Chemistry 4010 Fall 2019 Assignment 3 Solutions

1.

$$\begin{aligned}\frac{d[\mathrm{M}]}{dt} &= v_4 - v_1,\\ \frac{d[\mathrm{M_p}]}{dt} &= v_1 - v_2 + v_3 - v_4,\\ \frac{d[\mathrm{M_{pp}}]}{dt} &= v_2 - v_3.\end{aligned}$$

Note that

$$\begin{aligned}&\frac{d[\mathrm{M}]}{dt} + \frac{d[\mathrm{M_p}]}{dt} + \frac{d[\mathrm{M_{pp}}]}{dt} = 0.\\ &\therefore [\mathrm{M}] + [\mathrm{M_p}] + [\mathrm{M_{pp}}] = \mathrm{M_{tot}},\end{aligned}$$

where $\mathrm{M_{tot}}$ is a constant. We can therefore eliminate $[\mathrm{M_p}]$ from the differential equations using

$$[\mathrm{M_p}] = \mathrm{M_{tot}} - [\mathrm{M}] - [\mathrm{M_{pp}}].$$

This leaves us with the pair of differential equations

$$\begin{aligned}\frac{d[\mathrm{M}]}{dt} &= v_4 - v_1,\\ \frac{d[\mathrm{M_{pp}}]}{dt} &= v_2 - v_3.\end{aligned}$$

2. If $[\mathrm{MAPKK}]_{\mathrm{tot}} = 0$, then $v_1 = v_2 = 0$. Accordingly, M cannot be phosphorylated, so the equilibrium point is $([\mathrm{M}], [\mathrm{M_{pp}}]) = (\mathrm{M_{tot}}, 0)$.

3. My input file is the following:

```
# MAPK model (assignment 2)
dM/dt=v4-v1
dMpp/dt=v2-v3
Mp=Mtot-M-Mpp
v1=kcat1*MAPKKtot*M/Km1/(1+M/Km1+Mp/Km2)
```

```
v2=kcat2*MAPKKtot*Mp/Km2/(1+M/Km1+Mp/Km2)
v3=kcat3*MKPtot*Mpp/Km3/(1+Mpp/Km3+Mp/Km4+M/Km5)
v4=kcat4*MKPtot*Mp/Km4/(1+Mpp/Km3+Mp/Km4+M/Km5)

M(0)=500

param Km1=50, Km2=500, Km3=20, Km4=20, Km5=60
param kcat1=0.01, kcat2=15, kcat3=0.08, kcat4=0.06
param Mtot=500, MKPtot=100, MAPKKtot=0

@ METH=stiff, BOUNDS=1000
@ MAXSTOR=1000000

done
```

After some experimentation, I set the AUTO parameters as follows:

`Nmax:`	2000
`NPr:`	200
`Par Max:`	80

All other parameters were left at their default values. The resulting bifurcation diagram is shown in Fig. 1.

4. My phase diagram is shown in Fig. 2.

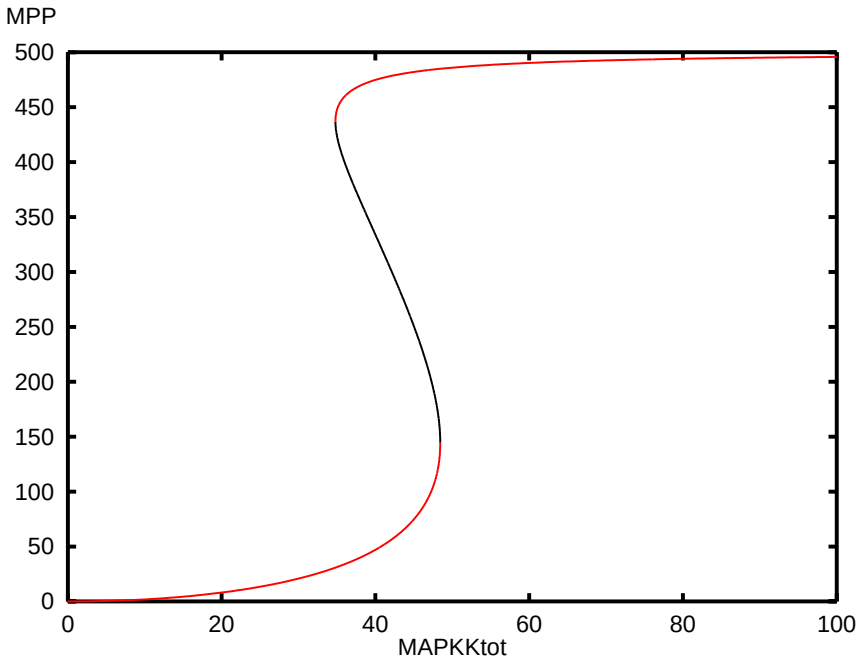

Figure 1: Bifurcation diagram for the MAPK model, with all parameters set as in the assigned problem.

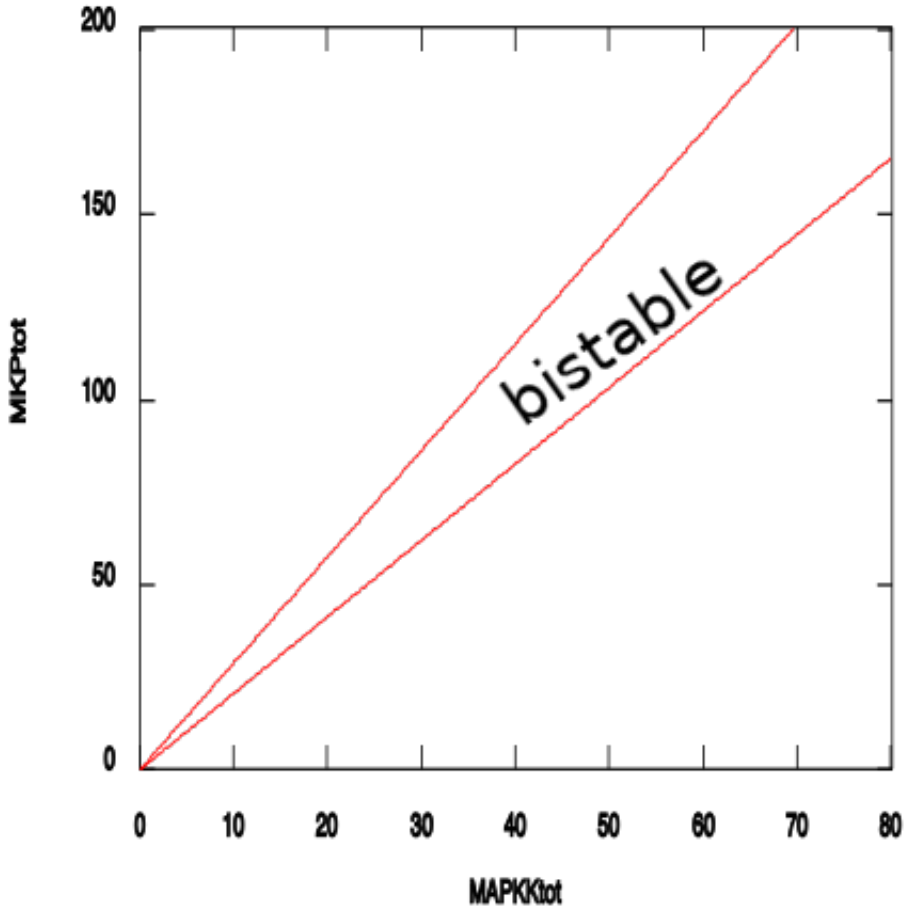

Figure 2: Phase diagram for the MAPK model obtained by continuation of the two saddle-node points in Fig. 1.