NTU Question 2

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25/02/2023

8.1

we have given the equation:

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_3} E + P$$

The rate of changes=speed for the four species are:

we are going to use the following strategies: we know that k[] means the concentration of something

for E we have rate forming E that is $k_2[ES]$ and $k_3[ES]$=rate taking away from E that is $k_1[E][S]$

$$\frac{\partial[E]}{\partial t} = k_2[ES] + k_3[ES] - k_1[E][S]$$

Similarly we could obtained the rate for S,ES and P as following:

$$\frac{\partial[S]}{\partial t} = k_2[ES] - k_1[E][S]$$

$$\frac{\partial[ES]}{\partial t} = k_1[E][S] - k_2[ES] - k_3[ES]$$

$$\frac{\partial[P]}{\partial t} = k_3[ES]$$

8.2

We first recall the that is:

$$y_1 = y_0 + (1/6) * (k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = hf(x_0, y_0)$$

$$k_2 = hf[x_0 + (1/2)h, y_0 + (1/2)k_1]$$

$$k_3 = hf[x_0 + (1/2)h, y_0 + (1/2)k_2]$$

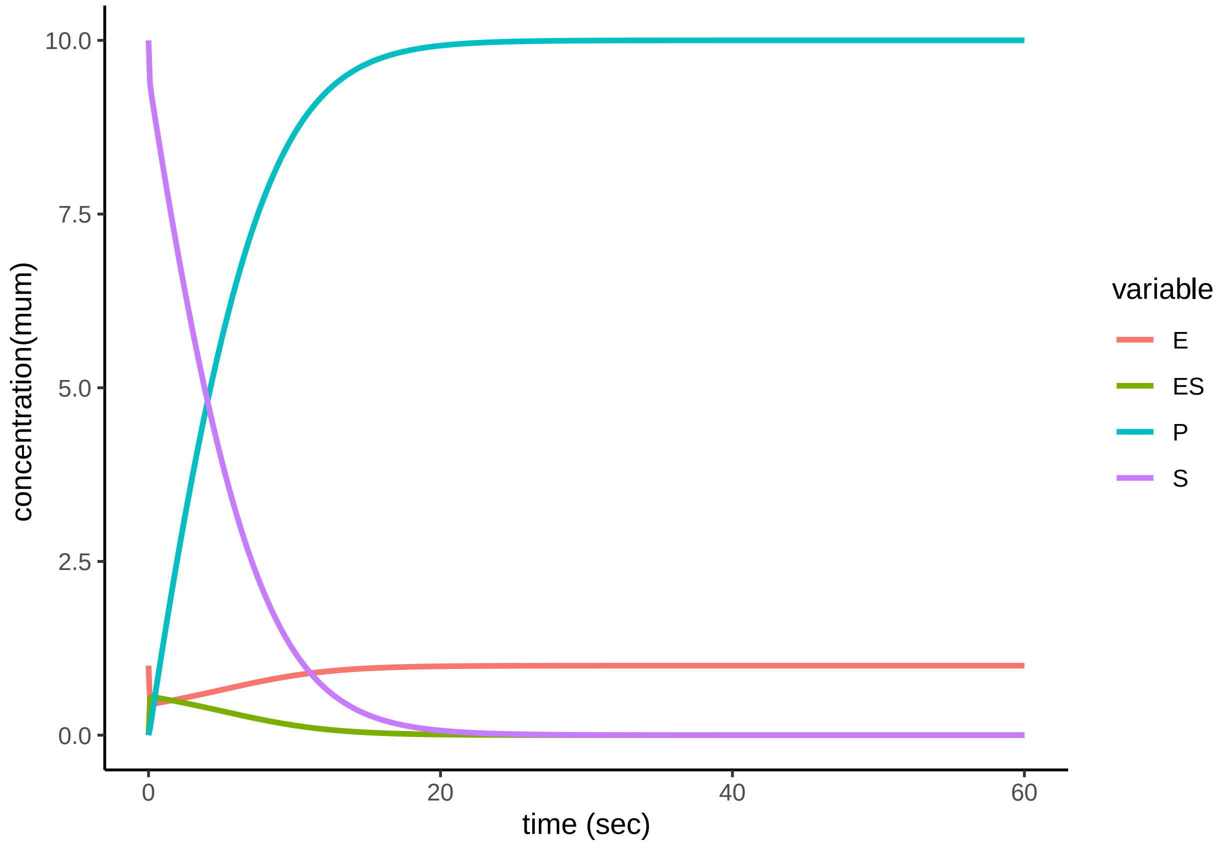
$$k_4 = hf(x_0 + h, y_0 + k_3)$$

Then we could produce the following R code:

```r
library("deSolve")
time <- seq(from=0, to=60, by = 0.1)
#convert parameters from mins into seconds
parameters <- c(k1<-100/60,k2<-600/60,k3<-150/60)
# initial conditions: also a named vector
state <- c(ES=0,S=10,E=1,P=0)
model2 <- function(t, state, parameters){
        with(as.list(c(state, parameters)),{
                dE<-(k2)*ES+(k3)*ES-k1*E*S
                 dS<-(k2)*ES-(k1)*E*S
                 dES<-(k1)*E*S-(k2)*ES-(k3)*ES
                 dP<-(k3)*ES
                 td<-c(dES,dS,dE,dP)
                return(list(td))
            }
        )
}

out <- ode(y = state, times = time, func = model2, parms = parameters)


# we could also get the graph as follow:
library(tidyverse)
```

```
## -- Attaching core tidyverse packages ------------------------ tidyverse 2.0.0 --
## v dplyr     1.1.0     v readr     2.1.4
## v forcats   1.0.0     v stringr   1.5.0
## v ggplot2   3.4.1     v tibble    3.1.8
## v lubridate 1.9.2     v tidyr     1.3.0
## v purrr     1.0.1
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
## i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to become error
```

```r
ode(y = state, times = time, func = model2, parms = parameters)%>%
  as.data.frame() -> out

out %>%
  gather(variable,value,-time) %>%
  ggplot(aes(x=time,y=value,color=variable))+
  geom_line(linewidth=1)+
  theme_classic()+
  labs(x='time (sec)',y='concentration(mum) ')
```

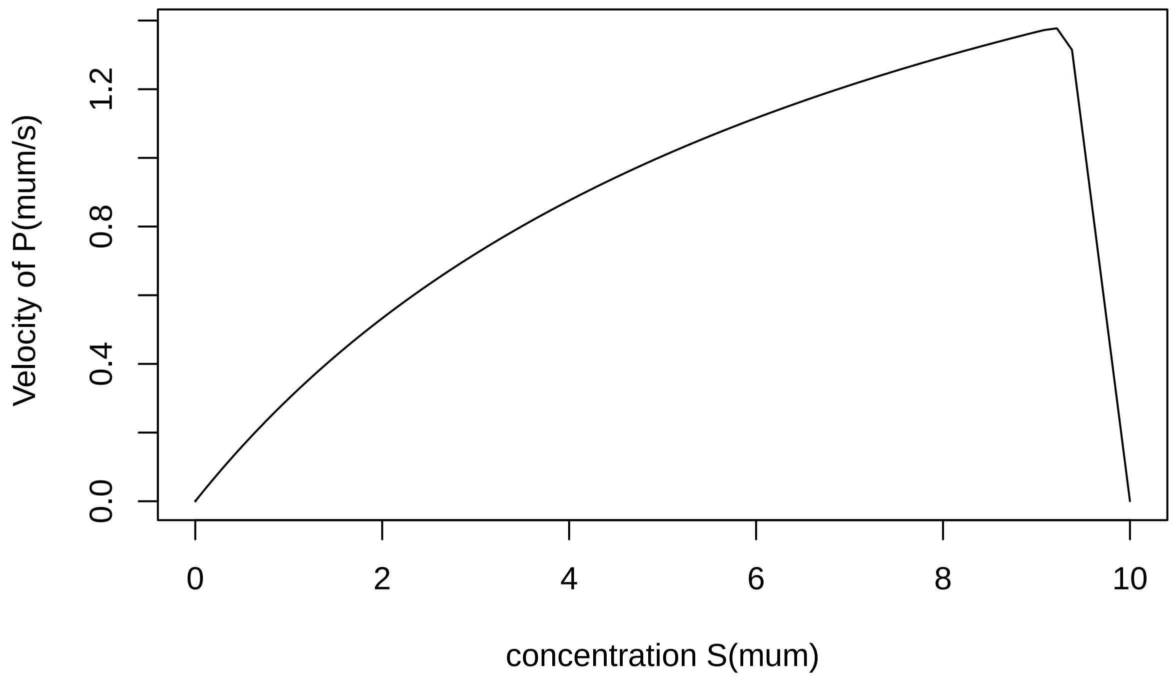



```
#find the value for each species
time1<- seq(from=0, to=0.001, by = 0.001)
parameters <- c(k1<-100/60,k2<-600/60,k3<-150/60)
# initial conditions: also a named vector
state <- c(ES=0,S=10,E=1,P=0)
out2<- ode(y = state, times = time1, func = model2, parms = parameters)
print(out2)
```

```
##    time         ES         S        E            P
## 1 0.000 0.00000000 10.000000 1.000000 0.000000e+00
## 2 0.001 0.01641304  9.983566 0.983587 2.057797e-05
```

8.3

```
#plot P against S, we know that velocity of P is k3*ES
k3<-150/60
plot(k3*ES~S,data=out,type='l',xlab="concentration S(mum)",ylab=" Velocity of P(mum/s)")
```



From the graph above, we can see that the maximum velocity of P is achieved when we have concentration S of value 9 μm and with velocity of P approximately 1.4μm/s.Before the maximum point, the relationship of concentration S and velocity P shows a increasing exponential relationship, ie: a curve but not a straight line. After the peak, it shows a negatively proportional relationship.