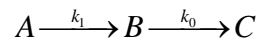


Assignment 8

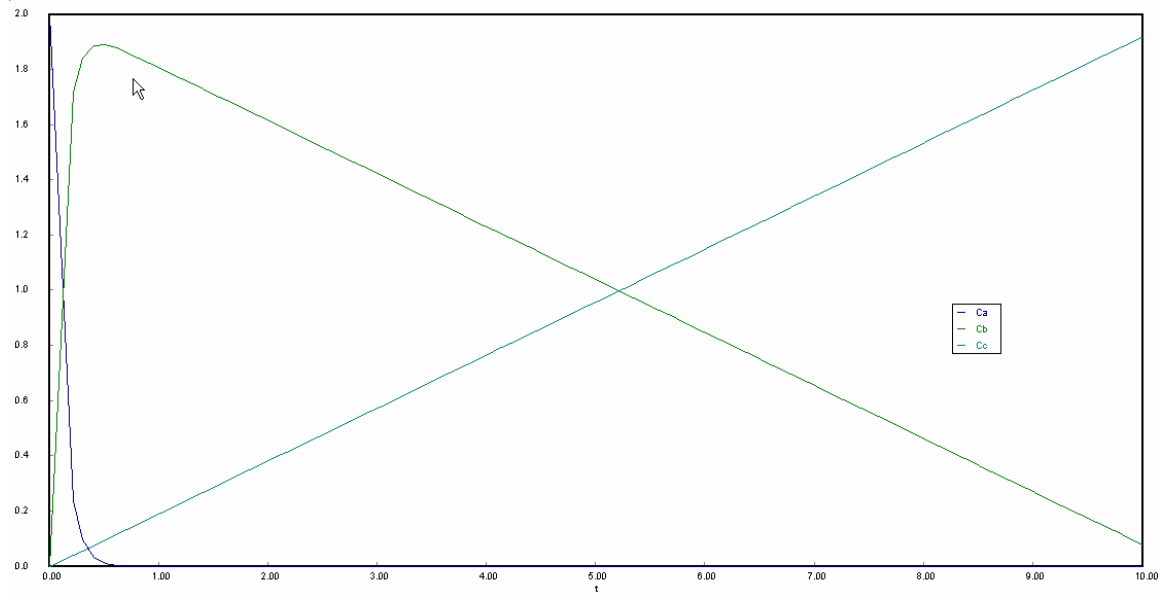
Problem 6.7 – Numerical Solutions



(a)(b)(c)

```
d(Ca)/dt = -k1 * Ca # in Stomach
Ca(0) = 2
d(Cb)/dt = k1 * Ca - k0 # in Blood
Cb(0) = 0
d(Cc)/dt = k0 # in wherever which is not important
Cc(0) = 0

k0 = 0.192
k1 = 10
t(0) = 0
t(f) = 10
```



(d)

$$d(Ca)/dt = -k_1 * Ca \text{ \# in Stomach}$$

$$Ca(0) = 1$$

$$d(Cb)/dt = k_1 * Ca - k_0 \text{ \# in Blood}$$

$$Cb(0) = 0$$

$$d(Cc)/dt = k_0 \text{ \# in wherever which is not important}$$

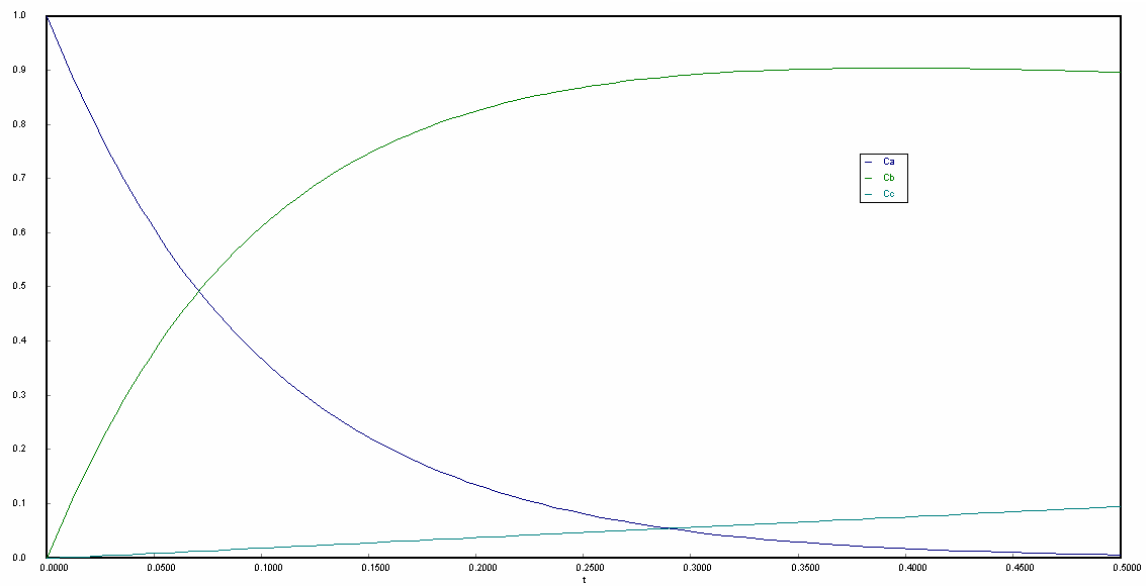
$$Cc(0) = 0$$

$$k_0 = 0.192$$

$$k_1 = 10$$

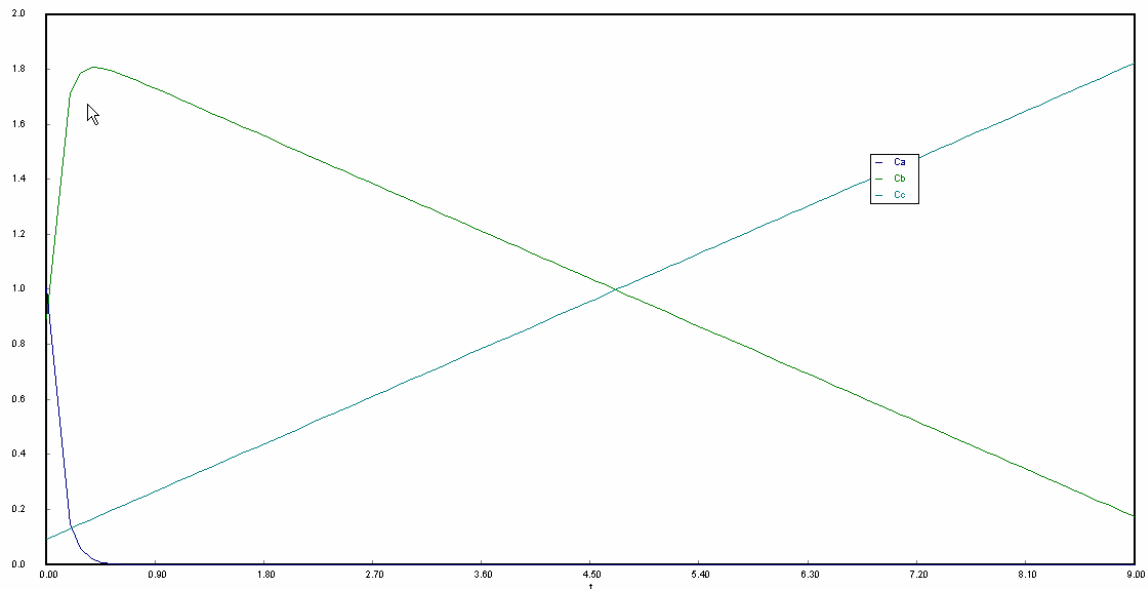
$$t(0) = 0$$

$$t(f) = 0.5$$



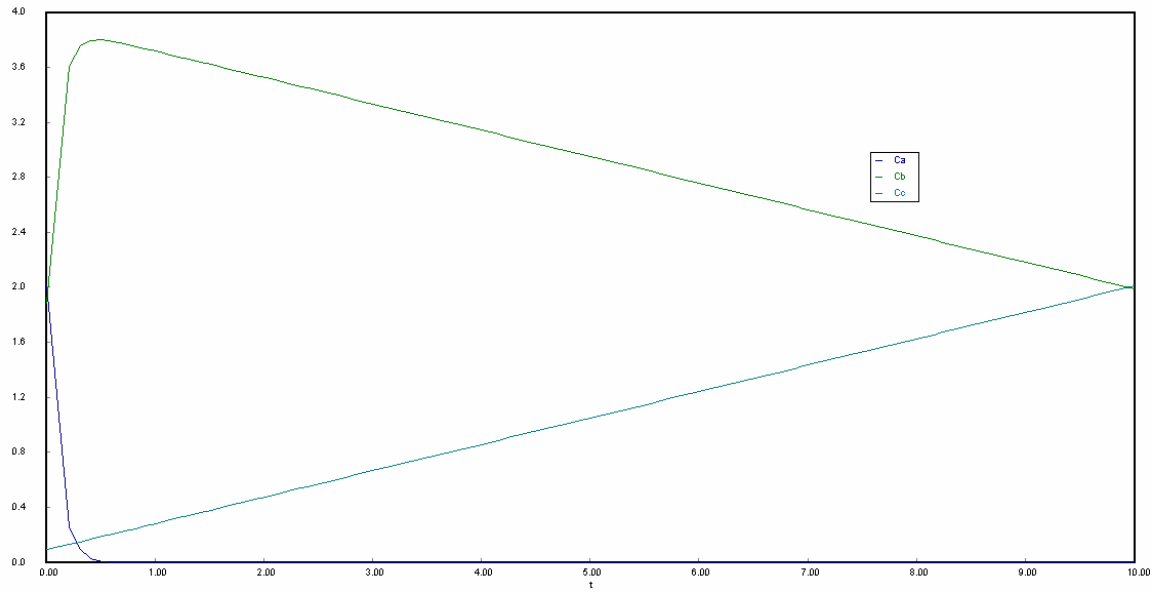
$d(Ca)/dt = -k_1 * Ca$ # in Stomach
 $Ca(0) = 1.0067379$
 $d(Cb)/dt = k_1 * Ca - k_0$ # in Blood
 $Cb(0) = 0.8972621$
 $d(Cc)/dt = k_0$ # in wherever which is not important
 $Cc(0) = 0.096$

$k_0 = 0.192$
 $k_1 = 10$
 $t(0) = 0$
 $t(f) = 9$



$d(Ca)/dt = -k_1 * Ca$ # in Stomach
 $Ca(0) = 2.0234759$
 $d(Cb)/dt = k_1 * Ca - k_0$ # in Blood
 $Cb(0) = 1.890524$
 $d(Cc)/dt = k_0$ # in wherever which is not important
 $Cc(0) = 0.096$

$k_0 = 0.192$
 $k_1 = 10$
 $t(0) = 0$
 $t(f) = 10$



(e)

$$Fa0 = 40 \text{ \# g/hr}$$

$$V = 40 \text{ \# liter}$$

Ca = Na/V # neglect the contribution from alcohol

$$d(Na)/dt = V * (-k1 * Na / V) + Fa0 \text{ \# in Stomach}$$

$$Na(0) = 0$$

$$d(Nb)/dt = (k1 * Na / V - k0) * V \text{ \# in Blood}$$

$$Nb(0) = 0$$

$$d(Nc)/dt = k0 * V \text{ \# in wherever which is not important}$$

$$Nc(0) = 0$$

$$k0 = 0.192$$

$$k1 = 10$$

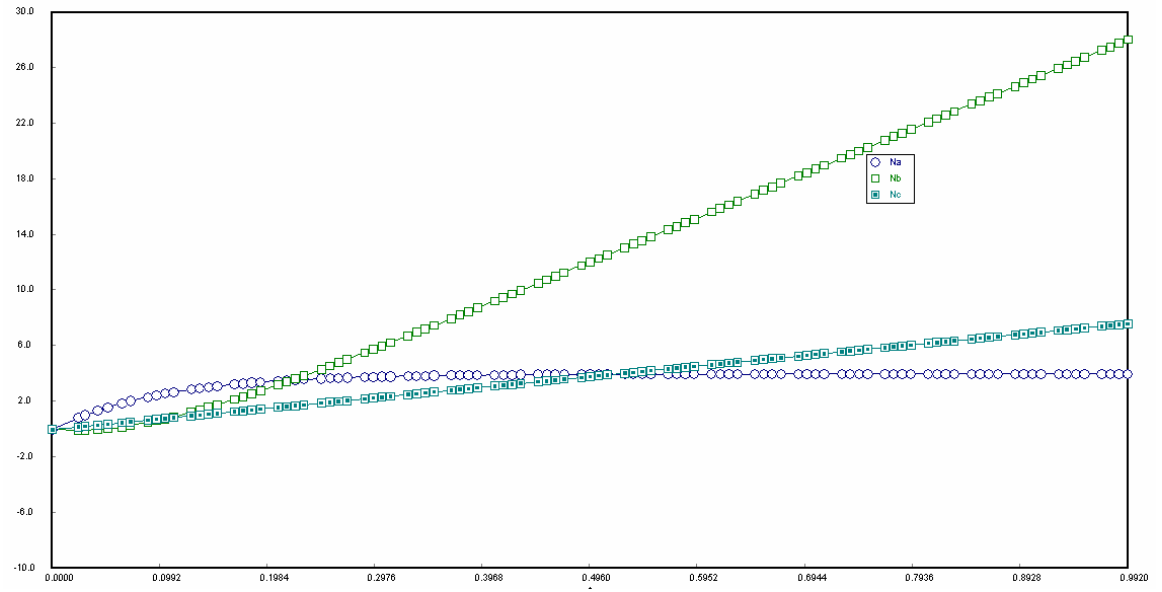
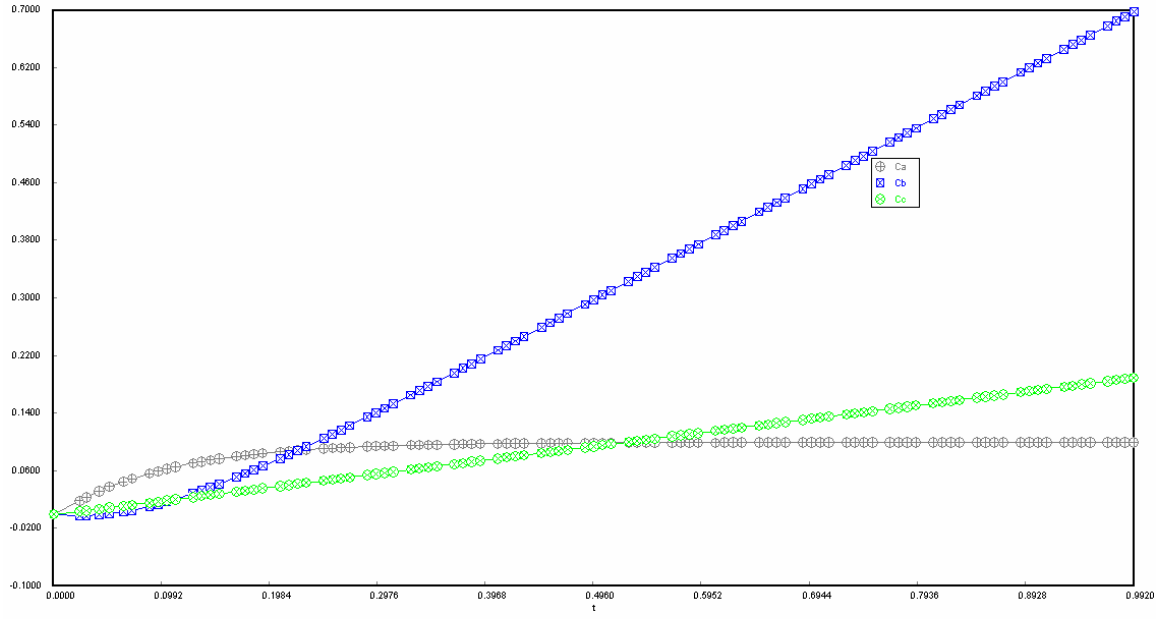
$$t(0) = 0$$

$$t(f) = 1$$

$$Ca = Na / V$$

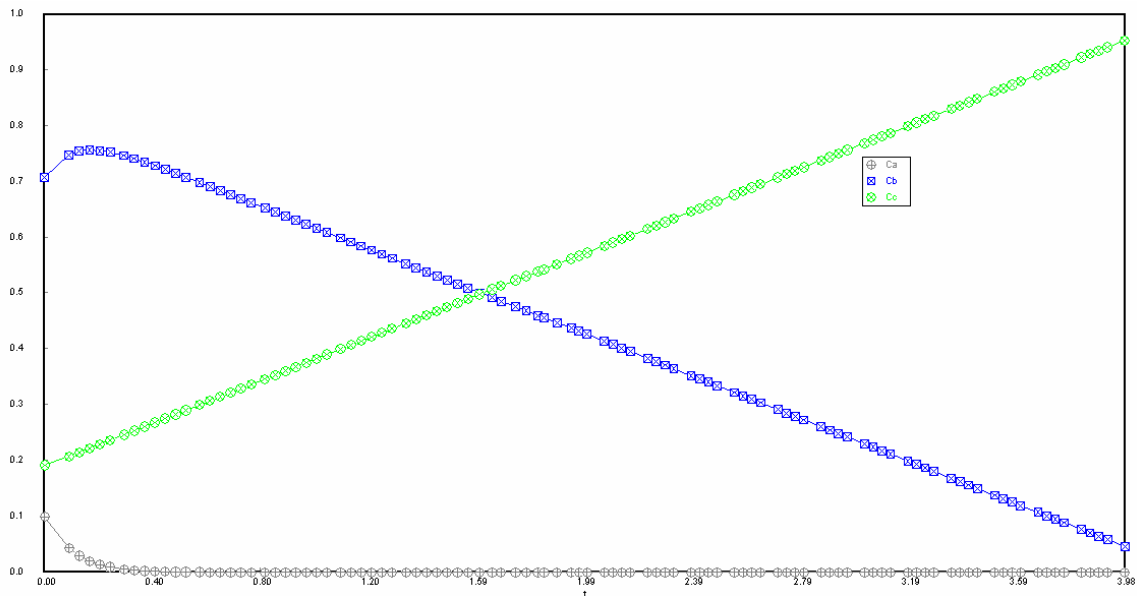
$$Cb = Nb / V$$

$$Cc = Nc / V$$



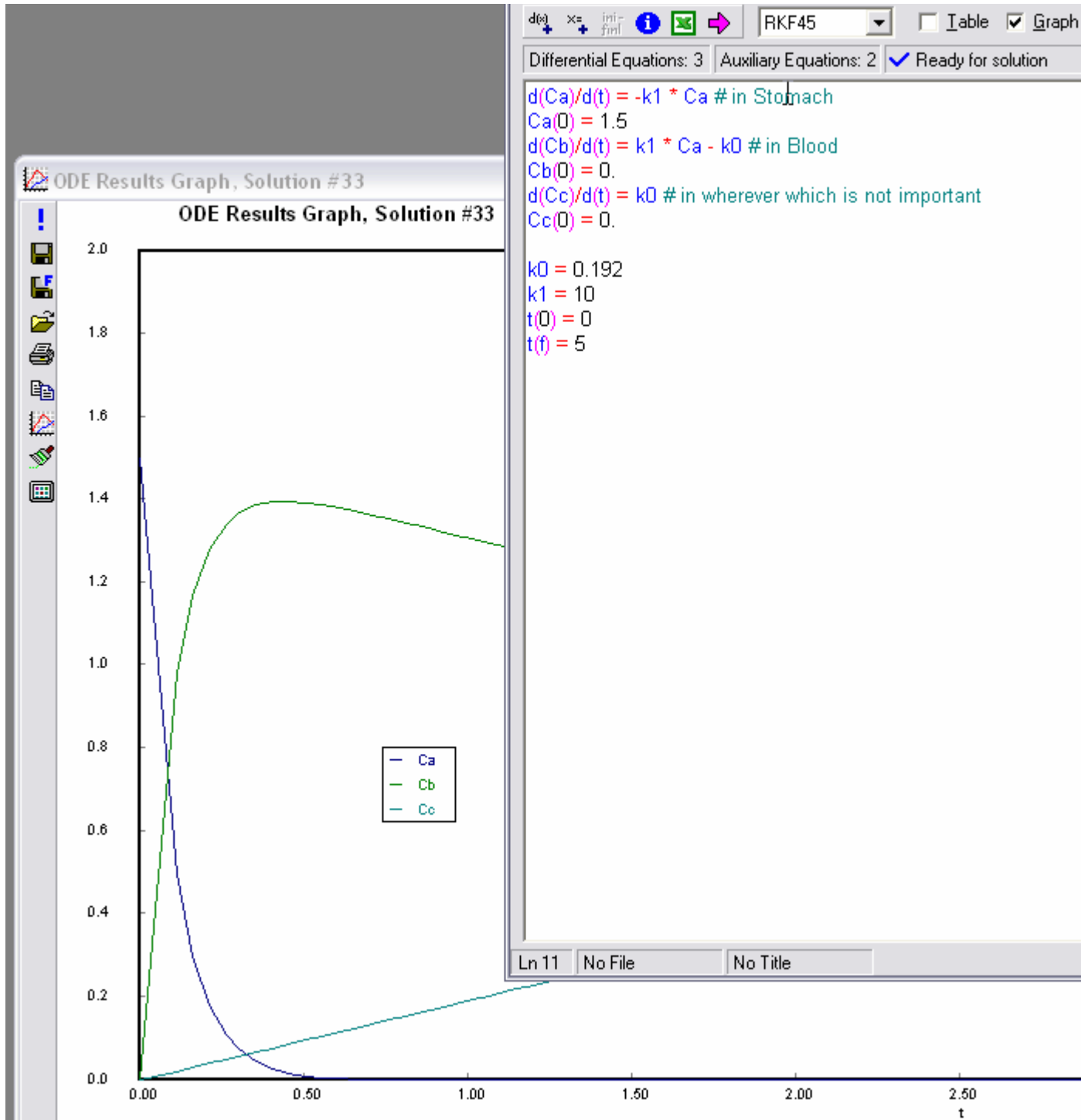
$Fa0 = 40 \text{ \# g/hr}$
 $V = 40 \text{ \# liter}$
 $\# Ca = Na/V \text{ \# neglect the contribution from alcohol}$
 $d(Na)/dt = V * (-k1 * Na / V) \text{ \# in Stomach}$
 $Na(0) = 3.99818$
 $d(Nb)/dt = (k1 * Na / V - k0) * V \text{ \# in Blood}$
 $Nb(0) = 28.32018$
 $d(Nc)/dt = k0 * V \text{ \# in wherever which is not important}$
 $Nc(0) = 7.68$

$k0 = 0.192$
 $k1 = 10$
 $t(0) = 0$
 $t(f) = 4$
 $Ca = Na / V$
 $Cb = Nb / V$
 $Cc = Nc / V$



- (a) ~6 hrs
- (b) ~7.5hrs
- (c) >10hrs
- (d) US:~5.5hrs; Sweden:~8hrs; Russia:>10hrs
- (e) US:~0hrs; Sweden:~1.5hrs; Russia:>4hrs

(f)



US: <5mins

- (g) It depends on person's metabolism, but since thin person have small body volume so I expect it take long to wait till the level of alcohol in blood goes down to the intoxication level.

Problem 6.12

$$A := 1 \quad B := 2$$

$$C := 3 \quad D := 4$$

$$k1A := 7 \text{ min}^{-1} \quad k2D := 3 \frac{\text{liter}^2}{\text{mol}^2 \cdot \text{min}} \quad k3E := 2 \frac{\text{liter}}{\text{mol} \cdot \text{min}}$$

$$CA := 0.1 \frac{\text{mol}}{\text{liter}} \quad CB := 0.93 \frac{\text{mol}}{\text{liter}} \quad CC := 0.51 \frac{\text{mol}}{\text{liter}} \quad CD := 0.049 \frac{\text{mol}}{\text{liter}}$$

$$r1A := -k1A \cdot CA \quad r2D := k2D \cdot CC^2 \cdot CA \quad r3E := k3E \cdot CD \cdot CC$$

$$r1B := \frac{1}{3} \cdot -r1A \quad r2C := \frac{-2}{3} \cdot r2D \quad r3D := \frac{-4}{3} \cdot r3E$$

$$r1C := r1B \quad r2A := \frac{-1}{3} \cdot r2D \quad r3C := r3D$$

$$r1D := 0 \quad r3A := 0$$

$$r1E := 0 \quad r2B := 0 \quad r3B := 0$$

$$r2E := 0$$

$$r1A = -11.667 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \quad r1B = 3.889 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \quad r1C = 3.889 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r2A = -0.434 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \quad r2B = 0 \quad r2C = -0.867 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r3A = 0 \quad r3B = 0 \quad r3C = -1.111 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r1D = 0 \quad r1E = 0$$

$$r2D = 1.3 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \quad r2E = 0$$

$$r3D = -1.111 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \quad r3E = 0.833 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r_A := r_{1A} + r_{2A} + r_{3A}$$

$$r_B := r_{1B} + r_{2B} + r_{3B}$$

$$r_C := r_{1C} + r_{2C} + r_{3C}$$

$$r_D := r_{1D} + r_{2D} + r_{3D}$$

$$r_E := r_{1E} + r_{2E} + r_{3E}$$

$$r_A = -12.1 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r_B = 3.889 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r_C = 1.911 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$r_D = 0.19 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$$

$$V = \frac{FA_0 - FA}{-r_A}$$

$$CA_0 := 3 \frac{\text{mol}}{\text{liter}}$$

$$v_0 := 100 \frac{\text{liter}}{\text{min}}$$

$$V := v_0 \cdot \frac{CA_0 - CA}{-r_A}$$

$$V = 399.444 \text{L}$$

(h)

```
# P6-12 (h)
# unit are all converted to time [=] min; volume [=] liter; mole
k1A = 7
k2D = 3
k3E = 2
r1A = -k1A * CA
r2D = k2D * CC ^ 2 * CA
r3E = k3E * CD * CC
rA = r1A - r2D / 3
rB = -r1A/3
rC = -r1A/3 - r2D / 3 ^ 2 - r3E
rD = r2D - r3E / 3 ^ 4
rE = r3E
V = 600
v0 = 100
tau = V / v0
CA0 = 3
CB0 = 0
CC0 = 0
CD0 = 0
CE0 = 0
```

```
f(CA) = (CA - CA0) - rA * tau
CA(0) = 3 > 0
f(CB) = (CB - CB0) - rB * tau
CB(0) = 0 > 0
f(CC) = (CC - CC0) - rC * tau
CC(0) = 0 > 0
f(CD) = (CD - CD0) - rD * tau
CD(0) = 0 > 0
f(CE) = (CE - CE0) - rE * tau
CE(0) = 0 > 0
```

POLYMATH Report

Nonlinear Equations

No Title
09-Apr-2006

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	CA	0.0672845	0	3.
2	CB	0.9419832	1.11E-16	0
3	CC	0.5142601	1.11E-16	0
4	CD	0.0347087	-6.939E-18	0
5	CE	0.2141915	-2.776E-17	0

	Variable	Value
1	k1A	7.
2	k2D	3.
3	k3E	2.
4	r1A	-0.4709916
5	r2D	0.0533829
6	r3E	0.0356986
7	rA	-0.4887859
8	rB	0.1569972
9	rC	0.08571
10	rD	0.0057848
11	rE	0.0356986
12	V	600.
13	v0	100.
14	tau	6.
15	CA0	3.
16	CB0	0
17	CC0	0
18	CD0	0
19	CE0	0

Nonlinear equations

- 1 $f(CA) = (CA - CA0) - rA * \tau = 0$
- 2 $f(CB) = (CB - CB0) - rB * \tau = 0$
- 3 $f(CC) = (CC - CC0) - rC * \tau = 0$
- 4 $f(CD) = (CD - CD0) - rD * \tau = 0$
- 5 $f(CE) = (CE - CE0) - rE * \tau = 0$

Explicit equations

- 1 $k1A = 7$
- 2 $k2D = 3$
- 3 $k3E = 2$
- 4 $r1A = -k1A * CA$
- 5 $r2D = k2D * CC^2 * CA$
- 6 $r3E = k3E * CD * CC$
- 7 $rA = r1A - r2D / 3$
- 8 $rB = -r1A / 3$
- 9 $rC = -r1A / 3 - r2D / 3^2 - r3E$

10 $rD = r2D - r3E / 3 * 4$

11 $rE = r3E$

12 $V = 600$

13 $v0 = 100$

14 $\tau = V / v0$

15 $CA0 = 3$

16 $CBO = 0$

17 $CC0 = 0$

18 $CD0 = 0$

19 $CE0 = 0$

Conditions for solution

CA	Absolutely Positive
CB	Absolutely Positive
CC	Absolutely Positive
CD	Absolutely Positive
CE	Absolutely Positive

General Settings

Total number of equations	24
Number of implicit equations	5
Number of explicit equations	19
Elapsed time	0.0000 sec
Solution method	CONSTRAINED
Convergence tolerance	0.0000001
Maximum # of iterations	150
# of iterations used	6

Data file: <c:\documents and settings\chung-kan huang\desktop\pol>

Problem 6.14

P6.14

all units are consist as I did in P6.12

$$kD1 = 0.25$$

$$kE2 = 0.1$$

$$kF3 = 5$$

$$v0 = 10$$

$$rD1 = kD1 * CA * CB ^ 2$$

$$rE2 = kE2 * CA * CD$$

$$rF3 = kF3 * CB * CC ^ 2$$

$$rA = -rD1 - 3 * rE2$$

$$rB = -2 * rD1 - rF3$$

$$rC = rD1 + rE2 - 2 * rF3$$

$$rD = rD1 - 2 * rE2 + rF3$$

$$rE = rE2$$

$$rF = rF3$$

$$d(CA)/d(V) = rA / v0$$

$$CA(0) = 1.5$$

$$d(CB)/d(V) = rB / v0$$

$$CB(0) = 2$$

$$d(CC)/d(V) = rC / v0$$

$$CC(0) = 0$$

$$d(CD)/d(V) = rD / v0$$

$$CD(0) = 0$$

$$d(CE)/d(V) = rE / v0$$

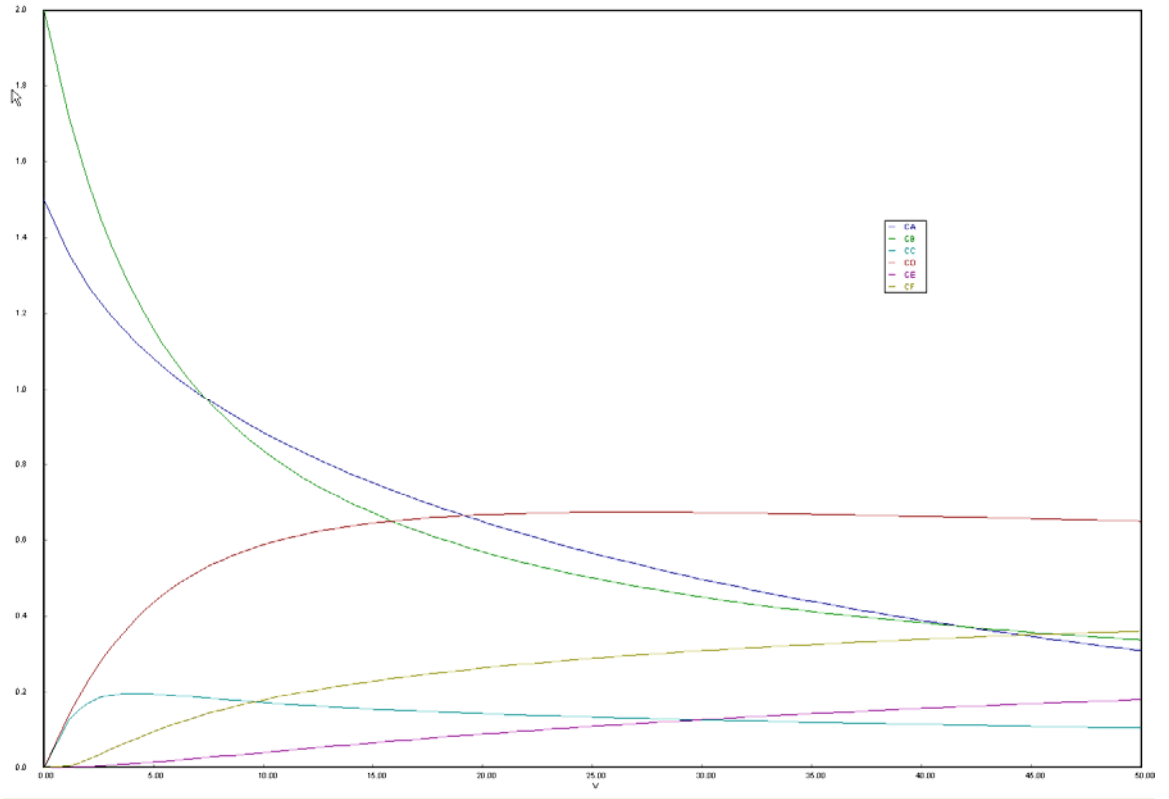
$$CE(0) = 0$$

$$d(CF)/d(V) = rF / v0$$

$$CF(0) = 0$$

$$V(0) = 0$$

$$V(t) = 50$$



V	CA	CB	CC	CD	CE	CF	rA	rB	rC	rD	rE	rF
0	1.5	2	0	0	0	0	-1.5	-3	1.5	1.5	0	0
1.115966	1.359484	1.719705	0.125761	0.140938	0.001159	0.006218	-1.080344	-2.177723	0.789579	1.115714	0.018335	0.127047
1.52497	1.318291	1.635981	0.151796	0.184361	0.002051	0.012906	-0.972546	-1.984744	0.564961	1.035646	0.023449	0.180344
2.011653	1.274456	1.545921	0.172456	0.2319	0.003365	0.023179	-0.867062	-1.786173	0.361296	0.947802	0.028691	0.224193
2.505479	1.227874	1.449841	0.186837	0.283281	0.005248	0.037397	-0.765747	-1.578521	0.196621	0.846708	0.033934	0.250629
3.054248	1.194999	1.382406	0.19288	0.319517	0.006924	0.049136	-0.701002	-1.434804	0.112389	0.771161	0.037358	0.256948
3.584893	1.160314	1.312172	0.196218	0.357182	0.00904	0.062694	-0.638682	-1.28784	0.048477	0.689819	0.040661	0.254442
4.207453	1.123385	1.239015	0.197039	0.39609	0.011719	0.078069	-0.578874	-1.139185	0.003175	0.604084	0.043773	0.244076
4.56167	1.103902	1.201286	0.196574	0.415936	0.013321	0.086442	-0.549921	-1.064823	-0.013285	0.560133	0.045232	0.236371
5.350479	1.063819	1.125947	0.194152	0.454918	0.017046	0.103968	-0.494811	-0.919809	-0.035404	0.472844	0.047846	0.217262
5.750479	1.044992	1.091737	0.192492	0.472257	0.019002	0.112257	-0.470583	-0.854988	-0.041594	0.433301	0.048895	0.207193
6.150479	1.027034	1.059865	0.190675	0.488161	0.020992	0.120154	-0.448866	-0.796563	-0.045472	0.397459	0.049763	0.197407
6.550479	1.009859	1.030106	0.188768	0.502764	0.023011	0.127676	-0.429293	-0.743795	-0.047718	0.364973	0.050471	0.188035
7.350479	0.977755	0.976143	0.184853	0.528543	0.027111	0.141675	-0.395422	-0.652695	-0.049093	0.30876	0.051487	0.170771
7.750479	0.962347	0.951606	0.182901	0.539925	0.029184	0.148192	-0.380663	-0.613281	-0.04881	0.284444	0.051826	0.162911
8.150479	0.947661	0.928507	0.180976	0.55042	0.031267	0.154415	-0.367108	-0.577346	-0.048137	0.262308	0.052071	0.155552
8.550479	0.933475	0.906723	0.179088	0.560108	0.033356	0.160362	-0.354611	-0.544504	-0.0472	0.242125	0.052232	0.148673
9.350479	0.906459	0.866667	0.17545	0.577334	0.037542	0.171503	-0.332303	-0.486793	-0.044872	0.206833	0.052343	0.136245
9.750479	0.893566	0.848209	0.173707	0.584991	0.039635	0.176729	-0.322295	-0.461371	-0.043595	0.191385	0.052309	0.130636
10.15048	0.881047	0.830689	0.172015	0.592081	0.041723	0.181746	-0.31294	-0.437925	-0.042291	0.177209	0.052225	0.125391
10.55048	0.868879	0.814036	0.170375	0.59865	0.043807	0.186566	-0.304172	-0.416257	-0.040987	0.16418	0.052095	0.120484
11.35048	0.845514	0.783081	0.16725	0.610386	0.047953	0.195665	-0.288166	-0.377576	-0.038436	0.141132	0.051723	0.111579
11.75048	0.83428	0.768668	0.165762	0.615624	0.050013	0.199967	-0.280833	-0.360271	-0.03721	0.130926	0.051488	0.107533
12.15048	0.823324	0.7549	0.16432	0.620485	0.052062	0.204116	-0.273891	-0.344157	-0.036025	0.121492	0.051226	0.103732
12.55048	0.812631	0.741734	0.162925	0.624996	0.054099	0.208123	-0.267307	-0.329127	-0.034884	0.112761	0.05094	0.101055
13.35048	0.791985	0.71705	0.160264	0.633072	0.058137	0.215739	-0.255091	-0.301946	-0.032738	0.097162	0.050307	0.093607
13.75048	0.782008	0.705463	0.158994	0.636668	0.060135	0.219364	-0.249409	-0.289632	-0.031735	0.090188	0.049965	0.090606
14.15048	0.772248	0.694339	0.157763	0.640029	0.06212	0.222875	-0.24398	-0.278075	-0.030776	0.083704	0.049609	0.087769
14.55048	0.762696	0.683649	0.156569	0.643136	0.064089	0.226278	-0.238786	-0.267215	-0.029862	0.077669	0.04924	0.085084
15.35048	0.744182	0.663473	0.154283	0.648691	0.067982	0.232785	-0.229036	-0.247365	-0.028158	0.066801	0.048472	0.080125
15.75048	0.735204	0.653941	0.153188	0.651168	0.069905	0.235899	-0.22445	-0.238281	-0.027365	0.061907	0.048075	0.077832
16.15048	0.726402	0.644752	0.152124	0.653462	0.071812	0.238925	-0.220039	-0.229701	-0.02661	0.057334	0.047672	0.075653
16.55048	0.71777	0.635888	0.151088	0.655855	0.073703	0.241868	-0.215791	-0.221588	-0.025891	0.053059	0.047262	0.073579
17.35048	0.700992	0.619065	0.149098	0.65936	0.077434	0.247522	-0.207748	-0.206631	-0.024551	0.045314	0.046431	0.069719
17.75048	0.692834	0.611076	0.14814	0.661033	0.079274	0.250238	-0.203933	-0.199728	-0.023928	0.041805	0.04601	0.067921
18.15048	0.684824	0.603348	0.147207	0.662574	0.081098	0.252887	-0.200246	-0.193174	-0.023334	0.038515	0.045587	0.066203
18.55048	0.676957	0.59587	0.146296	0.663991	0.082904	0.255469	-0.196679	-0.186946	-0.022766	0.035429	0.045162	0.064561
19.35048	0.661632	0.581613	0.144539	0.666486	0.084666	0.260448	-0.189879	-0.17538	-0.021708	0.029812	0.04431	0.061483
19.75048	0.654167	0.574812	0.14369	0.667576	0.086222	0.26285	-0.186634	-0.170005	-0.021214	0.027255	0.043884	0.06004
20.15048	0.646827	0.568217	0.142861	0.66857	0.08796	0.265196	-0.183485	-0.164879	-0.020742	0.024852	0.043458	0.058656
20.55048	0.63961	0.561817	0.142049	0.669474	0.091681	0.267489	-0.180428	-0.159987	-0.02029	0.022592	0.043032	0.057326
21.35048	0.625529	0.54957	0.140477	0.671032	0.095073	0.271924	-0.17457	-0.150848	-0.019445	0.018464	0.042186	0.054822
21.75048	0.618658	0.543706	0.139715	0.671695	0.096743	0.27407	-0.171762	-0.146576	-0.019048	0.016579	0.041765	0.053641
22.15048	0.611897	0.538007	0.138968	0.672287	0.098397	0.27617	-0.169029	-0.142487	-0.018669	0.014804	0.041346	0.052503
22.55048	0.605242	0.532464	0.138236	0.672813	0.100034	0.278227	-0.166368	-0.13857	-0.018305	0.013131	0.040929	0.051408
23.35048	0.592241	0.521822	0.136813	0.673678	0.103259	0.282214	-0.16125	-0.131215	-0.017621	0.010068	0.040103	0.049333
23.75048	0.585889	0.516711	0.136121	0.674025	0.104847	0.284144	-0.158787	-0.12776	-0.0173	0.008667	0.039694	0.048349
24.15048	0.579634	0.511733	0.135441	0.674319	0.106418	0.286044	-0.156384	-0.124442	-0.016991	0.007345	0.039288	0.0474
24.55048	0.573472	0.506883	0.134773	0.674563	0.107974	0.287904	-0.15404	-0.121253	-0.016694	0.006099	0.038885	0.046482
25.35048	0.561421	0.497545	0.133472	0.674912	0.111037	0.291517	-0.149516	-0.115241	-0.016134	0.003813	0.038088	0.044737
25.75048	0.555528	0.493049	0.132837	0.675023	0.112545	0.293273	-0.147333	-0.112403	-0.015869	0.002765	0.037695	0.043906
26.15048	0.54972	0.488662	0.132212	0.675094	0.114037	0.294997	-0.145199	-0.109671	-0.015614	0.001777	0.037305	0.043102
26.55048	0.543995	0.484438	0.131598	0.675128	0.115514	0.29669	-0.143114	-0.10704	-0.015369	0.000844	0.036919	0.042323
27.35048	0.532789	0.476118	0.130396	0.675092	0.118421	0.299987	-0.13908	-0.102057	-0.014904	-0.000867	0.036156	0.040835
27.75048	0.527303	0.472113	0.129809	0.675026	0.119852	0.301592	-0.137128	-0.099696	-0.014683	-0.001651	0.035781	0.040125
28.15048	0.521895	0.468233	0.12923	0.674931	0.121269	0.303169	-0.135218	-0.097418	-0.014471	-0.002391	0.035409	0.039436
28.55048	0.516561	0.464424	0.128659	0.674807	0.12267	0.30472	-0.133348	-0.095219	-0.014265	-0.003089	0.035041	0.038766
29.35048	0.506111	0.457058	0.127542	0.674483	0.12543	0.307744	-0.129724	-0.09104	-0.013875	-0.004369	0.034315	0.037484
29.75048	0.500992	0.453496	0.126994	0.674284	0.126788	0.309219	-0.127967	-0.089054	-0.013689	-0.004955	0.033958	0.03687
30.15048	0.495942	0.450011	0.126454	0.674064	0.128133	0.310669	-0.126245	-0.087133	-0.013509	-0.005507	0.033605	0.036272
30.55048	0.49096	0.4466	0.12592	0.673823	0.129463	0.312097	-0.124558	-0.085274	-0.013335	-0.006028	0.033255	0.035691
31.35048	0.481192	0.439991	0.124874	0.673283	0.132082	0.314885	-0.121282	-0.081733	-0.013003	-0.006981	0.032568	0.034575
31.75048	0.476405	0.436789	0.12436	0.672987	0.133371	0.316247	-0.119691	-0.080045	-0.012844	-0.007417	0.032229	0.034038
32.15048	0.47168	0.433653	0.123852	0.672674	0.134647	0.317587	-0.11813	-0.07841	-0.012691	-0.007826	0.031895	0.033516
32.55048	0.467015	0.43058	0.12335	0.672345	0.135909	0.318908	-0.116599	-0.076824	-0.012542	-0.008212	0.031564	0.033007
33.35048	0.457867	0.424616	0.122364	0.671646	0.138395	0.321489	-0.113623	-0.073795	-0.012256	-0.008915	0.030913	0.032027
33.75048	0.45338	0.421722	0.12188	0.671276	0.139619	0.322751	-0.112175	-0.072347	-0.01212	-0.009235	0.030593	0.031554
34.15048	0.448949	0.418885	0.1214	0.670895	0.14083	0.323995	-0.110754	-0.070942	-0.011987	-0.009535	0.030277	0.031094
34.55048	0.444575	0.416102	0.120926	0.670502	0.142029	0.325221	-0.109358	-0.069578	-0.011858	-0.009817	0.029964	0.030644
35.35048	0.43599	0.410693	0.119992	0.669686	0.144389	0.32762	-0.106642	-0.066965	-0.01161	-0.010328	0.029349	0.029777
35.75048	0.431777	0.408064	0.119532	0.669264	0.145551	0.328795	-0.105319	-0.065714	-0.011491	-0.010558	0.029047	0.029358
36.15048	0.427616	0.405484										