Exercise 1

- Example: suppose you start with 1M of A and no B and C. Which of the following series will lead to the greatest $[C]_{eq}$?
- (Remember $Keq_T = Keq_1 \times Keq_2$)
  - Series 1

$$\begin{array}{ccccccc} A & \rightleftharpoons & B & \Delta G^\circ & = & +18,85\,\mathrm{kJ\,mol^{-1}}; & K_{eq} = 5 \times 10^{-4} \\ B & \rightleftharpoons & C & \Delta G^\circ & = & -18,85\,\mathrm{kJ\,mol^{-1}}; & K_{eq} = 2 \times 10^{3} \end{array}$$

  - Series 2

$$\begin{array}{ccccccc} A & \rightleftharpoons & B & \Delta G^\circ & = & -18,85\,\mathrm{kJ\,mol^{-1}}; & K_{eq} = 2 \times 10^{3} \\ B & \rightleftharpoons & C & \Delta G^\circ & = & +18,85\,\mathrm{kJ\,mol^{-1}}; & K_{eq} = 5 \times 10^{-4} \end{array}$$

$$[A] + [B] + [C] = 1M$$

$$[A]_{eq} + [B]_{eq} + [C]_{eq} = 1M$$

Series 1:

At equilibrium:

$[B]eq = 5x10^{-4}.[A]eq$

$[C]eq = [A]eq$

$[A]eq + [A]eq + 5x10^{-4}.[A]eq = 1$ M

=> [A]eq = 0.5 M; [B]eq = 0.00025 M; [C]eq = 0.5 M

Series 2:

At equilibrium:

$[B]eq = 2x10^{3}.[A]eq$

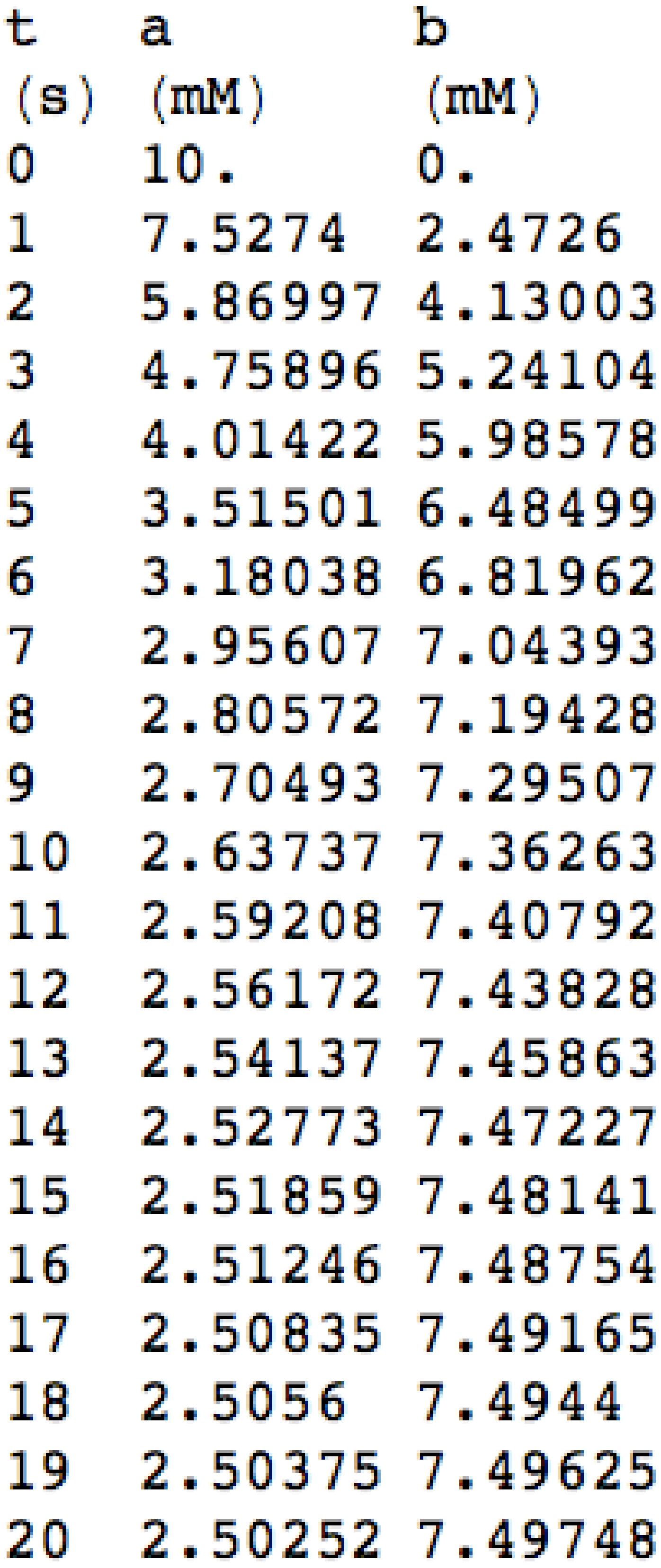
$[C]eq = [A]eq$

$[A]eq + [A]eq + 2x10^{3}.[A]eq = 1$ M

=> [A]eq = 0.0005 M; [B]eq = 0.999 M; [C]eq = 0.0005 M

Exercise 2: Experimental data

For a non catalyzed, chemical reaction; A<->B the following experimental data were obtained:

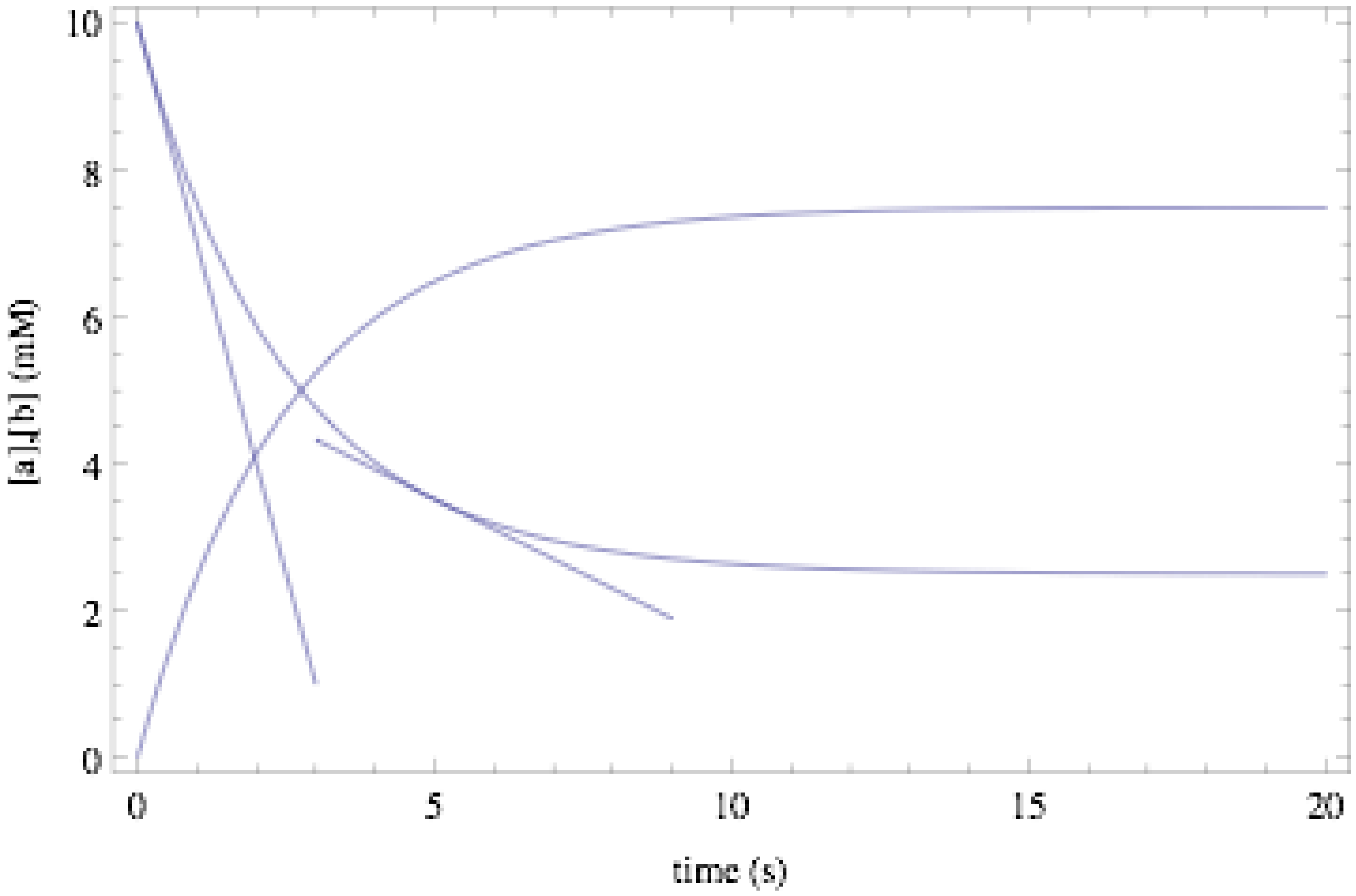


t (s)	a (mM)	b (mM)
0	10.	0.
1	7.5274	2.4726
2	5.86997	4.13003
3	4.75896	5.24104
4	4.01422	5.98578
5	3.51501	6.48499
6	3.18038	6.81962
7	2.95607	7.04393
8	2.80572	7.19428
9	2.70493	7.29507
10	2.63737	7.36263
11	2.59208	7.40792
12	2.56172	7.43828
13	2.54137	7.45863
14	2.52773	7.47227
15	2.51859	7.48141
16	2.51246	7.48754
17	2.50835	7.49165
18	2.5056	7.4944
19	2.50375	7.49625
20	2.50252	7.49748

Calculate:

- reaction rate at t=5 s
- Keq
- k(forward)
- k(reverse)
- mass action ratio at t=5 s
- reaction rate at t=20 s
- forward rate at t=20 s
- reverse rate at t=20 s

Exercise 2: Solution



v -d[A]/dt = slope of tangent at t=5
= 0.4 mM/s

K

K_{eq} Equilibrium ratio of [B]/[A] =
7.5/2.5 = 3

k_f
v = k_f*a - k_r*b;
rate of reaction (d[A]/dt) at t=0;
= -d[A]/dt
= slope of tangent at t=0
= 3.0 mM/s;
k_f = 3.0/10 = 0.3 1/s

k_r
$K_{eq} = k_f/k_r$;
k_r = 0.3/3 = 0.1 1/s

Γ [B]/[A] at t=5, 6.48/3.52 = 1.84

v_{20} at t=20 the reaction is very close to equilibrium as is evident from the constant concentrations of A and B, the velocity is close to 0

$v_{f,\ t=20}$ at t=20 v_f = 0.3*2.5 = 0.75 mM/s

$v_{r,\ t=20}$ at t=20 v_r = 0.1*7.5 = 0.75 mM/s

Exercise 3

- Calculate the maximal glucose gradient possible for a proton symport system with a stoichiometry of 2 protons per glucose molecule, if there is a pH difference of -0.3 (inside 6.7, outside 7.0), and the membrane potential is -200mV (negative inside).
- R=8.31447 J/K/mol, T=298.17 K, F=96.485 kJ/V

Exercise 3: Solution

- Calculate the maximal glucose gradient possible for a proton symport system with a stoichiometry of 2 protons per glucose molecule, if there is a pH difference of -0.3 (inside 6.7, outside 7.0), and the membrane potential is -200mV (negative inside)

$$\begin{array}{rcl} pH & = & -^{10}log[H^+] \\ pH = 7 & -> & [H^+] = 10^{-7} \\ pH = 6.7 & -> & [H^+] = 10^{-6.7} = 1.995 \cdot 10^{-7} \end{array}$$

$$\begin{array}{rcl} \Delta G_{H+} & = & RTln\frac{[H^+]_{in}}{[H^+]_{out}} + ZF \cdot \Delta\psi \\ \Delta G_{H+} & = & 8.31447 \cdot 298.17 \cdot ln(1.995) + 96.485 \cdot 10^3 \cdot -0.2 \\ \Delta G_{H+} & = & 1712.19 - 19297 \\ \Delta G_{H+} & = & -17584.8\,\mathrm{J/mol\ H^+} \end{array}$$

$$\begin{array}{rcl} \Delta G_{Glc} & = & RTln\frac{[Glc]_{in}}{[Glc]_{out}} \\ 2 \cdot 17584.8 & = & 8.31447 \cdot 298.17 \cdot ln\frac{[Glc]_{in}}{[Glc]_{out}} \\ \frac{[Glc]_{in}}{[Glc]_{out}} & = & 1.45 \cdot 10^6 \end{array}$$