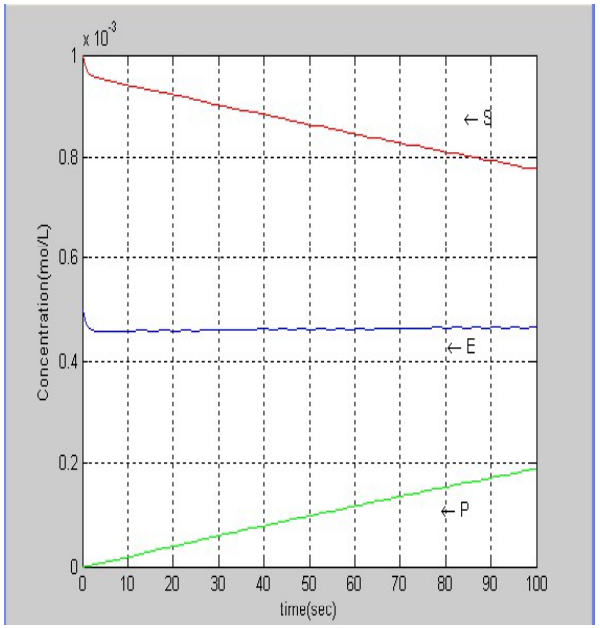


Parameter Variation

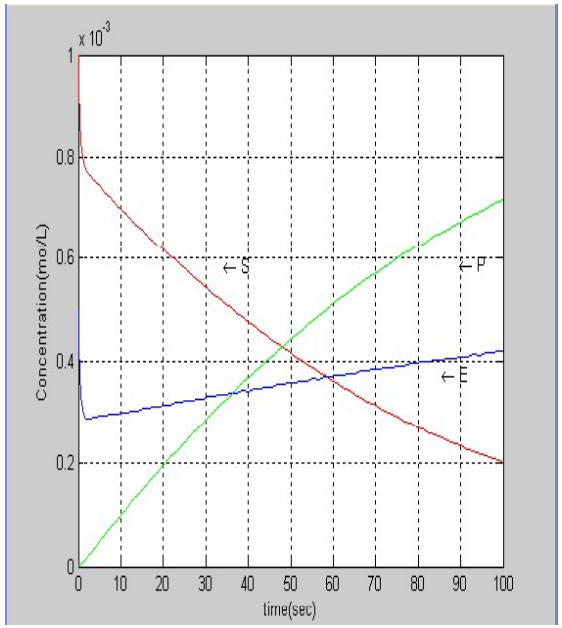
$k1=1e^{1}$



$k1=1e^{2}$

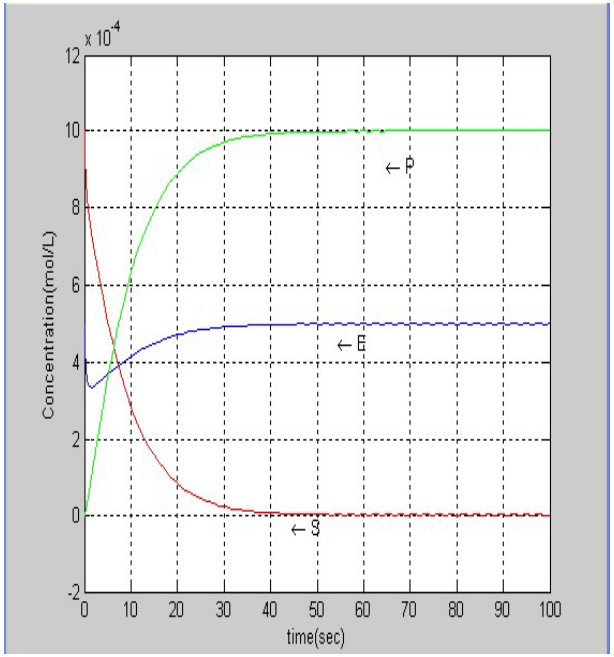


$k1=1e^{3}$

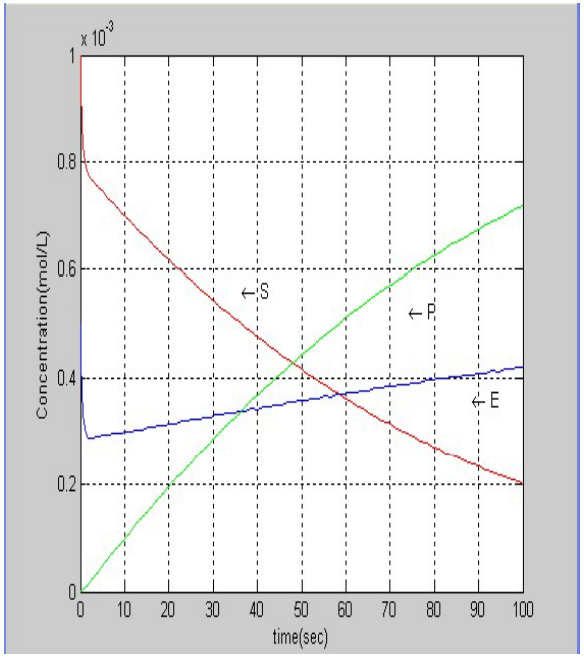


Parameter Variation

k2=0.5



k2=0.05



k2=0.005