

**Orysya Stus**  
**A10743411**  
**Worked With : Arnav Aggarwal**  
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# Homework 4

Please answer all questions in this notebook. You may do calculations by hand or using *Mathematica* but please show all working here. Please email the Mathematica notebook and a pdf of the notebook output to beng123@gmail.com with the subject line HOMEWORK 4 - YOUR NAME - YOUR PID. This homework is due at the start of class on Thursday 2/6/2014 (3:30 pm). Everything you need to know for Mathematica is in the corresponding notebook files. Remember that explanations should accompany the plots for each of the questions.

## Problem 1

Do question 8.4 in the book. Use the following values for your model:

$$v_{a\_exch} = 0.03 \text{ mM/min}$$

$$k_{ampform}^{\rightarrow} = 0.03/\text{minute}$$

$$k_{amp\_exch}^{\rightarrow} = 0.3/\text{minute}$$

You will have to find the steady state and update your model's initial conditions before proceeding to perturb the system.

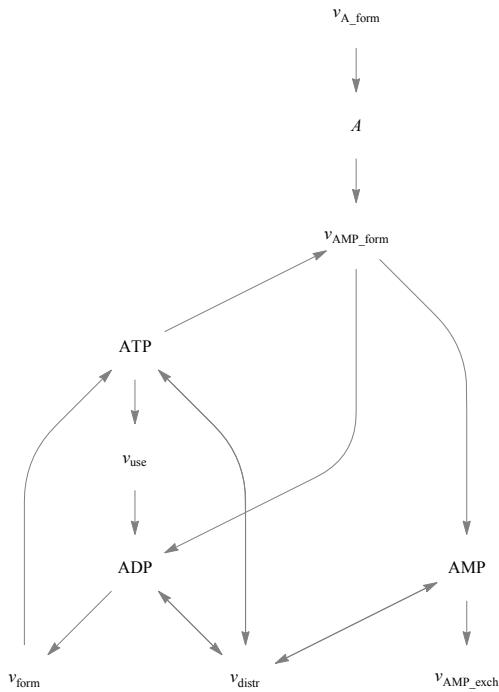
```

atpmode1 =
constructModel[{r["use", {m["ATP", None]}, {m["ADP", None]}, {1, 1}, False],
r["form", {m["ADP", None]}, {m["ATP", None]}, {1, 1}, False],
r["distr", {m["ADP", None]}, {m["AMP", None]}, m["ATP", None]}, {2, 1, 1}, True],
r["AMP_form", {m["A", None]}, m["ATP", None]}, {m["AMP", None]}, m["ADP", None}],
{1, 1, 1, 1}, False], r["A_form", {}, {m["A", None]}, {1}, False],
r["AMP_exch", {m["AMP", None]}, {}, {1}, False}],
InitialConditions → {m["ATP", None] → 1.6 Millimole Liter-1,
m["ADP", None] → 0.4 Millimole Liter-1, m["AMP", None] → 0.1 Millimole Liter-1,
m["A", None] → 1 Millimole Liter-1}, Parameters →
{Keq["distr"] → 1, k["distr"] → 1000 Liter Minute-1 Millimole-1,
k["AMP_form"] → 0.03 Millimole Liter-1 Minute-1, k["AMP_exch"] →
0.3 Millimole Liter-1 Minute-1, k["A_form"] → 0.03 Millimole Liter-1 Minute-1,
kuse → 6.25` Minute-1, kform → 25. ` Minute-1,
m["A", "Xt"] → 1 Millimole Liter-1}]

```

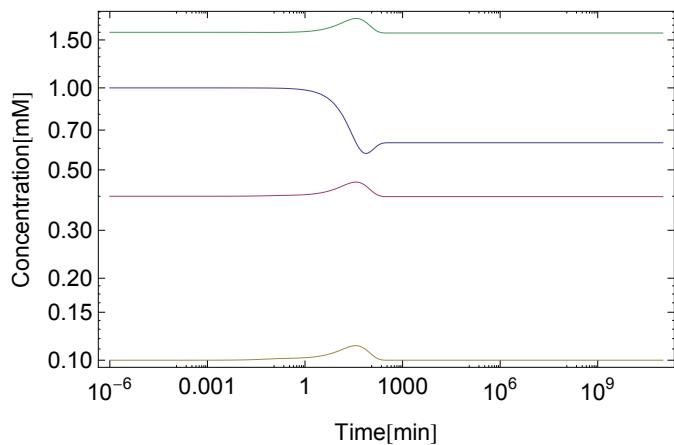
Overview	
Number of species(rows):	4
Number of columns(reactions):	6
Number of exchange reactions:	2
Number of irreversible reactions:	5
Matrix rank:	4
Dimensions null space:	2
Dimensions left null space:	0
Number of parameters	8
Number of custom rate equations	0
Number of equilibrium constants:	1
Number of forward rate constants:	6
Number of initial concentrations:	4
Number of genes:	0
Number of proteins:	0

```
visualizePathways[atpmodel]
```



A diagram showing the cycle of ATP, ADP, and AMP in relation to one another.

```
{concSol, fluxSol} = simulate[atpmodel, {t, 0, 100 000 000 000}];
plotSimulation[concSol, FrameLabel \rightarrow {"Time[min]", "Concentration[mM]"}]
```



A is in blue, ADP in purple, AMP in yellow, and ATP in green. This diagram shows the change in concentration of each of the said substances over a time period.

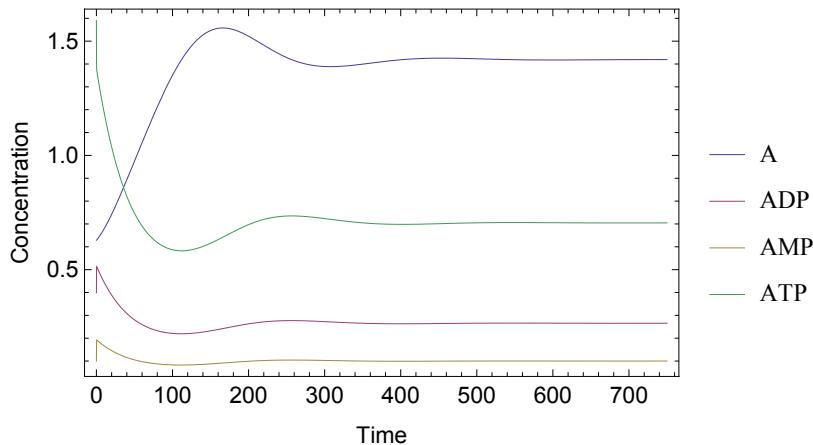
```

steadyState = concSol /. t → 100 000
{A → 0.628778, ADP → 0.398796, AMP → 0.1, ATP → 1.59039}

perturbedmodel = atpmodel;
updateInitialConditions[perturbedmodel, steadyState]

{concSolPerturbed, fluxSolPerturbed} =
  simulate[perturbedmodel, {t, 0, 1*^6}, Parameters → {k["use"] → 9.375}];
plotSimulation[concSolPerturbed, {t, 0, 750}, PlotFunction → Plot,
  Legend → True, FrameLabel → {"Time", "Concentration"}]

```



ATP, ADP, and AMP all decrease in concentration over a period of time in comparison to A. The formation of A is favored in this cycle.

Energy charge equation is now :

$$\frac{\text{occupancy}}{\text{capacity}} = \frac{\text{ATP} + 0.5\text{ADP} + \text{AMP}}{\text{ATP} + \text{ADP} + \text{AMP} + \text{A}}$$

## Problem 2

Do problem 7.2 in the textbook. Show working and answers below:

$$\frac{220 \text{ mV}}{7 \text{ nm}} * \frac{1 \text{ V}}{1000 \text{ mV}} * \frac{10^7 \text{ nm}}{1 \text{ cm}} = 3.14 * 10^5 \frac{\text{V}}{\text{cm}}$$

$$\frac{240 \text{ mV}}{7 \text{ nm}} * \frac{1 \text{ V}}{1000 \text{ mV}} * \frac{10^7 \text{ nm}}{1 \text{ cm}} = 3.43 * 10^5 \frac{\text{V}}{\text{cm}}$$

The range,  $(3.14 - 3.43) * 10^5 \text{ V/m}$ , is significantly higher than that of a car's ignition coil of 1000 V/cm. It is over 3 orders of magnitude higher than the potential gradient in air caused by cars.

## Problem 3

Do problem 7.4 in the textbook. Show working and answers below:

$$60 \frac{\mu\text{g}}{\text{mL}} * \frac{1\text{g}}{10^6 \mu\text{g}} * \frac{100\text{mL}}{30\text{g}} = 0.0002 = 0.02\%$$

The percentage shows the concentration of BPGM in erythrocytes over the total enzyme mass (30 g) .

## Problem 4

Do problem 7.6 in the textbook. Show working and answers below:

a :

$$\frac{160 \text{ g Hg}}{1 \text{ L blood}} * \frac{1 \text{ L}}{1000 \text{ mL}} * \frac{1 \text{ mL}}{5 * 10^9 \text{ cells}} = 3.2 * 10^{-11} \frac{\text{g Hg}}{\text{red blood cell}}$$

b : Assume hemoglobin has molecular mass of 60, 000 g/mol.

$$3.2 * 10^{-11} \frac{\text{g Hg}}{\text{red blood cell}} * \frac{1 \text{ mol Hg}}{60,000 \text{ g Hg}} * \frac{6.022 * 10^{23} \text{ molecules}}{\text{mol}} = 3.21 * 10^8 \frac{\text{molecules Hg}}{\text{red blood cell}}$$

c :

$$\text{Volume} = \pi r^2 h = \frac{\pi d^2 h}{4} = \frac{\pi * (8 * 10^{-6} \text{m})^2 * 1.8 * 10^{-6} \text{m}}{4} = 9.048 * 10^{-17} \text{m}^3$$

d :

$$\text{Sphere volume} = \frac{4}{3} \pi r^3 = \frac{\pi d^3}{6} = \pi * \frac{6.8 * 10^{-9} \text{m}^3}{6} = 1.646 * 10^{-25} \text{m}^3$$

$$\text{Fraction} = \frac{3.21 * 10^8 \text{ molecules Hg}}{9.048 * 10^{-17} \text{ m}^3} * \frac{1.646 * 10^{-25} \text{ m}^3}{\text{molecule Hg}} = 0.584 = 58.4\%$$

e :

$$\frac{(6.8 * 10^{-9} \text{m})^3 \text{Hg}}{\text{molecule Hg}} * 3.21 * 10^8 \text{ molecules Hg} = 1.01 * 10^{-16} \text{ m}^3 \text{ Hg}$$

This volume is somehow slightly greater than the total volume of the red blood cell indicating that the hemoglobin molecules are packed extremely tight in this cubic array, they are highly ordered inside the red blood cell and likely create a pressure on the cell membrane.

f :

Yes the hemoglobin can react with each other because they are so close. The interaction of hemoglobin S molecules in sickled red cells could affect the shape of the red blood cell. Because the sickled cells occupy a lower volume, the RBC may not have the support it needed from the pressure from regularly shaped hemoglobin and this may cause the disease.